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Surface critical behaviour of the smoothly inhomogeneous planar Ising model: the Pfaffian method

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Abstract. A semi-infinite nearest-neighbour square Ising lattice is investigated whose couplings $J(l)$ at a distance l from the boundary differ from homogeneity by an amount $J(l)-J(\infty)\sim -A/l$. On the basis of the Pfaffian method we obtain the critical behaviour at the surface of this system. The exponents $\eta_{\|}$, $\nu_{\|}$, β_1, γ_{11} and δ_{11} all display rich non-universal behaviour as a function of the amplitude A.

For A below a critical value there is a spontaneous surface magnetisation when the bulk ($l=\infty$) is critical and an asymmetry between the exponents on either side of the critical point.

1. Introduction

Instances of fully understood surface critical behaviour are rare. These acquire a particular significance in connection with current research in surface physics, which is concerned with such diverse phenomena as wetting, roughening, surface ordering and polymer adsorption. This work deals with a system for which a complete understanding can be gained.

We consider an inhomogeneous ferromagnetic Ising system with nearest-neighbour interactions on a semi-infinite square lattice. The coupling constants are represented in figure 1. There is a coupling J_1 in the vertical direction and there are couplings $J_2(l)$, depending on the column number l, in the horizontal direction. Furthermore there is a magnetic field h_1 acting only on the surface spins. Thus the system Hamiltonian is

$$H=-\sum_{l=1}^{\infty}\sum_{k=-\infty}^{\infty}(J_1\sigma_{l,k}\sigma_{l,k+1}+J_2(l)\sigma_{l,k}\sigma_{l+1,k})-h_1\sum_{k=-\infty}^{\infty}\sigma_{1,k}. \tag{1.1}$$

For the homogeneous case, $J_2(l)=J_2$, a great wealth of exact results has been obtained by McCoy and Wu (1973), who have given a detailed account of their method. Quantities of interest are the correlation function $g_{\|}(r)$ between two spins a distance r apart on the surface (see figure 1), the surface susceptibility χ_{11} and the surface magnetisation m_1, as functions of the temperature T and the surface field h_1. At the bulk critical temperature T_c, these quantities exhibit singularities with critical exponents which differ, in general, from the corresponding bulk exponents. For example, at $T=T_c$ the pair correlation $g(r)$ in the bulk decays as $1/r^{\eta}$ with $\eta=\frac{1}{4}$ (Wu *et al* 1976), whereas the surface pair correlation $g_{\|}(r)$ decays as $1/r^{\eta_{\|}}$ with $\eta_{\|}=1$ (McCoy and Wu 1967). McCoy and Wu (1969) and McCoy (1969) also carried out a thorough

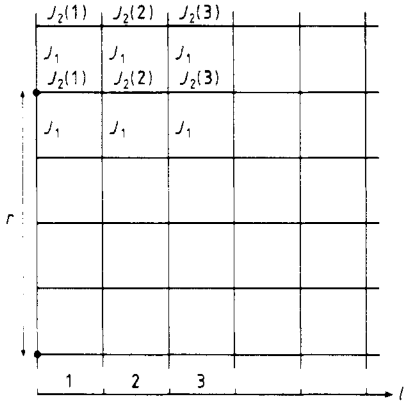

Figure 1. The semi-infinite square Ising lattice with inhomogeneous couplings described by equation (1.1). All vertical nearest-neighbour bonds have strength J_1. The horizontal nearest-neighbour bonds $J_2(l)$ are constant in a given column l, but vary smoothly with the distance l from the border. The variable r indicates the distance between two border spins.

study of the Hamiltonian of equation (1.1) in the case where $J_2(l)$ is a random variable (see also McCoy and Wu 1973). We shall come back to some of their remarkable findings for the random case, comparing them to our own results at the end of § 9.

In this paper we consider the case in which the nearest-neighbour couplings $J_2(l)$ monotonically tend towards a bulk value $J_2(\infty)$ in such a way that for asymptotically large l

$$J_2(l) - J_2(\infty) \simeq -A_0 l^{-1} + \ldots \tag{1.2}$$

where the amplitude A_0 is a constant and the ellipsis indicates higher powers of $1/l$. Hence the presence of the surface affects the couplings deep into the bulk. We shall concentrate in particular on temperatures T near the critical point T_c of a homogeneous bulk, and put

$$t = (T - T_c)/T_c. \tag{1.3}$$

The quantities t, h_1 and A_0 are the basic parameters of the model system.

Recently much attention has been given to systems determined by equation (1.1) and by the more general decay proportional to $A_0 l^{-p}$ (with $p > 0$). Hilhorst and van Leeuwen (1981) showed, for a similar system on a triangular lattice, that for $p > 1$ the usual boundary critical behaviour (i.e. as exhibited by a semi-infinite *homogeneous* system) is not modified, but that for $p \leqslant 1$ a variety of interesting and unexpected modifications occur. They presented exact results for the case $A_0 > 0$ (weakening of the couplings near the surface) and showed that $p = 1$ is a very special marginal case with continuously varying exponents. The difficult case of $A_0 < 0$ (enhancement of the couplings near the surface) was analysed by Burkhardt and Guim (1984). For $A_0 < 0$ surface magnetisation may occur when there is no bulk magnetisation. A coherent presentation for the general amplitude A_0 and exponent p has been given by Burkhardt *et al* (1984).

The approach of Hilhorst and van Leeuwen, and of Burkhardt and Guim, is based on a sequence of exact reformulations of the problem, constructed with the aid of the well known star-triangle transformation. In the limit of couplings $J_2(l)$ that vary only smoothly with l the problem can be cast in the form of two coupled partial differential equations. A less rigorous but very illuminating approach has been formulated by Burkhardt (1982a, b) and by Cordery (1982), who show that the exact results can be understood on the basis of simple renormalisation group and scaling arguments. These arguments predict that in general, for a semi-infinite system whose bulk correlation length diverges with an exponent ν, the surface critical behaviour is modified only if the exponent p of the inhomogeneous part of the couplings satisfies $p \leq 1/\nu$.

In this paper we describe a different method of solution, which was reported earlier (Blöte and Hilhorst 1983). We build on the analysis by McCoy and Wu (1973), which is characterised by the use of Pfaffians. Our analysis, just like the star-triangle approach, becomes exact in the limit of smoothly varying couplings $J_2(l)$. On the one hand our results are more restricted than those of Burkhardt *et al* (1984) in that we consider only the case $p = 1$ as given by equation (1.2); on the other hand we consider deviations from bulk criticality ($t \neq 0$) and are also able to include a surface magnetic field h_1. Where the two methods overlap, the results agree.

The paper is set up as follows. In § 2 we first recall the Pfaffian approach to the calculation of the boundary behaviour of the two-dimensional Ising model. We then derive a differential equation basic to the remainder of our paper and discuss its validity for smoothly varying couplings. The general solution of the equation is given in § 3 and is related to the zero-field boundary spin-spin correlation function. In § 4 we extract from the general expression the temperature-dependent correlation length. The cases $t > 0$ and $t < 0$, as well as different intervals for the amplitude A_0, have to be distinguished. For A_0 below a critical value $A_{0,c}$ the correlation length exponents $\nu_\parallel$ and $\nu'_\parallel$ (for $t > 0$ and $t < 0$ respectively) are unequal. In particular, $\nu_\parallel$ turns out to be non-universal as it varies linearly with A_0. In § 5 we discuss the spontaneous magnetisation, which is always present when $t < 0$ and, for $A_0 < A_{0,c}$, also when $t = 0$. Its exponent, denoted β_1 or $\beta_1^{(1)}$, is again non-universal. The correlation function in the scaling limit $r \to \infty$, $t \to 0$ is considered in § 6. In § 7 we consider the boundary magnetic susceptibility; again, for $A_0 < A_{0,c}$ we find $\gamma_{11} \neq \gamma'_{11}$ for its exponents. The behaviour of the correlation function at criticality is derived in § 8, and the small-h_1 behaviour of the boundary magnetisation on the critical isotherm in § 9. The exponents $\eta_\parallel$ and δ_{11} are also found to vary continuously with the amplitude A_0. In § 10 we make a number of concluding remarks. These concern the universality of our results, the validity of the usual relations between the exponents, and a very remarkable special case in which the presence of the boundary is not 'noticed' by the system.

2. A differential equation based on the Pfaffian solution of the Ising model

We shall let $m_1(t, h_1)$ denote the average magnetisation of a boundary spin at the reduced temperature t and for a boundary magnetic field h_1. Furthermore $g_\parallel(r, t)$ will be the pair correlation function between two spins on the boundary a distance r apart, in zero field (see figure 1). For $r \to \infty$ we have

$$\lim_{r\to\infty} g_{\parallel}(r, t) = m_1^2(t) \tag{2.1}$$

where

$$m_1(t) = \lim_{h_1 \downarrow 0} m_1(t, h_1) \tag{2.2}$$

is the spontaneous boundary magnetisation. Another quantity of interest will be the zero-field boundary susceptibility $\chi_{11}(t)$, defined as

$$\chi_{11}(t) = \lim_{h_1 \downarrow 0} (m_1(t, h_1) - m_1(t))/h_1. \tag{2.3}$$

It may also be obtained as a sum over the pair correlation:

$$\chi_{11}(t) = \sum_{r=-\infty}^{\infty} (g_{\parallel}(r, t) - m_1^2(t)). \tag{2.4}$$

