Boundary magnetization and spin correlations in inhomogeneous two-dimensional Ising systems

Theodore W. Burkhardt and Ihnsouk Guim
Department of Physics, Temple University, Philadelphia, Pennsylvania 19122

H. J. Hilhorst and J. M. J. van Leeuwen
Laboratorium voor Technische Natuurkunde, Technische Hogeschool, Postbus 5046, 2600-GA Delft, The Netherlands
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We consider a system of Ising spins on a semi-infinite triangular lattice with nearest-neighbor coupling constants that depend on the distance m from the boundary. An exact technique for calculating the boundary magnetization and the boundary pair correlation function is described. It relies on repeated application of a mapping based on the star-triangle transformation. The case of coupling constants that differ from the bulk coupling by an amount Am^{-y} for large m is examined in detail. For $y<1$ the inhomogeneity of the couplings leads to an interesting variety of modifications in the boundary critical behavior. For $y=1$, $A>A_c$ (A_c being a positive critical value), and for $y<1$, $A>0$, there is a spontaneous surface magnetization at the bulk critical temperature.

I. INTRODUCTION

The boundary critical behavior of the two-dimensional Ising model with free surfaces and with homogeneous nearest-neighbor interactions has been discussed comprehensively by McCoy and Wu.[1] The boundary spins exhibit "ordinary" surface critical behavior,[2] i.e., they order at the bulk critical temperature T_c. The surface critical behavior is characterized by critical exponents that differ, in general, from the bulk critical exponents. For example, the boundary magnetization m_1 vanishes as $(T_c-T)^{1/2}$ as T approaches T_c from below, whereas the bulk magnetization varies as $(T_c-T)^{1/8}$. At $T=T_c$ the pair correlation function $g_{\parallel}(r)$ of surface spins separated by r falls off as r^{-1} for large r, while the bulk correlation function decays as $r^{-1/4}$.

The ordinary surface transition is driven by the bulk transition and is insensitive to modifications in the surface coupling strengths. Au-Yang[3] has obtained exact results for the two-dimensional Ising model with distinct surface and bulk couplings $J_{\parallel}$ and J_B, respectively. She finds that the amplitudes of quantities such as the surface magnetization depend on $J_{\parallel}$, but the surface critical exponents do not. Owing to the one-dimensional nature of the surface, there is ordinary surface critical behavior for any finite $J_{\parallel}$. However, in the Ising model with a bulk dimension greater than 2, there are "surface," "special," and "extraordinary" transitions[2] for appropriately enhanced surface couplings.

In this paper we consider a semi-infinite system of Ising spins on a triangular lattice with nearest-neighbor couplings $K_1(m)$, $m=\frac{1}{2},\frac{3}{2},\ldots$ and $K_2(m)$, $m=1,2,\ldots$ (see Fig. 1) that depend on the distance m from the surface. We are particularly interested in the case of couplings that differ from the bulk couplings K_{1B},K_{2B} at considerable distances from the surface. If the difference $K_i(m)-K_{iB}$, $i=1,2$ vanishes for $m>l$, where l is a finite penetration depth, ordinary critical behavior is expected, since l is negligible in comparison with the bulk correlation length sufficiently close to the bulk critical temperature. In this paper we obtain exact results for ferromagnetic $K_i(m)$ that vary asymptotically as

$$K_i(m)=K_{iB}+A_i m^{-y}\ ,\quad m\gg 1\ . \tag{1.1}$$

The critical behavior we describe below is entirely determined by this asymptotic form, i.e., is independent of the m dependence of $K_i(m)$ for smaller m, as long as all the $K_i(m)$ are finite, which we assume to be the case.

Since the dimensionless $K_i(m)$ are defined by $K_i=J_i/k_BT$, the m dependence of Eq. (1.1) could arise from an inhomogeneous temperature or from inhomogeneous interaction constants J_i. The latter could conceivably result from surface-induced elastic deformations of the lattice in a real system.

As the exponent y is reduced in Eq. (1.1), the inhomogeneity of the coupling constants penetrates deeper into

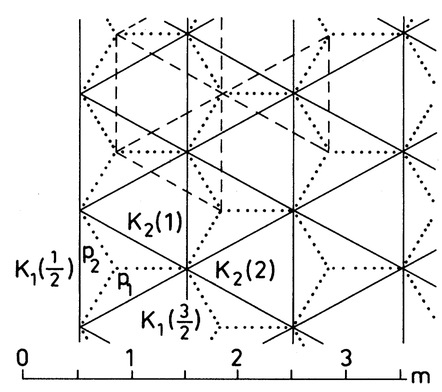

FIG. 1. Initial triangular lattice (solid lines) with coupling constants $K_1(m)$, $m=\frac{1}{2},\frac{3}{2},\ldots$, and $K_2(m)$, $m=1,2,\ldots$. Intermediate hexagonal lattice (dotted lines) with couplings $p_1(m)$, $m=1,2,\ldots$, and $p_2(m)$, $m=\frac{1}{2},\frac{3}{2},\ldots$. New triangular lattice (dashed lines).

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the system. We shall see that for $y>1$ there is ordinary surface critical behavior with the same critical exponents as in the homogeneous semi-infinite case $A=0$. For $y\leq 1$ the inhomogeneous couplings produce a variety of interesting modifications in the behavior at the boundary. In particular, for $y=1$, $A>A_c$ (A_c being a positive critical value) and for $y<1$, $A>0$, there is a spontaneous surface magnetization at the bulk critical temperature T_c that vanishes for $T>T_c$. When $y=1$, the pair correlation function $g_{\parallel}(r)$ of the surface spins decays with a nonuniversal A-dependent exponent $\eta_{\parallel}$. For $y<1$, there is an anomalous exponential decay of the form $\exp[-(r/\xi_{\parallel})^{1-y}]$ at bulk criticality for either sign of A.

This paper gives a detailed account of work that has already been reported in short communications. Hilhorst and van Leeuwen[4] showed how to calculate $g_{\parallel}(r)$ in the case of m-dependent couplings with the help of a mapping based on the star-triangle transformation. They obtained exact results for the case $A<0$. Burkhardt and Guim[5] extended the same approach to $A>0$. Blöte and Hilhorst[6] have examined the case $y=1$ more thoroughly using a Pfaffian method, described and applied to the case of random $K_i(m)$ in Ref. 1.

Burkhardt[7] and Cordery[8] have shown that the exact Ising results are compatible with simple scaling or renormalization-group arguments that are applicable to any semi-infinite system with a divergent bulk correlation length. The scaling theory predicts that inhomogeneous couplings with the m dependence of Eq. (1.1) modify the surface critical behavior for $y<\nu^{-1}$, where ν is the usual bulk critical exponent, but not for $y>\nu^{-1}$.

The paper is organized as follows. In Sec. II the star-triangle method for calculating the boundary magnetization and pair correlation function is described. The method is applicable, in principle, to $K_i(m)$ with an arbitrary m dependence. In Sec. III exact results are obtained for $K_i(m)$ with the asymptotic form given in Eq. (1.1). The Ising results are summarized and compared with the predictions of the scaling or renormalization-group theory in Sec. IV. A brief account of the scaling theory is given in Appendix A. The reader who is primarily interested in a summary of the Ising results may proceed directly to Sec. IV.

II. METHOD OF CALCULATION

A. Difference equations for the coupling constants

We now describe a method for calculating the boundary magnetization and the boundary pair correlation function of the Ising system represented in Fig. 1, where the nearest-neighbor couplings $K_1(m)$ and $K_2(m)$ are arbitrary functions of the distance m from the surface. The method utilizes an exact mapping, based on the star-triangle transformation,[9] that replaces a semi-infinite triangular lattice of Ising spins with coupling constants $K_1(m,n)$ and $K_2(m,n)$ by a similar system with transformed coupling constants $K_1(m,n+1)$ and $K_2(m,n+1)$. The boundary magnetization and boundary pair correlation functions of the nth and $(n+1)$st systems satisfy simple recurrence relations. One can calculate these quantities for the initial system of interest $(n=0)$ from an infinite sequence of mappings.