Formal expressions for the quantities $m_1(t, h_1)$ and $g_{\parallel}(r, t)$, for arbitrary couplings $J_2(l)$, can be found in McCoy and Wu (1973). These authors employed the Pfaffian method developed by Kasteleyn (1961, 1963), and some of their results will serve as a starting point for this work. The Pfaffian method reduces calculations in the two-dimensional Ising model to the problem of finding the determinant of a matrix, the rows and columns of which each correspond to a definite lattice site. In the case such as that shown in figure 1, one can Fourier transform in the translationally invariant vertical direction, thereby introducing a wavenumber θ. The original determinant then reduces to the product of smaller, θ-dependent determinants. The calculation of each of these can be done recursively in the column variable l, and involves a quantity $x_l(\theta)$. The expression for $g_{\parallel}(r, t)$ thus obtained by McCoy and Wu reads, in a boundary field $h_1 = 0$,

$$g_{\parallel}(r, t) = \frac{1}{2\pi i} \int_{-\pi}^{\pi} d\theta \frac{\exp(-ir\theta)}{x_1(\theta)} \tag{2.5}$$

where $x_1(\theta)$ is the solution of the recursion relation

$$x_{l-1}(\theta) = a(\theta) + \frac{b^2(\theta) x_l(\theta)}{a(\theta) x_l(\theta) + z_2^2(l)}, \qquad (l = 2, 3, \ldots) \tag{2.6}$$

in which

$$a(\theta) = -2z_1 \sin\theta |1 + z_1 \exp(i\theta)|^{-2}, \qquad b(\theta) = (1 - z_1^2)|1 + z_1 \exp(i\theta)|^{-2} \tag{2.7}$$

$$z_1 = \tanh(J_1/k_B T) \qquad z_2(l) = \tanh(J_2(l)/k_B T) \qquad (l = 1, 2, \ldots, \infty). \tag{2.8}$$

The recursion relation should be solved with the boundary condition that $\lim_{l\to\infty} x_l(\theta) \equiv x_\infty(\theta)$ be the stable stationary solution when (2.6) is iterated in the direction of decreasing l. This fully defines how to calculate $g_{\parallel}(r, t)$.

Again using the Pfaffian method McCoy and Wu find for the boundary magnetisation $m_1(t, h_1)$ in arbitrary boundary field h_1 the expression

$$m_1(t, h_1) = z + (1 - z^2) z \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \frac{1}{z^2 + d(\theta) x_1(\theta)} \tag{2.9}$$

where

$$z = \tanh(h_1/k_B T) \tag{2.10}$$

and

$$d(\theta) = -2 \sin \theta |1 + \exp(i\theta)|^{-2}. \tag{2.11}$$

The recursion relation (2.6), while trivial for a homogeneous lattice, cannot be solved exactly in the general case. However, if the couplings $J_2(l)$ vary sufficiently smoothly, then l may be regarded as a continuous variable, and, in an appropriately taken limit, (2.6) reduces to a differential equation. There are two ways at least to derive this equation. One of them, to be presented here, is based on considering the temperature region near bulk criticality, i.e.

$$|t| \ll 1. \tag{2.12}$$

The other one is based on taking the anisotropic limit and is given in the appendix.

The bulk critical temperature T_c is the value of T for which the criticality relation

$$z_2 = (1 - z_1)/(1 + z_1) \tag{2.13}$$

(Onsager 1944) is satisfied, where we have set $z_2 \equiv z_2(\infty)$. A pair satisfying relation (2.13) will be denoted (z_{1c}, z_{2c}). We may now indicate three small parameters in our problem. Firstly, if (2.12) holds then z_1 and z_2 will, in general, deviate from z_{1c} and z_{2c} by amounts of the order of t. Secondly, we shall be interested only in the large-r behaviour of the correlation function $g_{\|}(r, t)$, which is determined by the small-θ behaviour of $x_1(\theta)$. Thus we assume

$$\theta \ll 1. \tag{2.14}$$

Thirdly, we impose that the couplings $J_2(l)$ differ only little from their bulk value $J_2(\infty)$. This condition is realised if $J_2(l)$ is of the form

$$J_2(l) = J_2(\infty) - \varepsilon A_0 \Delta(\varepsilon l) \tag{2.15}$$

where ε is a small constant and $\Delta(x)$ an arbitrary function which remains finite for $x \to 0$ and has the large-x expansion

$$\Delta(x) \simeq x^{-1} + a_2 x^{-2} + a_3 x^{-3} + \dots \qquad (x \to \infty) \tag{2.16}$$

so that (1.2) is ensured. In what follows we shall employ the special choice

$$\Delta(x) = 1/(1 + x). \tag{2.17}$$

We emphasise that the amplitude A_0 in (2.15) is not required to be small.

It is now natural to assume that t and θ are also of the order of ε. With the aid of (2.12), (2.14) and (2.15) we can then expand the coefficients in the recursion relation (2.6) and obtain to first order in t and θ

$$\begin{aligned} a(\theta) &\simeq -2 z_{1c} \theta / (1 + z_{1c})^2 \\ b(\theta) &\simeq z_{2c}(1 + 2 J_1 t / k_B T_c) \end{aligned} \tag{2.18}$$

$$z_2(l) \simeq z_{2c} - (1 - z_{2c}^2)(J_2(\infty) t + \varepsilon A_0 \Delta(\varepsilon l))/k_B T_c. \tag{2.19}$$

Substitution into (2.6) yields the equation

$$y_{l-1} = -c\theta + (1 + c_1 t) y_l / (1 - c\theta y_l - c_2 t - \varepsilon A \Delta(\varepsilon l)) \tag{2.20}$$

where we have defined

$$y_i = x_i / z_{2c} \tag{2.21}$$

$$A = 4A_0 / k_B T_c \sinh(2J_2(\infty)/k_B T_c) \tag{2.22}$$

$$c = 2z_{1c}/(1 - z_{1c}^2) \tag{2.23}$$

$$\left.\begin{aligned} c_1 &= 4J_1/k_B T_c \\ c_2 &= 2(1 - z_{2c}^2) J_2(\infty)/z_{2c} k_B T_c. \end{aligned}\right. \tag{2.24}$$

From (2.20) we see that $y_{l-1} - y_l$ is of the order of ε. We can formally derive a differential equation by introducing

$$s \equiv \varepsilon l + 1 \tag{2.25}$$

$$y(s) \equiv y_l \tag{2.26}$$

putting $t = \varepsilon \bar{t}$, $\theta = \varepsilon \bar{\theta}$, and taking the limit $\varepsilon \to 0$ in (2.20). In the discussion in § 10 we further comment on this limit. The result is

$$\frac{\mathrm{d}y(s)}{\mathrm{d}s} = -c\theta(y^2(s) - 1) - \left(\frac{A}{s} + \gamma t\right) y(s) \tag{2.27}$$

where we have again written t for $\bar{t}$ and θ for $\bar{\theta}$, and used the explicit form (2.17) for $\Delta(x)$, and where

$$\gamma = c_1 + c_2 = 2[2z_{2c}J_1 + (1 - z_{2c}^2)J_2]/z_{2c}k_B T_c. \tag{2.28}$$

One easily finds that the proper boundary condition for equation (2.27) is

$$y(\infty) = -(\gamma t + \rho)/2c\theta \tag{2.29}$$

where

$$\rho = (\gamma^2 t^2 + 4c^2\theta^2)^{1/2}. \tag{2.30}$$

One can convert the nonlinear first-order equation (2.27) into a linear second-order differential equation by introducing

$$u(s\rho) = \exp\left[\int_1^s \left(c\theta y(s') + \frac{A}{2s'} + \tfrac{1}{2}\gamma t\right) \mathrm{d}s'\right]. \tag{2.31}$$

Inversely we have

$$y(s) = -\frac{1}{2c\theta}\left(\frac{A}{s} + \gamma t\right) + \frac{1}{c\theta}(\gamma^2 t^2 + 4c^2\theta^2)^{1/2} \frac{\mathrm{d}}{\mathrm{d}z} \ln u(z)\bigg|_{z=s\rho}. \tag{2.32}$$

From (2.27) and (2.31) one obtains

$$\frac{\mathrm{d}^2 u(z)}{\mathrm{d}z^2} = \left(\frac{1}{4} - \frac{\kappa}{z} - (\tfrac{1}{4} - \mu^2)\frac{1}{z^2}\right) u(z) \qquad (0 < z < \infty) \tag{2.33}$$

where

$$\kappa = -\tfrac{1}{2}A\gamma t/\rho = -\tfrac{1}{2}A \,\mathrm{sgn}\, t/(1 + 4c^2\theta^2/\gamma^2 t^2)^{1/2} \tag{2.34}$$

$$\mu = \tfrac{1}{2}(1 - A). \tag{2.35}$$

The boundary condition (2.29) becomes

$$u(\infty)=0. \tag{2.36}$$

Equation (2.33), which is Whittaker's differential equation, constitutes together with (2.36) our reformulation of the problem. We shall see in the following sections that its solutions imply a richness of new phenomena. After giving the general solution of (2.33) in § 3, we shall discuss the case of arbitrary $t\neq 0$ in §§ 4–7, and the special case $t=0$ in §§ 8 and 9.