The star-triangle mapping we use is quite similar to the mapping on which the exact differential renormalization-group transformation of Hilhorst, Schick, and van Leeuwen[10] for the two-dimensional Ising model is based. However, in the application considered here, the transformation does not reduce the number of spins, nor is there a rescaling of lengths.

The star-triangle transformation replaces a star of four Ising spins (see Fig. 2) with nearest-neighbor couplings p_1,p_2,p_3 by a triangle of three Ising spins with couplings K_1,K_2,K_3. The relationship between the K's and p's, which follows from a simple decimation or dedecoration of the central spin of the star, is given by[9]

$$K_1=\frac{1}{4}\ln\frac{\cosh(p_1+p_2+p_3)\cosh(-p_1+p_2+p_3)}{\cosh(p_1-p_2+p_3)\cosh(p_1+p_2-p_3)}\ , \tag{2.1}$$

and its cylic permutations in the indices 1,2,3. In the application of this paper (see Fig. 1), $K_2=K_3$ and $p_2=p_3$. Thus Eq. (2.1) implies

$$K_i=F_i(p_1,p_2)\ ,\ \ i=1,2 \tag{2.2a}$$

$$F_1(p_1,p_2)=\tfrac{1}{4}\ln[\cosh(p_1+2p_2)\times\cosh(p_1-2p_2)/\cosh^2 p_1]\ , \tag{2.2b}$$

$$F_2(p_1,p_2)=\tfrac{1}{4}\ln[\cosh(p_1+2p_2)/\cosh(p_1-2p_2)]\ . \tag{2.2c}$$

To map the semi-infinite triangular lattice of spins with couplings $K_i(m,n)$ onto a similar system with couplings $K_i(m,n+1)$, we first replace all the right-pointing triangles of system n by stars. Labeling the $K_i(m,n)$ and the couplings $p_i(m,n)$ of the resulting hexagonal lattice as in Fig. 1, one sees that

$$K_1(m,n)=F_1(p_1(m+\tfrac{1}{2},n),\ p_2(m,n))\ ,\ \ m=\tfrac{1}{2},\tfrac{3}{2},\ldots \tag{2.3a}$$

$$K_2(m,n)=F_2(p_1(m,n),p_2(m-\tfrac{1}{2},n))\ ,\ \ m=1,2,\ldots\ . \tag{2.3b}$$

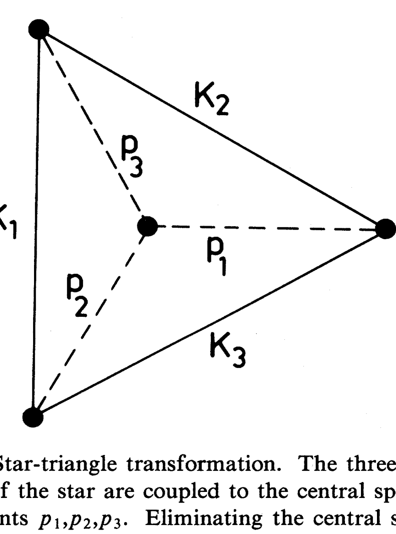

FIG. 2. Star-triangle transformation. The three spins (dots) at the tips of the star are coupled to the central spin with coupling constants p_1,p_2,p_3. Eliminating the central spin leads to interactions K_1,K_2,K_3, given by Eq. (2.1), between the three remaining spins.

Next, we replace the left-pointing stars of the hexagonal lattice by triangles. Using the same labeling scheme for the couplings $K_i(m,n+1)$ of the resulting triangular lattice as for the original triangular lattice, we find

$$K_1(\tfrac{1}{2},n+1)=F_1(0,\, p_2(\tfrac{1}{2},n))\ , \tag{2.4a}$$

$$K_1(m,n+1)=F_1(p_1(m-\tfrac{1}{2},n),\, p_2(m,n))\ , \quad m=\tfrac{3}{2},\tfrac{5}{2},\ldots \tag{2.4b}$$

$$K_2(m,n+1)=F_2(p_1(m,n),\, p_2(m+\tfrac{1}{2},n))\ , \quad m=1,2,\ldots . \tag{2.4c}$$

Difference equations giving the $K_i(m,n+1)$ in terms of the $K_i(m,n)$ may be obtained by eliminating the p_i from Eqs. (2.3) and (2.4). The introduction of alternate variables,

$$X=\exp(-4K_1)\ ,\quad Y=\sinh^2(2K_2)\ , \tag{2.5}$$

$$C_1=\cosh^2 p_1\ ,\quad C_2=\cosh^2(2p_2)\ , \tag{2.6}$$

greatly simplifies the derivation. In terms of these variables the star-triangle transformation given in Eqs. (2.2) has the purely rational form

$$X=\frac{C_1}{C_1+C_2-1}\ ,\quad Y=\frac{C_1C_2-C_1-C_2+1}{C_1+C_2-1}\ , \tag{2.7a}$$

with inverse transformation

$$C_1=\frac{1-X+Y}{1-X}\ ,\quad C_2=\frac{1+Y}{X}\ . \tag{2.7b}$$

The difference equations relating the coupling constants of the nth and $(n+1)$st triangular lattices are given by

$$X(\tfrac{1}{2},n+1)=X(\tfrac{1}{2},n)/[1+Y(1,n)]\ , \tag{2.8a}$$

$$X(m,n+1)=[1-X(m-1,n)+Y(m-\tfrac{1}{2},n)]X(m,n)/D(m,n)\ , \quad m=\tfrac{3}{2},\tfrac{5}{2},\ldots \tag{2.8b}$$

$$Y(m,n+1)=[1-X(m+\tfrac{1}{2},n)+Y(m+1,n)]Y(m,n)/D(m+\tfrac{1}{2},n)\ , \quad m=1,2,\ldots \tag{2.8c}$$

where

$$D(m,n)=1-X(m-1,n)+Y(m+\tfrac{1}{2},n)+X(m,n)Y(m-\tfrac{1}{2},n)-X(m-1,n)Y(m+\tfrac{1}{2},n)\ . \tag{2.8d}$$

In this paper we study the influence of smoothly inhomogeneous couplings as given by Eq. (1.1) on the boundary critical behavior at the bulk critical temperature, i.e., the K_{iB} of Eq. (1.1) satisfy the bulk criticality condition[11]

$$\exp(2K_{1B})\sinh(2K_{2B})=1\ , \tag{2.9}$$

which in terms of the variables X and Y of Eqs. (2.5) takes the form

$$X_B=Y_B\ . \tag{2.10}$$

B. Boundary magnetization and pair correlation function

The boundary magnetization $m_1(n)$ and the boundary pair correlation $g_{\parallel}(r,n)$ of the system with coupling constants $K_i(m,n)$ are defined by

$$m_1(n)=\langle\sigma_0\rangle_n\ , \tag{2.11a}$$

$$g_{\parallel}(r,n)=\langle\sigma_0\sigma_r\rangle_n-\langle\sigma_0\rangle_n\langle\sigma_r\rangle_n\ , \tag{2.11b}$$

where σ_0 and σ_r are boundary spin variables (that take the values ± 1) separated by r lattice constants. The transformation equations

$$m_1(n)=[1-e^{-4K_1(1/2,n+1)}]^{1/2}m_1(n+1)\ , \tag{2.12a}$$

$$g_{\parallel}(r,n)=\tfrac{1}{4}[1-e^{-4K_1(1/2,n+1)}]\times[g_{\parallel}(r+1,n+1)+2g_{\parallel}(r,n+1)+g_{\parallel}(r-1,n+1)]\ ,\quad r\geq 1 \tag{2.12b}$$

under the mapping of Eqs. (2.8) follow from a straightforward derivation.