3. Solution of the differential equation. The resulting integral for the correlation function

The solution to the differential equation (2.33) with boundary condition (2.36) is the Whittaker function

$$u(z)=W_{\kappa,\mu}(z) \tag{3.1}$$

(Abramowitz and Stegun (AS) 1965, ch 13). It is usually written as

$$W_{\kappa,\mu}(z)=\exp(-\tfrac{1}{2}z)z^{1/2+\mu}U(\tfrac{1}{2}+\mu-\kappa,1+2\mu,z) \tag{3.2}$$

with

$$U(a,b,z)=\frac{\Gamma(1-b)}{\Gamma(1+a-b)}M(a,b,z)-\frac{z^{1-b}}{1-b}\frac{\Gamma(b)}{\Gamma(a)}M(1+a-b,2-b,z) \tag{3.3}$$

(see AS, equation (13.1.3)). Here $M(a,b,z)$ is the Kummer function

$$M(a,b,z)=1+\frac{az}{b}+\frac{(a)_2z^2}{(b)_2 2!}+\frac{(a)_3z^3}{(b)_3 3!}+\dots \tag{3.4}$$

with the usual notation

$$(a)_n=a(a+1)(a+2)\dots(a+n-1) \qquad (n=1,2,\dots). \tag{3.5}$$

Derivatives $U'(a,b,z)$ can be expressed in the $U(a,b,z)$ themselves with the aid of the property

$$zU'(a,b,z)=(a-b+z)U(a,b,z)-U(a-1,b,z). \tag{3.6}$$

From (2.5), (2.21), (2.32) with $s=1$, and using (3.6) as well as several other relationships between the functions U (see AS, ch 13.4), we obtain for $g_\parallel(r,t)$ the expression

$$g_\parallel(r,t)\simeq\frac{g_0}{2\pi\mathrm{i}}\int_{-\pi}^{\pi}\mathrm{d}\theta\,\theta\exp(-\mathrm{i}r\theta)\frac{1-2\mu}{1-2\mu-2\kappa}\frac{U(\frac{1}{2}+\mu-\kappa,2\mu+1,\rho)}{U(-\frac{1}{2}+\mu-\kappa,2\mu-1,\rho)} \tag{3.7}$$

with

$$g_0=2c/z_{2c}=4z_{1c}/(1-z_{1c})^2. \tag{3.8}$$

With the aid of (3.3) the functions U in (3.7) can be expressed in terms of Kummer functions. Upon rewriting the resulting expression and using (2.34) and (2.35) we find

$$g_\parallel(r,t)\simeq\frac{g_0}{2\pi\mathrm{i}}\int_{-\pi}^{\pi}\mathrm{d}\theta\,\theta\exp(-\mathrm{i}r\theta)\frac{N(\theta)}{D(\theta)} \tag{3.9}$$

with the numerator $N(\theta)$ and denominator $D(\theta)$ given by

$$N(\theta)=\frac{\Gamma(-2\mu)}{\Gamma(\frac{1}{2}-\mu-\kappa)}\rho^{2\mu}M(\tfrac{1}{2}+\mu-\kappa,1+2\mu,\rho)+\frac{\Gamma(2\mu)}{\Gamma(\frac{1}{2}+\mu-\kappa)}M(\tfrac{1}{2}-\mu-\kappa,1-2\mu,\rho) \tag{3.10}$$

and

$$D(\theta)=\frac{\Gamma(-2\mu)}{\Gamma(\frac{1}{2}-\mu-\kappa)}2\rho^{2\mu}(1-A)M(-\tfrac{1}{2}+\mu-\kappa,2\mu-1,\rho)$$
$$+\frac{\Gamma(2\mu)}{\Gamma(\frac{1}{2}+\mu-\kappa)}\frac{2c^2\theta^2}{1+A}M(\tfrac{3}{2}-\mu-\kappa,3-2\mu,\rho). \tag{3.11}$$

The integrand in (3.9) depends on θ and on t both explicitly and via ρ and κ. It depends on the amplitude A explicitly and via μ and κ. In the next sections the equations (3.9)-(3.11) will be the starting point for the asymptotic evaluation of $g_{\parallel}(r,t)$ when t is small.

4. The analytic structure of the integrand of (3.9). Correlation lengths

4.1. General considerations

The boundary correlation length $\xi_{\parallel}(t)$ is defined by

$$g_{\parallel}(r,t)\sim\exp(-r/\xi_{\parallel}(t)) \qquad (r\to\infty). \tag{4.1}$$

For $t\to 0$ one expects the correlation length to diverge and therefore we write

$$\xi_{\parallel}(t)\simeq\hat{\xi}_{+}t^{-\nu_{\parallel}} \qquad \xi_{\parallel}(t)\simeq\hat{\xi}_{-}(-t)^{-\nu'_{\parallel}} \tag{4.2}$$

for $t>0$ and $t<0$ respectively. In *homogeneous* semi-infinite Ising systems one usually finds that $\xi_{\parallel}$ is equal to the bulk correlation length ξ. For a square lattice this means (Wu *et al* 1976)

$$\xi_{\parallel}(t)=\xi(t)=\hat{\xi}_0|t|^{-\nu} \qquad (t\to 0) \tag{4.3}$$

with $\nu=1$ and, for the direction parallel to the J_1 bond (i.e. parallel to the boundary)

$$\hat{\xi}_0=z_{1c}k_BT_c/[(1-z_{1c}^2)J_1+2z_{1c}J_2]. \tag{4.4}$$

We shall see below that for inhomogeneous ($A\neq 0$) semi-infinite lattices both the amplitude and the exponent of $\xi_{\parallel}$ may be altered.

From (3.9) one can see that $\xi_{\parallel}(t)$ is determined by the non-analyticity of $N(\theta)/D(\theta)$ in the complex θ plane with the smallest imaginary part. Since both $N(\theta)$ and $D(\theta)$ depend on θ only via the root

$$R(\theta/t)=(1+4c^2\theta^2/\gamma^2t^2)^{1/2} \tag{4.5}$$

the ratio $N(\theta)/D(\theta)$ has the same singularities as this root, namely branch points at

$$\theta_{\pm}=\pm\tfrac{1}{2}\mathrm{i}\gamma t/c. \tag{4.6}$$

We shall cut the complex θ plane along the imaginary axis from $\pm\frac{1}{2}\mathrm{i}\gamma|t|/c$ to $\pm\mathrm{i}\infty$. From (3.9) and (4.6) we then see that *if there are no other singularities*, we have

$$\xi_{\parallel}(t)\simeq 2c/\gamma|t|. \tag{4.7}$$

With the aid of (2.13), (2.23), (2.28), and (4.4) one can show that (4.7) is identical to (4.3). Therefore equation (4.7), to the extent that it will remain unmodified by the considerations below, represents the well known correlation length divergence prevailing both in the bulk and on the boundary of homogeneous semi-infinite systems.

We should now consider the possibility of additional poles in $N(\theta)$ or zeros in $D(\theta)$. Since $1/\Gamma(z)$ is analytic for all z and M is a power series, we do not expect poles in $N(\theta)$. The remainder of this section will be devoted, therefore, to the study of the zeros of $D(\theta)$. A useful observation is that with the definition

$$\bar{\theta} = \theta/t \tag{4.8}$$

we can expand the function $D(\theta)$ in the form

$$\begin{aligned} D(\theta) = {} & \frac{\Gamma(-2\mu)}{\Gamma(\frac{1}{2}-\mu-\kappa(\bar{\theta}))}|\gamma t|^{2\mu} R^{2\mu}(\bar{\theta})(B_0(\bar{\theta}) + tB_1(\bar{\theta}) + t^2 B_2(\bar{\theta}) + \ldots) \\ & + \frac{\Gamma(2\mu)}{\Gamma(\frac{1}{2}+\mu-\kappa(\bar{\theta}))} t^2\bar{\theta}^2(C_0(\bar{\theta}) + tC_1(\bar{\theta}) + t^2 C_2(\bar{\theta}) + \ldots) \end{aligned} \tag{4.9}$$

where we have indicated explicitly the dependence of κ on $\bar{\theta}$, and where the expansion coefficients $B_k(\bar{\theta})$ and $C_k(\bar{\theta})$ are functions of $\bar{\theta}$ only. They are well behaved for $\bar{\theta} \to 0$. In particular we have

$$B_0(\bar{\theta}) = 2(1-A) \tag{4.10}$$

$$C_0(\bar{\theta}) = 2c^2/(1+A). \tag{4.11}$$

We wish to solve the equation $D(\theta) = 0$ for small t. The strategy will be to find the values of θ for which the dominant term in (4.9) vanishes. If necessary, corrections to these leading-order values may then be found perturbatively as a series in the appropriate powers of t. The powers occurring in (4.9) are t^k and $|t|^{2\mu-2+k}$, $k = 2, 3, 4, \ldots$. The dominant term is the one with $|t|^{2\mu}$ if $\mu < 1$ (hence $A > -1$), and the one with t^2 if $\mu > 1$ (hence $A < -1$). We therefore distinguish these two cases in §§ 4.2 and 4.3 respectively.

4.2. *The correlation length for $A > -1$*

For $A > -1$ we have $\mu < 1$ and the leading term in the function $D(\theta)$ given by (4.9) is the one proportional to $B_0(\bar{\theta})$. In this term $B_0(\bar{\theta})$ is a constant and $R(\bar{\theta})$ has no zeros other than at the branch point discussed above. Therefore any additional zeros of $D(\theta)$ must be the solutions of

$$1/\Gamma(\tfrac{1}{2} - \mu - \kappa(\bar{\theta})) = 0. \tag{4.12}$$

Using the expressions (2.34) and (2.35) for κ and μ, and using (4.8), we find from (4.12)

$$1 + (\operatorname{sgn} t)/(1 + 4c^2\theta^2/\gamma^2 t^2)^{1/2} = -2n/A \qquad (n = 0, 1, 2, \ldots). \tag{4.13}$$

Four cases have to be distinguished.

(1) $t > 0$, $A > 0$. There are no solutions to (4.13).

(2) $t < 0$, $A > 0$. For $n = 0, 1, 2, \ldots$ there are pairs of imaginary solutions given by

$$\theta_n = \pm \mathrm{i}\frac{\gamma t}{2c}\frac{[2n(2n+2A)]^{1/2}}{2n+A} \qquad (n = 0, 1, 2, \ldots). \tag{4.14}$$

(3) $t>0$, $-1<A<0$. There is the same set of poles (4.14), except that the pole at $\theta=0$ is absent: $n=1,2,3,\ldots$.