The thermal averages of interior spins (as opposed to boundary spins) have considerably more complicated transformation properties. The mapping replaces each interior spin in a thermal average by triple-spin as well as single-spin terms. Each mapping generates correlation functions of larger numbers of spins, and the methods of this paper are no longer applicable.

Useful expressions for the boundary magnetization $m_1=m_1(0)$ and the boundary pair correlation function $g_{\parallel}(r)=g_{\parallel}(r,0)$ of the initial system may be obtained by iterating Eqs. (2.12) with the boundary condition $g_{\parallel}(0,n)=1-m_1^2(n)$. These read

$$m_1=\lim_{n\to\infty}[f(n)]^{1/2}m_1(n)=\pm[f(\infty)]^{1/2}\ , \tag{2.13a}$$

$$g_{\parallel}(r)=\sum_{n=1}^{\infty}4^{-n}\frac{r}{n}\binom{2n}{n+r}f(n)[1-m_1^2(n)]\ , \tag{2.13b}$$

$$f(n)=\prod_{j=1}^{n}[1-X(\tfrac{1}{2},j)]\ , \tag{2.13c}$$

A derivation of Eq. (2.13b) is given in Appendix B. In writing the limit in Eq. (2.13a) as $\pm[f(\infty)]^{1/2}$, we have set $m_1(\infty)=\pm 1$, since a nonvanishing $f(\infty)$ requires

$$X(\tfrac{1}{2},n)=\exp[-4K_1(\tfrac{1}{2},n)]\to 0\quad \text{as } n\to\infty\ .$$

Equations (2.13) completely determine m_1 and $g_{\parallel}(r)$ in terms of the sequence of $X(\tfrac{1}{2},n)$ generated by repeated mappings.

If the initial couplings are given by Eq. (1.1) with critical bulk couplings K_{iB}, the quantity $X(\tfrac{1}{2},n)$ tends smoothly to zero in the limit $n\to\infty$, as discussed below. The asymptotic form of $X(\tfrac{1}{2},n)$ for large n reveals whether or not the boundary magnetization vanishes. It is useful to rewrite Eq. (2.13a) as

$$\ln|m_1|=\tfrac{1}{2}\ln f(n_0)-\tfrac{1}{2}\int_{n_0}^{\infty}dn\, X(\tfrac{1}{2},n)\ , \tag{2.14}$$

where n_0 is sufficiently large that $\ln[1-X(\frac{1}{2},n)]$ may be replaced by $-X(\frac{1}{2},n)$ and the sum over n by an integral. From Eq. (2.14) it is clear that $m_1=0$ unless the integral converges, i.e., unless $X(\frac{1}{2},n)$ tends toward zero faster than n^{-1} as n approaches infinity.

The asymptotic form of $X(\frac{1}{2},n)$ for large n also determines the behavior of $g_{\parallel}(r)$ for large r. This behavior may be conveniently calculated from the formulas

$$g_{\parallel}(r) \sim r \int_r^{\infty} dn\, n^{-3/2} e^{-r^2/n} F(n,n_0)[1-F(\infty,n)] , \tag{2.15a}$$

$$F(n_2,n_1)=\exp\left[-\int_{n_1}^{n_2} dj\, X(\tfrac{1}{2},j)\right] . \tag{2.15b}$$

These expressions follow from Eqs. (2.13) upon replacing sums by integrals and rewriting the binomial coefficients using Stirling's approximation. The quantity n_0 in Eq. (2.15a) is a finite cutoff, on which the critical exponents and correlation length of $g_{\parallel}(r)$ do not depend.