(4) $t<0$, $-1<A<0$. The only solution is the second-order pole at $\theta_0=0$. The location of the pole and the branch cuts have been indicated in figure 2 for these four

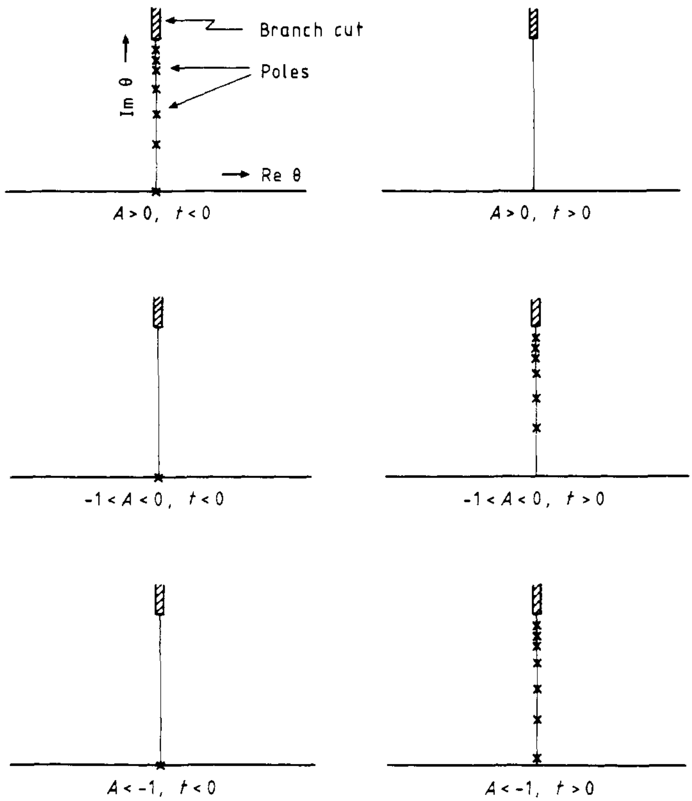

Figure 2. Analytic structure of the integrand of (3.19) in the complex θ plane. The six figures correspond to the cases (1) to (6) distinguished in the text. They are symmetric with respect to both axes. In three cases there is an infinite sequence of poles (equation (4.14) and (4.19)) accumulating towards the branch point. All distances are proportional to t, except that for $A<-1$, $t>0$, one pole is at a distance of order $t^{(1-A)/2}$ from the origin (equation (4.21)).

cases. From equation (4.14) it may be seen that the poles θ_n, $n=1, 2, \ldots$ are all of order t and that for $n\to\infty$ they have accumulation points that coincide with the branch points. We shall not need higher-order corrections for these poles. Some caution is required for the double pole at $\theta_0=0$, however, which in principle could move away from the origin in a higher-order calculation. However, for $\theta=0$ and $t<0$ the expression (4.12), which multiplies the first part of $D(\theta)$, vanishes, and the remaining part of $D(\theta)$ is proportional to θ^2. Hence for $t<0$ the value $\theta_0=0$ is an exact double zero of the denominator. We shall see later that this zero is responsible for the spontaneous boundary magnetisation. We can now conclude that in cases (2) and (3) ($t>0$, $-1<A<0$ or $t<0$, $A>0$) the correlation length $\xi_{\|}(t)$ is determined by the root

θ_1 according to

$$\xi_{\|}(t) = 1/|\theta_1| = \frac{c}{\gamma}\frac{2+A}{(1+A)^{1/2}}\frac{1}{|t|} \qquad (t>0, -1<A<0) \text{ or } (t<0, A>0). \tag{4.15}$$

In cases (1) ($t>0, A>0$) and (4) ($t<0, -1<A<0$) the correlation length is determined by the branch cut and given by (4.7). At $A=0$ the two expressions (4.14) and (4.15) join continuously. It is clear that in all these cases the correlation length exponent, defined by (4.2), is given by $\nu_{\|}=1$. However, in the regions (2) and (3) the correlation length amplitudes $\hat{\xi}_{\pm}$ differ from their bulk value $\hat{\xi}_0$ given by (4.3) and (4.7). In table 1 we list the ratios $\xi_{\pm} \equiv \hat{\xi}_{\pm}/\hat{\xi}_0 = (\gamma/2c)\hat{\xi}_{\pm}$ for the different cases.

Table 1. Survey of the critical boundary behaviour of the semi-infinite inhomogeneous two-dimensional Ising model described in this work. These results apply in the limits $t\to 0$, $h_1 \to 0$ and $r\to\infty$. All quantities are defined in the text.

	$t<0$	$t=0$	$t>0$
$A\leqslant -1$	$\gamma'_{11}=2+A$ $\nu'_{\|}=1$ $\xi_-=1$ $\beta_1^{(0)}=0$ $\beta_1^{(1)}=-1-A$	$\eta_{\|}=0$ $\eta'_{\|}=-1-A$ $\delta_{11}=1/(-1-A)$	$\gamma_{11}=\frac{1}{2}(1-A)$ $\nu_{\|}=\frac{1}{2}(1-A)$
$A=-1$	$m_1(t,0)\sim[\ln(-t^{-1})]^{-1/2}$	$g_{\|}(r)\sim 1/\ln r$ $m_1(0,h_1)\sim(\ln h_1^{-1})^{-1/2}$	$\xi_{\|}\sim(\ln t^{-1})^{1/2}t^{-1}$
$-1\leqslant A\leqslant 0$	$\gamma'_{11}=-A$ $\nu'_{\|}=1$ $\xi_-=1$ $\beta_1=\frac{1}{2}(1+A)$	$\eta_{\|}=1+A$ $\delta_{11}=(1-A)/(1+A)$	$\gamma_{11}=-A$ $\nu_{\|}=1$ $\xi_+=\frac{1}{2}(2+A)/(1$ $+A)^{1/2}$
$A=0$	$\chi_{11}(t,0)\sim\ln(-t^{-1})$	$m_1(0,h_1)=h_1\ln h_1^{-1}$	$\chi_{11}(t,0)\sim\ln t^{-1}$
$A\geqslant 0$	$\gamma'_{11}=-A$ $\nu'_{\|}=1$ $\xi_-=\frac{1}{2}(2+A)/(1+A)^{1/2}$ $\beta_1=\frac{1}{2}(1+A)$	$\eta_{\|}=1+A$ $\delta_{11}=(1-A)/(1+A)$ $(A<1)$	$\gamma_{11}=-A$ $\nu_{\|}=1$ $\xi_+=1$
		$m_1(0,0)\sim(-A-1)^{1/2}$ $\chi_{11}(0,0)\sim(-A-2)^{-1}$ $\chi_{11}(0,0)\sim A^{-1}$	as $A\uparrow -1$ as $A\uparrow -2$ as $A\downarrow 0$.

4.3. *The correlation length for $A<-1$*

4.3.1. First-order calculation. For $A<-1$ we have $\mu>1$ and the leading term in the expression (4.9) for $D(\theta)$ is the one proportional to $C_0(\bar{\theta})$. Since $C_0(\bar{\theta})$ is a constant, the zeros of $D(\theta)$ are, to leading order, the solutions of

$$\bar{\theta}^2/\Gamma(\tfrac{1}{2}+\mu-\kappa(\bar{\theta}))=0. \tag{4.16}$$

There is obviously the double zero

$$\theta_0=0 \qquad (t \text{ arbitrary}, A<-1) \tag{4.17}$$

and in addition there are the solutions of

$$1-(\operatorname{sgn} t)/(1+4c^2\theta^2/\gamma^2t^2)^{1/2}=2(n+1)/A \qquad (n=0,1,2,\ldots). \tag{4.18}$$

This leads us to distinguish two more cases.

(5) $t>0$, $A<-1$. We find the solutions

$$\theta_n = \pm \mathrm{i}\, \frac{\gamma t}{2c} \frac{[2n(2n-2A)]^{1/2}}{2n-A} \qquad (n=1,2,\dots). \tag{4.19}$$

(6) $t<0$, $A<-1$. There are no solutions to (4.16) other than (4.17). The poles and branch points for these cases are shown in figure 2. As before, the values θ_n given by (4.19) are of the order of t and accumulate at the branch points. At $A=-1$, the expression (4.19) joins continuously with (4.14) (see case (3)); when A passes from above through $A=-1$, then θ_1 of (4.19) merges with the origin, sticks to it, and becomes the solution θ_0 of (4.14). Similarly, the solution θ_n of (4.19) becomes the solution θ_{n-1} of (4.14).

4.3.2. Second-order correction to the root θ_0. For $t>0$ we have from (2.30) and (2.31) that $\frac{1}{2}-\mu-\kappa(0)=A$, so that (except when A is a non-positive integer) the first series of terms in (4.9) does not vanish. Hence the root $\theta_0=0$ found in (4.17) is not an exact zero of $D(\theta)$. We consider now the equation obtained by also keeping the next-to-leading term, i.e. the one with $B_0(\bar\theta)$. Using (4.10), (4.11), and the fact that for $t>0$ we have $\frac{1}{2}+\mu-\kappa(0)=1$ we obtain

$$\frac{\Gamma(-2\mu)}{\Gamma(1-2\mu)}\, \gamma^{2\mu}|t|^{2\mu}(1-A)+\Gamma(2\mu)t^2\bar\theta^2\frac{c^2}{1+A}=0 \tag{4.20}$$

whence

$$\theta_0=\pm\mathrm{i}\,\frac{(\gamma t)^{(1-A)/2}}{c}\left(\frac{-1-A}{\Gamma(1-A)}\right)^{1/2} \qquad (t>0,\ A<-1). \tag{4.21}$$

Hence in this case the root $\theta_0=0$ of (4.17) has a next-order correction and becomes the expression (4.21). The correlation length is given by

$$\xi_\parallel(t)=c\left(\frac{\Gamma(1-A)}{-1-A}\right)^{1/2}(\gamma t)^{(A-1)/2} \qquad (t>0,\ A<-1). \tag{4.22}$$

Thus we witness the appearance of a correlation length exponent $\nu_\parallel$ which *varies continuously* with the amplitude A of the applied perturbation,

$$\nu_\parallel=\tfrac{1}{2}-\tfrac{1}{2}A \qquad (A<-1). \tag{4.23}$$

For $t<0$ we have that $\frac{1}{2}-\mu-\kappa(0)=0$. Hence $\theta_0=0$ is an exact double zero of $D(\theta)$. One can divide this zero out and investigate the remaining expression for further zeros. Upon considering again the leading term it appears that the next singularity is the branch point. Hence for $t<0$ and $A<-1$ we again obtain the expression (4.7). Therefore

$$\nu'_\parallel=1 \qquad (A<-1) \tag{4.24}$$

and we see that we have a case of exponent asymmetry: $\nu'_\parallel\neq\nu_\parallel$. The results for the exponents are also shown in table 1 and figure 3.