C. Differential equations for the coupling constants

When the difference equations (2.8) are iterated numerically with initial coupling constants that vary with m according to Eq. (1.1) and approach bulk critical couplings for large n, both $X(m,n)$ and $Y(m,n)$ tend asymptotically to zero for fixed m in the large-n limit. For large n, $X(m,n)$ and $Y(m,n)$ increase smoothly and monotonically with m and approach the bulk critical values $X_B=Y_B$ asymptotically for large m. In the case of $X(m,n)$ and $Y(m,n)$ which vary sufficiently slowly with m and n, the difference equations (2.8) may be replaced by the differential equations

$$\frac{\partial \ln X(\frac{1}{2},n)}{\partial n} = -[1+Y(1,n)]^{-1}Y(1,n) , \tag{2.16a}$$

$$\frac{\partial \ln X}{\partial n} = -(1-X+Y)^{-1}\left[Y\frac{\partial X}{\partial m}+(1-X)\frac{\partial Y}{\partial m}\right] , \tag{2.16b}$$

$$\frac{\partial \ln Y}{\partial n} = -(1-X+Y)^{-1}\left[(1+Y)\frac{\partial X}{\partial m}-X\frac{\partial Y}{\partial m}\right] . \tag{2.16c}$$

To determine the asymptotic behavior of $X(\frac{1}{2},n)$ for large n, we exactly solve the coupled nonlinear flow equations (2.16b) and (2.16c), with boundary condition (2.16a) and with initial couplings given by Eq. (1.1). Equations (2.16b) and (2.16c) are translationally invariant in m and n, i.e., if $X(m,n)$ and $Y(m,n)$ solve the equations, $X(m-m_0,n-n_0)$ and $Y(m-m_0,n-n_0)$ do also. The constant n_0 may be chosen arbitrarily, but m_0 is fixed by Eq. (2.16a). Having obtained an explicit solution to the differential flow equations, we will argue that it also satisfies the difference equations (2.8) in the large-n limit.

The partial differential equations (2.16b) and (2.16c) assume the much simpler form

$$u\frac{\partial u}{\partial m}=v\frac{\partial v}{\partial n} , \quad u\frac{\partial v}{\partial m}=v\frac{\partial u}{\partial n} , \tag{2.17}$$

in terms of the variables

$$u=2(XY)^{1/2}/(1+Y) , \quad v=2(1-X+Y)^{1/2}/(1+Y) . \tag{2.18}$$

The inverse transformation, which is double valued, as discussed below, is given by

$$X^{1/2}=\frac{u(v^2+Q^2)}{2vQ} , \tag{2.19a}$$

$$Y^{1/2}=Q/v , \tag{2.19b}$$

$$Q(u,v)=[1-\tfrac{1}{4}(v-u)^2]^{1/2}\mp[1-\tfrac{1}{4}(v+u)^2]^{1/2} . \tag{2.19c}$$

Thus the original couplings K_1 and K_2 are related to u and v by

$$\exp(-2K_1)=\frac{u(v^2+Q^2)}{2vQ} , \tag{2.20a}$$

$$\sinh(2K_2)=Q/v . \tag{2.20b}$$

Before proceeding, we note that the domain of ferromagnetic couplings, $K_1 \geq 0$ and $K_2 \geq 0$, is mapped via Eqs. (2.5) onto the strip $0 \leq X \leq 1$ and $Y \geq 0$. The critical line of Eq. (2.9), which corresponds to $X=Y$, divides the strip into a region $X>Y$ of subcritical couplings ($T>T_c$) and a region $X<Y$ of supercritical couplings. This is summarized in Fig. 3.

Equations (2.18) map *both* the subcritical and supercritical domains of ferromagnetic couplings onto a triangle in the u,v plane with sides along the lines $u=0$, $u=v$, and $u+v=2$ as shown in Fig. 3. The critical line corresponds to the side $u+v=2$. The double-valued property of the inverse mapping (2.19) stems from the $\mp$ sign in Eq. (2.19c). The upper and lower signs correspond to couplings on the weak-coupling ($T>T_c$) and strong-coupling ($T<T_c$) sides of the critical line, respectively. The vari-