4.3.3. Second-order correction to the roots θ_n, $n=1,2,\dots$. For $A<-1$ the leading-order expression (4.19) for the zeros θ_n of the denominator D coincides with the leading-order

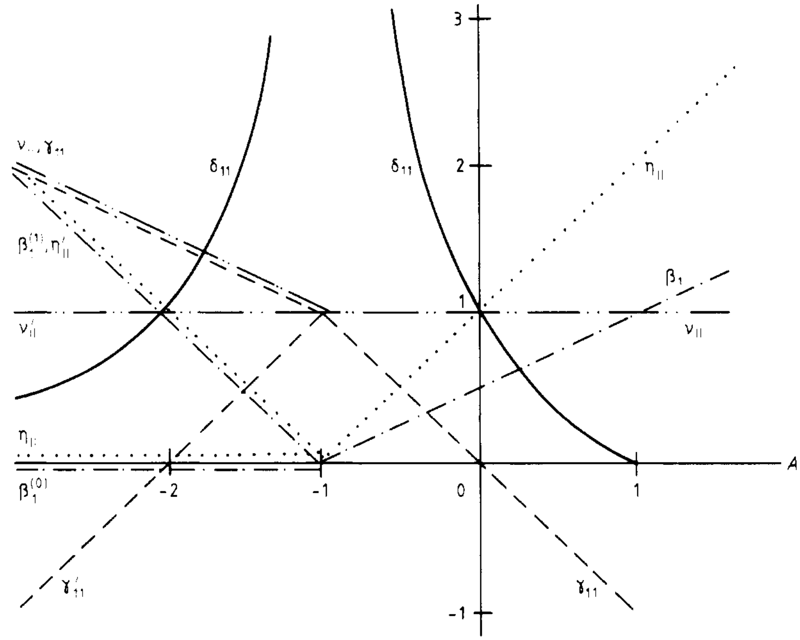

Figure 3. The critical exponents as a function of the amplitude A of the inhomogeneous perturbation.

zeros of the numerator N. It is easy, however, to calculate higher-order corrections. These show that the poles and zeros of N/D get separated and allow one to find the residues. We shall not pursue these corrections here.

4.4. Special case: A equal to an integer m

4.4.1. $A = m \neq 0, 1$. When the amplitude A is equal to an integer m, we have $2\mu = 1 - m$ and some of the Γ and M functions involved in the definition (3.2) develop singularities. Nevertheless the limit $A \to m$ of the right-hand side of (3.3) exists. The resulting function $U(a, b, z)$ (with $b = 1 + 2\mu = 2 - m$) is a series with terms proportional to $z^{-|1-m|/2-(1-m)/2+k}$ and $z^{+|1-m|/2-(1-m)/2+k} \ln z$, for $k = 0, 1, 2, \ldots$. (see AS, equations (13.1.6) and (13.1.7)). When A is an integer, equations (3.9) and (3.10) cannot be used and one has to repeat the calculation starting from (3.7) and using the explicit expression for $U(a, b, z)$. For $A \neq 0$, 1 one finds that the leading-order analysis of the preceding subsections is not affected, and that the results for the correlation length and critical exponents simply carry over to integer A.

4.4.2. $A = -1$. For $A = -1$ we have from (2.34) and (2.35) that $\mu = 1$ and $\kappa = \frac{1}{2}\gamma t/\rho$. We try to find the location of poles of the integrand of (3.7) assuming that $|\theta/t| \ll 1$, which means

$$\rho = \gamma|t|(1 + 2c^2\theta^2/\gamma^2 t^2 + \ldots) \tag{4.25}$$

$$\kappa = \tfrac{1}{2}(\operatorname{sgn} t)(1 - 2c^2\theta^2/\gamma^2 t^2 + \ldots). \tag{4.26}$$

For $|t| \ll 1$ the functions U in (3.7) have the small-ρ expansions

$$U(\tfrac{3}{2}-\kappa, 3, \rho) = \frac{1}{\Gamma(\frac{3}{2}-\kappa)}\rho^{-2} + \mathrm{O}(\rho^{-1}) \tag{4.27}$$

$$U(\tfrac{1}{2}-\kappa, 1, \rho) = -\frac{1}{\Gamma(\frac{1}{2}-\kappa)}\left(\ln\rho + \frac{\Gamma'(\frac{1}{2}-\kappa)}{\Gamma(\frac{1}{2}-\kappa)} - 2\Gamma'(1) + \mathrm{O}(\rho\ln\rho)\right). \tag{4.28}$$

Using (4.25)-(4.28) and taking into account the factor $\theta/(2\kappa+1)$ in (3.7) we find after a straightforward calculation that the integrand of (3.7) has a pole at $\theta = 0$ for $t<0$ and poles at $\theta = \pm i\gamma t c^{-1}[\ln(1/\gamma t)]^{-1/2}$ for $t>0$. Hence we have

$$\xi_{\parallel}(t) \simeq \frac{c[\ln(1/\gamma t)]^{1/2}}{\gamma t} \qquad (t\downarrow 0, A=-1) \tag{4.29}$$

as shown in table 1.

4.4.3. A = 0. For $A=0$ we have from (2.34) and (2.35) that $\mu = \frac{1}{2}$ and $\kappa = 0$. In this case the differential equation (2.33) has the trivial solution $u(\rho) = \exp(-\frac{1}{2}\rho)$ which via (2.32) leads to

$$y(1) = -(\gamma t + \rho)/2c\theta \tag{4.30}$$

in agreement with (2.29). The only singularities of $1/y(1)$ are the branch cuts starting at $\pm\frac{1}{2}i\gamma t/c$ and a pole at $\theta = 0$ for $t<0$. Hence $\xi_{\parallel}(t)$ is given by (4.7) for all $t \ll 1$, in agreement with Wu *et al* (1976).

5. The spontaneous magnetisation

For a homogeneous semi-infinite lattice the spontaneous boundary magnetisation $m_1(t)$, defined by (2.1), is known to vanish above bulk criticality ($t>0$) and to be non-zero below it ($t<0$) (McCoy and Wu 1973). It will turn out that in the inhomogeneous case, $A \neq 0$, the same is true. Anticipating what follows we associate critical exponents β_1 and $\beta_1^{(1)}$ with the leading and the next-to-leading (non-integer) singular powers respectively in the series for $m_1(t)$ as $t\uparrow 0$, and we write

$$m_1(t) \simeq b_0(-t)^{\beta_1} + \ldots + b_1(-t)^{\beta_1^{(1)}} \qquad (t\uparrow 0). \tag{5.1}$$

Here the ellipsis represents terms with integer powers between β_1 and $\beta_1^{(1)}$.

For the calculation of the spontaneous magnetisation $m_1(t)$ we employ (2.1) and (3.9). Since $N(\theta)/D(\theta)$ is odd in θ, we have to evaluate

$$m_1^2(t) = -\lim_{r\to\infty}\frac{g_0}{2\pi}\int_{-\pi}^{\pi} d\theta\,\theta\sin r\theta\frac{N(\theta)}{D(\theta)}. \tag{5.2}$$

The result depends on the $\theta\to 0$ behaviour of the integrand. With the aid of the properties of the M and Γ functions one easily finds from (3.10) and (3.11) the small-θ expansions

$$N(\theta) = 1 + \mathrm{O}(\theta^2) \qquad (t<0) \tag{5.3}$$

$$D(\theta) = 2c^2\theta^2\{-(\gamma|t|)^{2\mu-2}\Gamma(A+1)[1+\ldots] + (A+1)^{-1}[1+\ldots]\} + \mathrm{O}(\theta^4) \qquad (t<0). \tag{5.4}$$

Here the ellipsis indicates a power series in t. For $t>0$ both $N(\theta)$ and $D(\theta)$ remain finite in the small-θ limit. For $t<0$ the double zero of $D(\theta)$ at $\theta=0$ leads to a simple pole in the integrand of (5.2). Using (5.3) and (5.4) as well as the fact that

$$\lim_{r\to\infty}\int_{-\pi}^{\pi} d\theta \frac{\sin r\theta}{\theta} = \int_{-\infty}^{\infty} dx \frac{\sin x}{x} = \pi \tag{5.5}$$

we find

$$m_1^2(t)\begin{cases} =0 & (t>0) \quad (5.6)\\ \simeq \dfrac{-(A+1)(2cz_{2c})^{-1}}{[1+\ldots]-\Gamma(A+2)(\gamma|t|)^{-A-1}[1+\ldots]} & (t<0). \quad (5.7)\end{cases}$$

Two cases have to be distinguished. For $A>-1$ we have to leading order in t

$$m_1(t)\simeq[2cz_{2c}\Gamma(1+A)]^{-1/2}(-\gamma t)^{(1+A)/2} \qquad (A>-1, t<0) \tag{5.8}$$

i.e. the spontaneous magnetisation decays to zero with a non-universal exponent β_1 which depends on the strength A of the inhomogeneity,

$$\beta_1=\tfrac{1}{2}+\tfrac{1}{2}A \qquad (A>-1). \tag{5.9}$$

In the special case $A=0$ this agrees with the result $\beta_1=\frac{1}{2}$ obtained by McCoy and Wu for a homogeneous system. For $A<-1$ we have from (5.7)

$$m_1(t)\simeq(2cz_{2c})^{-1/2}(|A|-1)^{1/2}+[1+\ldots+\tfrac{1}{2}\Gamma(A+2)(-\gamma t)^{-A-1}] \qquad (A<-1, t<0). \tag{5.10}$$

Hence

$$\beta_1=0 \qquad \beta_1^{(1)}=-A-1 \qquad (A<-1). \tag{5.11}$$

From (5.6) and (5.7) it is evident that $m_1(t)$ is discontinuous at $t=0$ when $A<-1$. In § 8 we show that the value $m_1(0)$ is given by the limit $t\uparrow 0$. From (5.10) we then see that $m_1(0)$ vanishes with a square-root singularity as $A\uparrow -1$.

The results of § 4.4.2, finally, imply that when $A=-1$ and $t<0$ we have $N(\theta)/D(\theta)\simeq[2c^2\theta^2\ln(\gamma|t|)]^{-1}$ for $\theta\to 0$. It follows that

$$m_1(t)\simeq[cz_{2c}\ln(1/\gamma|t|)]^{-1/2} \qquad (A=-1, t<0). \tag{5.12}$$

For $A=-2,-3,\ldots$ the non-analytic term in brackets in (5.10) develops a logarithmic correction factor, as signalled by the divergence of its coefficient.

6. The correlation function $g_{\|}(r)$ in the scaling limit

Once the non-analyticities of the integrand of (3.9) in the complex θ plane have been determined, the integration path can be shifted to the lower half-plane and we obtain $g_{\|}(r,t)$ as

$$g_{\|}(r,t)=m_1^2(t)+\sum_n g_n(r,t)+g_{bc}(r,t). \tag{6.1}$$

Here $g_n(r,t)$ is the contribution of the pole at $-i|\theta_n|$ and $g_{bc}(r,t)$ is the contribution from the integration along the lower branch cut. From (3.9) we have explicitly

$$g_n(r,t)=-g_0[\theta\exp(-ir\theta)N(\theta)]_{\theta=-i|\theta_n|}\lim_{\theta\to -i|\theta_n|}\frac{\theta+i|\theta_n|}{D(\theta)} \tag{6.2}$$

and, upon putting $\theta = -\mathrm{i}\tau$,

$$g_{\mathrm{bc}}(r, t) = \frac{g_0}{2\pi \mathrm{i}} \int_{\tau_0}^{\infty} \mathrm{d}\tau\, \tau \exp(-r\tau) \lim_{\varepsilon \downarrow 0} \left(\frac{N(-\mathrm{i}\tau - \varepsilon)}{D(-\mathrm{i}\tau - \varepsilon)} - \frac{N(-\mathrm{i}\tau + \varepsilon)}{D(-\mathrm{i}\tau + \varepsilon)} \right) \tag{6.3}$$

where

$$\tau_0 = \gamma |t| / 2c \tag{6.4}$$

corresponds to the location of the branch point. The term in large round brackets in (6.3) is the discontinuity of the function $N(\theta)/D(\theta)$ across the branch cut. We now use again the expansion of this function in powers of t at fixed $\theta^2/t^2 = -(\gamma^2/4c^2)(\tau^2/\tau_0^2)$. It is useful to introduce the variable

$$u = \left(\frac{\tau^2}{\tau_0^2} - 1 \right)^{1/2} \tag{6.5}$$

The leading behaviour of (6.3) comes from the dominant non-analytic term in the expansion of $N(\theta)/D(\theta)$. It will be convenient to denote the order of this term by $p-2$, so that we can write, at fixed θ and to leading order as $t \to 0$,

$$\lim_{\varepsilon \downarrow 0} \left(\frac{N(-\mathrm{i}\tau - \varepsilon)}{D(-\mathrm{i}\tau - \varepsilon)} - \frac{N(-\mathrm{i}\tau + \varepsilon)}{D(-\mathrm{i}\tau + \varepsilon)} \right) = \mathrm{i} |t|^{p-2} I_A^{\pm}(u) \qquad (t \gtrless 0). \tag{6.6}$$

Explicit expressions for $I_A^{\pm}(u)$ can easily be obtained. We have $p = 1 + A$ for $-1 < A < 1$ and $p = -1 - A$ for $-2 < A < -1$. From (6.3) and (6.6) we obtain

$$\begin{aligned} g_{\mathrm{bc}}(r, t) &= \frac{\gamma^2}{4\pi c z_{2\mathrm{c}}} |t|^p \int_0^{\infty} \mathrm{d}u\, u \exp[-r\tau_0(1+u^2)^{1/2}] I_A^{\pm}(u) \\ &= |t|^p F_A^{\pm}(rt) \qquad (t \gtrless 0) \end{aligned} \tag{6.7}$$

which defines the scaling function $F_A^{\pm}(x)$.

When $At > 0$, there are no poles and equation (6.7) completes the derivation of the scaling form of the correlation function $g_{\parallel}(r, t)$. In the remaining cases, the evaluation of the contributions $g_n(r, t)$ given by (6.2) is straightforward. We only give the results. For $A > -1$ and $At < 0$ we have for $n = 1, 2, \ldots$

$$g_n(r, t) = \frac{1}{2cz_{2\mathrm{c}}} (\gamma |At|)^{1+A} \frac{(A)_n}{n!\Gamma(A)} (2n + A)^{-2-A} \exp(-r|\theta_n|) \tag{6.8}$$

with θ_n given by (4.14) and $(A)_n$ by (3.5). The expression (6.8) is always positive. It has the same scaling form, with the same exponent $p = 1 + A$ (at least for $-1 < A < 1$) as the branch cut contribution (6.7). By using (6.8) and (6.7) in (6.1) we obtain the scaling form of $g_{\parallel}(r, t)$. The sum over n is easily shown to be convergent.

For $A < -1$ and $t < 0$ there is only the branch cut term (6.7).

For $A < -1$ and $t > 0$ the pole at θ_0 leads to the purely exponentially decaying expression

$$g_0(r, t) = \frac{1}{2cz_{2\mathrm{c}}} (|A| - 1) \exp(-r|\theta_0|) \tag{6.9}$$

which in view of (4.21) depends only on the scaling variable $rt^{(1-A)/2}$. The contributions from the remaining poles (cf § 4.3.3) and from the branch cut merely constitute corrections to this result, which vanish in the scaling limit $t \to 0$, $r \to \infty$ at $rt^{(1-A)/2}$ fixed.

7. Boundary susceptibility

The boundary susceptibility $\chi_{11}(t)$ defined by (2.3) can be calculated in several different ways. At this point the easiest way is to substitute in expression (2.4) the results obtained in the two preceding sections. Alternatively one may define

$$\frac{1}{\bar{x}_1(\theta)}=\frac{1}{x_1(\theta)}-\frac{1}{\theta}\lim_{\theta\to 0}\left(\frac{\theta}{x_1(\theta)}\right) \tag{7.1}$$

(which subtracts the most singular part responsible for the spontaneous magnetisation). Substituting this, via (2.9), in either (2.3) or (2.4) one obtains

$$\chi_{11}(t)\simeq 1-\frac{1}{2\pi}\int_{-\pi}^{\pi}\frac{\mathrm{d}\theta}{\theta\bar{x}_1(\theta)}. \tag{7.2}$$

In either way one easily finds that for $|t|\to 0$ the susceptibility behaves as

$$\chi_{11}(t)\sim t^{-\gamma_{11}} \qquad \chi_{11}(t)\sim(-t)^{-\gamma_{11}} \tag{7.3}$$

for $t>0$ and $t<0$ respectively, with

$$\gamma_{11}=\gamma'_{11}=-A \qquad (-1<A<0) \text{ and } (A>0) \tag{7.4}$$

$$\gamma_{11}=\tfrac{1}{2}(1-A) \qquad \gamma'_{11}=2+A \qquad (A\leqslant -1). \tag{7.5}$$

These results are also shown in table 1 and figure 3. It is remarkable that for $A<-1$ the exponents γ_{11} and γ'_{11} are different.

8. The special case $T=T_c$. The correlation function exponent $\eta_{\parallel}$

Several of the results obtained in the previous sections for $T\neq T_c$ (i.e. $t\neq 0$) cannot be generalised to the case $T=T_c$ by just taking the limit $t\to 0$. In this section we therefore analyse separately the case where the bulk temperature is equal to T_c. For $t=0$ we have from (2.30) and (2.34) that $\rho=2c|\theta|$ and $\kappa=0$. The parameter μ, directly equivalent to the amplitude A of the perturbation, is still arbitrary. By employing several relations between special functions one can show that the general solution $u(z)=W_{\kappa,\mu}(z)$ to (2.33) and (2.36) reduces, for $\kappa=0$, to

$$u(z)=(z/\pi)^{1/2}K_\mu(\tfrac{1}{2}z) \tag{8.1}$$

where K_μ is the modified Bessel function. This result is obtained in an alternative way if by substituting $u(z)=z^{1/2}v(z)$ one reduces (2.33) to Bessel's differential equation for $v(z)$. From (8.1), (2.5), (2.21) and (2.32) with $s=1$ we find for $g_{\parallel}(r,t=0)$ the expression

$$g_{\parallel}(r,0)=-\frac{1}{2\pi z_{2c}}\int_{-\pi}^{\pi}\mathrm{d}\theta\frac{\sin r\theta}{y(1)} \tag{8.2}$$

with

$$y(1)=\frac{1-A}{2c\theta}+(\operatorname{sgn}\theta)K'_\mu(c|\theta|)/K_\mu(c|\theta|). \tag{8.3}$$