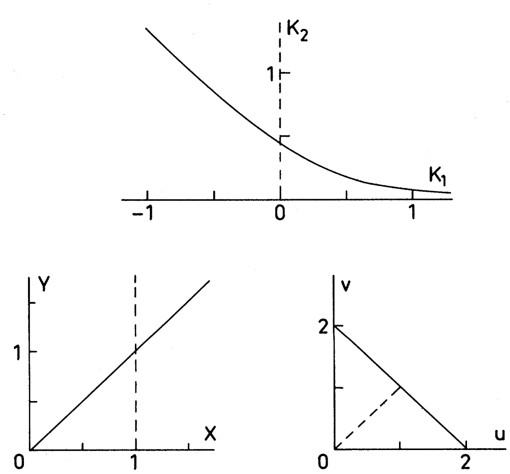

FIG. 3. Domains of the variables K_1,K_2, X,Y and u,v, as discussed below Eqs. (2.20). The solid lines indicate the critical line. The dashed lines separate regions with $K_1>0$ and $K_1<0$.

ables u and v have an interesting duality property[12] that we do not utilize.

In seeking a solution of the nonlinear partial differential equations (2.17), it is advantageous to perform the hodograph transformation,[13] i.e., we regard u and v rather than m and n as the independent variables. This results in the equivalent pair of equations

$$v\frac{\partial m}{\partial u}=u\frac{\partial n}{\partial v}\ ,\quad v\frac{\partial m}{\partial v}=u\frac{\partial n}{\partial u}\ , \tag{2.21}$$

which are linear in m and n and readily soluble by separation of variables. The solutions involve (modified) Bessel functions I_n, K_n, $n=0,1$. We consider superpositions of the form

$$m=m_0+u\int_0^\infty d\rho[w_1(\rho)I_1(\rho u)I_0(\rho v)+w_2(\rho)I_1(\rho u)K_0(\rho v)+w_3(\rho)K_1(\rho u)I_0(\rho v)+w_4(\rho)K_1(\rho u)K_0(\rho v)]\ , \tag{2.22a}$$

$$n=n_0+v\int_0^\infty d\rho[w_1(\rho)I_0(\rho u)I_1(\rho v)-w_2(\rho)I_0(\rho u)K_1(\rho v)-w_3(\rho)K_0(\rho u)I_1(\rho v)+w_4(\rho)K_0(\rho u)K_1(\rho v)]\ . \tag{2.22b}$$

Here, m_0 and n_0 are constants, and $w_1(\rho),\ldots,w_4(\rho)$ are weight functions. These quantities are determined in the next section.

The appropriate boundary conditions to be imposed on the solution (2.22) to the differential flow equations follow from the original difference equations (2.8). The difference equations determine all the $X(m,n)$ and $Y(m,n)$ from the initial values $X(m,0)$ and $Y(m,0)$. The differential equations (2.21) follow from Eqs. (2.8b) and (2.8c) and must be supplemented by the surface boundary condition (2.16a), which follows from Eq. (2.8a). The differential equations (2.21) and the boundary condition (2.16a) determine $u(m,n)$ and $v(m,n)$ for all m,n from the initial values $u(m,0)$ and $v(m,0)$.

III. SURFACE CRITICAL BEHAVIOR

A. Homogeneous couplings

Before considering the surface critical behavior for smoothly inhomogeneous couplings, we discuss the case of *homogeneous* initial couplings that satisfy the bulk criticality condition (2.10), i.e.,

$$X(m-\tfrac{1}{2},0)=Y(m,0)=X_B,\quad m=1,2,\ldots$$

corresponding to Eq. (1.1) with $A_i=0$. The couplings generated from these initial values (with $X_B=\frac{1}{3}$, corresponding to $K_{1B}=K_{2B}=\frac{1}{4}\ln 3$) by $n=500$ computer applications of the mapping of Eqs. (2.8) are shown in Fig. 4. The couplings are no longer homogeneous everywhere, but the criticality condition $X=Y$ is still satisfied locally, i.e., the points representing X and Y lie on a single curve.