When μ is not an integer (that is, A not an odd integer), the integrand in (8.2) can be analysed with the aid of the small-z expansion

$$K_\mu(z)=\frac{\pi}{2\sin\mu\pi}[(\tfrac{1}{2}z)^{-\mu}(a_0(-\mu)+a_2(-\mu)z^2+\ldots)-(\tfrac{1}{2}z)^{\mu}(a_0(\mu)+a_2(\mu)z^2+\ldots)] \tag{8.4}$$

where

$$a_k(\mu)=1/2^k(\tfrac{1}{2}k)!\Gamma(\mu+\tfrac{1}{2}k+1) \qquad (k=0,2,4,\ldots). \tag{8.5}$$

For integer μ the expression (8.4) is replaced by its limiting value, in which also logarithms of z appear. The dominant small-θ behaviour of (8.4) depends on the value of A. Distinguishing the different cases we find

$$\begin{aligned}
&y(1)\simeq\frac{c\theta}{1+A}\left(1+\ldots-|\tfrac{1}{2}c\theta|^{-A-1}\frac{\Gamma(\frac{3}{2}+\frac{1}{2}A)}{\Gamma(\frac{1}{2}-\frac{1}{2}A)}\right) && (A<-1, A\neq-3,-5,\ldots)\\
&y(1)\simeq-c\theta\ln|1/\theta| && (A=-1)\\
&y(1)\simeq-\frac{\Gamma(\frac{1}{2}+\frac{1}{2}A)}{\Gamma(\frac{1}{2}-\frac{1}{2}A)}(\operatorname{sgn}\theta)|\tfrac{1}{2}c\theta|^{-A} && (-1<A<1)\\
&y(1)\simeq-1/(c\theta\ln|1/\theta|) && (A=1)\\
&y(1)\simeq\frac{1-A}{c\theta}\left(1+\ldots+|\tfrac{1}{2}c\theta|^{A-1}\frac{\Gamma(\frac{3}{2}-\frac{1}{2}A)}{\Gamma(\frac{1}{2}+\frac{1}{2}A)}\right) && (A>1, A\neq3,5,\ldots).
\end{aligned} \tag{8.6}$$

For $A<-1$ and $A>1$, the ellipsis indicates the integer powers of θ^2 which dominate the leading non-analytic behaviour. The latter is of relative order $|\theta|^{|A|-1}$. For $A=\pm3$, $\pm5,\ldots$ it is replaced by terms proportional to $|\theta|^{|A|-1}\ln|\theta|$. The equations (8.6) show furthermore that as $A\to1$ $(A\to-1)$ from either side, the amplitude of the leading term vanishes (blows up), and that at the points $A=\pm1$ logarithmic corrections appear. With the aid of (8.2) and the expressions (8.6) it is easy to calculate the asymptotic large-r behaviour of $g_\parallel(r,0)$. We find that for $r\to\infty$

$$\begin{aligned}
&g_\parallel(r,0)\simeq\frac{|A|-1}{2cz_{2c}}+\frac{1}{cz_{2c}\sqrt{\pi}}\frac{\Gamma(-\frac{1}{2}A)}{\Gamma(-\frac{1}{2}-\frac{1}{2}A)}\left(\frac{c}{r}\right)^{|A|-1} && (A<-1)\\
&g_\parallel(r,0)\simeq\frac{1}{2cz_{2c}}\frac{1}{\ln r} && (A=-1)\\
&g_\parallel(r,0)\simeq\frac{1}{cz_{2c}\sqrt{\pi}}\frac{\Gamma(1+\frac{1}{2}A)}{\Gamma(\frac{1}{2}+\frac{1}{2}A)}\left(\frac{c}{r}\right)^{1+A} && (A>1).
\end{aligned} \tag{8.7}$$

These equations show again that at the bulk critical temperature $t=0$ there is a spontaneous boundary magnetisation provided that the enhancement of the couplings becomes sufficiently strong $(A<-1)$. As $A\uparrow-1$ we have

$$m_1(t=0)\sim(|A|-1)^{1/2} \qquad (A\uparrow-1). \tag{8.8}$$

This square-root behaviour agrees with the result by Burkhardt and Guim (1984) and by Burkhardt *et al* (1984). For $A\geqslant-1$ we have $m_1(t=0)=0$.

Upon combining these $t=0$ results with the $t\neq0$ results obtained in § 5 we see that when t passes through $t=0$, $m_1(t)$ vanishes continuously if $A\geqslant-1$, but jumps to zero (as soon as t becomes positive) if $A<-1$. In this sense the transition is discontinuous for $A<-1$; however, we have also seen in § 4 that at the transition point $t=0$ the correlation length diverges.

The equations (8.7) also show that at bulk criticality the boundary correlation function decays as a power law for all values of A. Upon defining $\eta_\parallel$ by

$$g_\parallel(r,0)\sim 1/r^{\eta_\parallel} \tag{8.9}$$

we see that

$$\eta_\parallel=\begin{cases}1+A & (A>-1)\\ 0 & (A<-1).\end{cases} \tag{8.10}$$

For $A<-1$ the next-to-leading term in (8.7) is associated with an exponent that we shall call $\eta_\parallel'$:

$$\eta_\parallel'=|A|-1. \tag{8.11}$$

An exceptional case is $A=-1$, where $\eta=0$ and $g_\parallel(r,0)$ decays as the inverse of a logarithm. The correlation function exponents have all been listed in table 1 (see also figure 3).

9. Magnetisation along the critical isotherm

In this section we consider the boundary magnetisation $m_1(t=0, h_1)$ in a small boundary field h_1 at bulk criticality. For $h_1\to 0^\pm$ we expect to obtain again the spontaneous boundary magnetisation $\pm m_1(0)$ given by (8.8). For $h_1\neq 0$ we shall obtain that

$$m_1(0,h_1)=(\operatorname{sgn} h_1)m_1(0)+(\text{Taylor series in } h_1)+m_{1,\text{sg}}(0,h). \tag{9.1}$$

The exponent δ_{11} associated with the boundary magnetisation is defined by

$$m_{1,\text{sg}}(0,h_1)\sim(\operatorname{sgn} h_1)|h_1|^{1/\delta_{11}} \qquad \text{as } h_1\to 0. \tag{9.2}$$

Whenever $1/\delta_{11}>1$, the singular behaviour (9.2) will be dominated by the linear term of the Taylor series in (9.1).

We shall obtain $m_1(0, h_1)$ from the basic relation (2.9). It will again be sufficient to know the small-θ behaviour of the quantities involved. Setting

$$H_1=h_1/k_BT_c \tag{9.3}$$

we have, when $|H_1|\ll 1$ and $|\theta|\ll 1$,

$$m_1(0,h_1)\simeq H_1+\frac{H_1}{2\pi}\int_{-\pi}^{\pi}\frac{\mathrm{d}\theta}{H_1^2-\frac{1}{2}z_{2c}\theta y_1(\theta)}. \tag{9.4}$$

For $y_1(\theta)$ we can now use the expressions (8.6). The evaluation of the integral (9.4) for small H_1 requires again that one distinguishes different cases, according to the value of the amplitude A. This leads to the following expressions:

$$m_{1,\text{sg}}(0,h_1)\simeq\frac{\pi}{\sin\pi A}C_A(\operatorname{sgn} h_1)|h_1/k_BT_c|^{|A|-1} \qquad (A<-1, A\neq -2,-3,-4,\ldots) \tag{9.5a}$$

$$m_{1,\mathrm{sg}}(0, h_1) \simeq \frac{\pi}{2\sin[\pi/(1-A)]} C_A(\operatorname{sgn} h_1)|h_1/k_BT_c|^{(1+A)/(1-A)}$$

$$(-1<A<1, A\neq 1-1/k, k=1,2,3,\ldots) \tag{9.5b}$$

$$m_{1,\mathrm{sg}}(0, h_1) = 0 \qquad (A>1). \tag{9.5c}$$

The proportionality factor C_A is a positive constant given by

$$C_A = -\frac{A}{2}\left(\frac{2}{c}\right)^{3/2}\left(-\frac{1+A}{z_{2c}}\right)^{1/2-A}[\Gamma(\tfrac{1}{2}-\tfrac{1}{2}A)\Gamma(-\tfrac{1}{2}-\tfrac{1}{2}A)]^{-1} \qquad (A<-1)$$

$$C_A = \frac{2}{\pi(1-A)}\left(\tfrac{1}{2}z_{2c}\left(\frac{2}{c}\right)^A \frac{\Gamma(\frac{1}{2}+\frac{1}{2}A)}{\Gamma(\frac{1}{2}-\frac{1}{2}A)}\right)^{-1/(1-A)} \qquad (-1<A<1). \tag{9.6}$$

For $A\to -1$ the constant C_A tends to zero and instead of (9.5*a*) and (9.5*b*) we find

$$m_{1,\mathrm{sg}}(0, h_1) \simeq (\operatorname{sgn} h_1)/[2cz_{2c}\ln(k_BT_c/|h_1|)]^{1/2} \qquad (A=-1). \tag{9.7}$$

For $A\to -k$, where k is a positive integer, the factor $1/\sin \pi A$ in (9.5*a*) diverges and the expression is replaced by

$$m_{1,\mathrm{sg}}(0, h_1) \simeq (-1)^A C_A(\operatorname{sgn} h_1)|h_1/k_BT_c|^{|A|-1}\ln(k_BT_c/|h_1|) \qquad (A=-2,-3,\ldots). \tag{9.8}$$

For $A\to 1-1/k$, where $k=1,2,3,\ldots$, the factor $1/\sin[\pi/(1-A)]$ in (9.5*b*) diverges and the expression is replaced by

$$m_{1,\mathrm{sg}}(0, h_1) \simeq (-1)^{k-1} C_A(\operatorname{sgn} h_1)|h_1/k_BT_c|^{(1+A)/(1-A)}\ln(k_BT_c/|h_1|)$$

$$(A=1-1/k, k=1,2,3,\ldots). \tag{9.9}$$

For $k=1$ this last expression describes the boundary magnetisation of a homogeneous $(A=0)$ semi-infinite system, and reduces to

$$m_{1,\mathrm{sg}}(0, h_1) \simeq \frac{4}{\pi z_{2c}}\frac{h_1}{k_BT_c}\ln(k_BT_c/|h_1|). \tag{9.10}$$

This agrees with the result obtained by McCoy and Wu (1973, ch VI, equation (5.37)) in their detailed study of the homogeneous case. The exponents δ_{11} implied by the equations have been listed in table 1 and are also shown in figure 3.

For the further discussion of our results we define the $2n$th moment $\chi^{(2n)}(t, h_1)$ of the boundary magnetisation by

$$\chi^{(2n)}(t, h_1) = \frac{\partial^{2n-1} m_1(t, h_1)}{\partial h_1^{2n-1}} \qquad (n=1,2,\ldots). \tag{9.11}$$

Clearly $\chi^{(2)}(t, h_1)$ is the ordinary magnetic boundary susceptibility $\chi_{11}(t, h_1)$ discussed in § 7. Because of the presence of the singular terms in the expansion (9.1) of $m_1(0, h_1)$ we see that

$$\chi^{(2n)}(0,0) = \infty \qquad \text{for } A\in[-2n, 1-1/n] \qquad (n=1,2,\ldots) \tag{9.12}$$

i.e. successive moments diverge in a nested sequence of successively larger intervals. Our analysis does not allow us to calculate the coefficients of the regular terms in the h_1 expansion of $m_1(0, h_1)$. It can be shown, nevertheless, that the coefficient of h_1^{2k-1}

diverges as the inverse of the distance between A and the end points of the kth interval in (9.12). Hence

$$\begin{aligned} \chi^{(2n)}(0,0) &\sim (|A|-2n)^{-1} \qquad \text{as } A\uparrow -2n \\ \chi^{(2n)}(0,0) &\sim (A-1+1/n)^{-1} \qquad \text{as } A\downarrow 1-1/n. \end{aligned} \tag{9.13}$$

The behaviour (9.12) and (9.13) is strongly reminiscent of what was found by McCoy (1969) (see also McCoy and Wu 1973) for the quantities $\chi^{(2n)}$ when the $J_2(l)$ are identically distributed *random variables.* In that case the $\chi^{(2n)}$ diverge in nested intervals on the *temperature* axis, the scale of the intervals being set by the width of the random distribution.

10. Discussion

Our basic equation, (2.27), has been derived in the limit of small t, θ, and ε. The amplitude A_0 of the *asymptotic* ($l\to\infty$) behaviour of the perturbation remains *fixed* in this limit, and we have shown that knowledge of this A_0 suffices to find the critical behaviour. For *finite* values of l, however, the strength of the applied perturbation becomes small with ε. One can therefore ask what the implications of our results are for fixed, finite, perturbations $J_2(l)-J_2(\infty)$ with a given A_0. We argue here that for arbitrary finite-l behaviour of the $J_2(l)$, the universal critical properties of the system, such as its exponents, are determined solely by the amplitude A_0 and are as given in this paper. In order to see this one can study the effect of taking into account terms proportional to l^{-2}, l^{-3}, ... in the asymptotic expansion (1.2). One way to do this would be to trace the influence of such terms on the differential equation (2.27) and its solution (e.g. taking $J_2(l)-J_2(\infty)=-A_0/(L+l)=-A_0l^{-1}(1-Ll^{-1}+L^2l^{-2}-\ldots)$ just leads to a shift of the spatial variable in (2.27)). Here we rather invoke the renormalisation group arguments developed by Burkhardt (1982a, b) and Cordery (1982), who show that all $1/l^k$ terms with $k=2,3,\ldots$ are irrelevant for the determination of the universal critical quantities. We conclude therefore that for arbitrary interactions characterised by an asymptotic $1/l$ behaviour (i) the critical amplitudes given in this work will be modified by higher-order terms in $1/l$, but (ii) the exponents (table 1 and figure 3) are exact. Independent confirmation of the latter comes from the work of Burkhardt *et al* (1984), whose results coincide with ours in the domain of overlap, $h=t=0$. There is also agreement with results for the spontaneous boundary magnetisation obtained by Peschel (1984) in the anisotropic limit of our model. Furthermore we have shown that for $A=0$ the problem greatly simplifies and our results for *both* exponents *and* amplitudes reduce to the exactly known values.

A completely analogous situation prevails in the star-triangle solution (Hilhorst and van Leeuwen 1981, Burkhardt and Guim 1982, 1983, 1984, Burkhardt *et al* 1984). There the system of interest is the 'initial condition' for a sequence of n transformations. Its critical behaviour is then extracted from the large n limit, which is described by a set of differential equations. Although these equations are not strictly valid at finite n, it suffices that for a given initial condition one approaches, as $n\to\infty$, the solution of the differential equations. It has been amply demonstrated that this is the case for the systems of interest (see, for example, Burkhardt *et al* 1984).

The general theory of surface critical phenomena (see Binder 1983) predicts certain relationships between the critical exponents. One can easily verify that these also hold for our non-universal (A-dependent) exponents. In particular we see from table 1 that

$$\begin{aligned} \gamma_{11} &= \nu_{\|}(1-\eta_{\|}) \\ \gamma'_{11} &= \nu'_{\|}(1-\eta'_{\|}) \end{aligned} \tag{10.1}$$

$$\begin{aligned} \beta_1 &= \tfrac{1}{2}\nu(d-2+\eta_{\|}) \qquad (A \geq -1) \\ \beta_1^{(0)} &= \tfrac{1}{2}\nu(d-2+\eta_{\|}) \qquad (A < -1) \end{aligned} \tag{10.2}$$

(where $\nu = 1$ is the bulk correlation length exponent, and $d = 2$ the lattice dimension), and

$$\begin{aligned} \gamma'_{11} + \beta_1 &= \beta_1 \delta_{11} \qquad (-1 \leq A \leq 1) \\ \gamma'_{11} + \beta_1^{(1)} &= \beta_1^{(1)} \delta_{11} \qquad (A < -1). \end{aligned} \tag{10.3}$$

It is worthwhile to notice that a remarkable special case is obtained when the amplitude A takes the value $-\frac{3}{4}$. We then have

$$\beta_1 = \beta = \tfrac{1}{8} \qquad \eta_{\|} = \eta = \tfrac{1}{4} \qquad (A = -\tfrac{3}{4}) \tag{10.4}$$

where β and η refer to the bulk. Hence for this value of A the spontaneous magnetisation and pair correlation function exponents 'do not notice' the presence of the border. Similarly

$$\delta_{11} = 7 \qquad \gamma_{11} = \gamma'_{11} = \tfrac{3}{4} \qquad (A = -\tfrac{3}{4}) \tag{10.5}$$

are the exponents associated with the spontaneous column magnetisation and the column susceptibility of an *infinite homogeneous* Ising model in which a magnetic field is applied to a single column only.

In summary, we have presented a full analysis of the surface critical behaviour of the Hamiltonain (1.1) for the case of an inhomogeneity of the type (1.2). This class of inhomogeneities is marginal: it leads to non-universal critical exponents, dependent on the amplitude A of the perturbation (compare with the analogous behaviour in the case of a line defect (Bariev 1979, McCoy and Perk 1980)). The consequences for the observable quantities on the boundary of such a system have been derived and spelled out in this work. Together with the study of Burkhardt *et al* (1984) this work establishes a rather complete understanding of power-law-type inhomogeneities in the couplings of semi-infinite planar Ising lattices.

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Appendix

We study the recursion relation (2.6) in the anisotropic limit $J_1 \to 0$, $J_2(l) \to \infty$, and show that it also leads to a differential equation of the form (2.27). It is convenient to use the standard variables λ and ε (here ε has a different meaning than in §§ 2 and 10) defined by

$$J_1/k_BT = \varepsilon \tag{A1a}$$

$$\exp(-2J_2(\infty)/k_BT) = \lambda\varepsilon \tag{A1b}$$

in which $\lambda = 1$ corresponds to criticality, and $\varepsilon \to 0$ to the anisotropic limit. In terms of these variables (2.7) and (2.8) become

$$\begin{aligned} z_1 &\simeq \varepsilon \\ z_2 &\simeq 1 - 2\lambda\varepsilon \end{aligned} \tag{A2}$$

$$\begin{aligned} a(\theta) &\simeq -2\varepsilon \sin\theta \\ b(\theta) &\simeq 1 - 2\varepsilon \cos\theta. \end{aligned} \tag{A3}$$

Furthermore we put

$$z_2(l) = \tanh J_2(l)/k_B T = 1 - 2\lambda_l \varepsilon \tag{A4}$$

so that by (1.2) we have that $\lambda_l \to \lambda$ for $l \to \infty$. With the choice

$$\lambda_l = 1 + \Delta\lambda + A/(\varepsilon l + 1) \tag{A5}$$

we see that $\Delta\lambda$ plays the role of the deviation from criticality. Upon putting $\varepsilon l + 1 = s$ and $x_l = x(s)$, and using (A1)-(A5) in the recursion (2.6), we find that in the limit $\varepsilon \to 0$ it reduces to the differential equation

$$\frac{\mathrm{d}x}{\mathrm{d}s} = -2\sin\theta(1 - x^2(s)) - \left(8\sin^2\tfrac{1}{2}\theta + 4\Delta\lambda + \frac{4A}{s}\right) x(s). \tag{A6}$$

For small θ this is the same as equation (2.27), although the constants appearing in it have a slightly different meaning. We remark that it has not been needed to assume that the λ_l are close to the critical value $\lambda = 1$.

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