For $m\geq n$ the coupling constants have not yet been affected by the surface-induced inhomogeneity, which penetrates one layer deeper with each iteration, and still have the value $X_B=\frac{1}{3}$. For $\frac{1}{3}n<m<n$, X and Y are practically indistinguishable from $\frac{1}{3}$, and for $m<\frac{1}{3}n$, X and Y lie very close to the straight line $X=Y=m/n$. For other initial couplings X_B in the ferromagnetic domain $0\leq X_B\leq 1$ similar results are obtained. After many iterations the numerical results correspond closely to the analytical expression

$$X=Y=\begin{cases} m/n, & m/n<X_B \\ X_B, & m/n>X_B \end{cases}\ . \tag{3.1}$$

These computer results point the way toward a particular class of analytical solutions of the differential flow equations (2.16). The subspace $X=Y$, in which the criticality condition is satisfied locally, is clearly an invariant subspace of the equations. In this subspace Eqs. (2.16) take the form

$$\frac{\partial \ln X(\frac{1}{2},n)}{\partial n}=-[1+X(1,n)]^{-1}X(1,n)\ , \tag{3.2a}$$

$$\frac{\partial \ln X}{\partial n}=-\frac{\partial X}{\partial m}\ . \tag{3.2b}$$

One may readily verify that Eq. (3.1) does indeed solve Eq. (3.2b). A more general solution may be obtained by replacing m and n by $m-m_0$ and $n-n_0$, respectively, as discussed below Eq. (2.16). However, boundary condition (3.2a) clearly requires $m_0=0$ for large fixed n. This value of m_0 is compatible with the numerical results shown in Fig. 4.

One may verify that the slanted portion $X=Y=m/n$ of the critical similarity solution satisfies the difference equations (2.8) for large n, as well as the differential equations (2.16). The matching of the slanted and horizontal branches at $m/n\approx X_B$ can also be studied analytically with the difference equations. The flow equations (3.2) imply that the result $X=Y=m/n$ in the limit of fixed m, $n\to\infty$ holds quite generally if the initial couplings are locally critical and vary sufficiently smoothly with m.

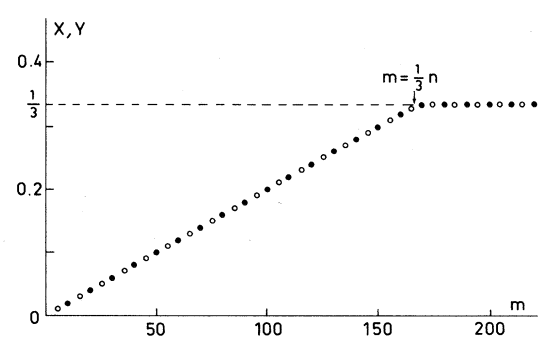

FIG. 4. X and Y (open and solid circles, respectively) after 500 iterations of the difference equations (2.8) with initially homogeneous couplings $X=Y=\frac{1}{3}$.

To see this, we solve Eqs. (3.2) as follows. Regarding m as the dependent variable rather than X, we rewrite Eq. (3.2b) as

$$\frac{\partial m}{\partial n}=X , \tag{3.3}$$

which has the general solution

$$m=nX+F(X) . \tag{3.4}$$

The function $F(X)$ is fixed by the initial couplings $X(m,0)$. Boundary condition (3.2a) further restricts $F(X)$. In the large-n limit in which one expects the differential flow equations to be applicable, Eq. (3.2a) is satisfied for any $F(X)$ that vanishes as $X\to 0$. Thus Eq. (3.4) yields $X=m/n$ for $n\to\infty$, m fixed, as in Eq. (3.1).

Inserting the result $X(\frac{1}{2},n)=(2n)^{-1}$, $n\gg 1$ for the critical subspace $X=Y$ into Eqs. (2.14) and (2.15), we obtain predictions for the surface magnetization m_1 and the surface pair correlation $g_{\parallel}(r)$. We find $m_1=0$, as expected, and $g_{\parallel}(r)\sim r^{-\eta_{\parallel}}$, $\eta_{\parallel}=1$ for large r. This is the same value of $\eta_{\parallel}$ obtained by McCoy and Wu[1] for the semi-infinite Ising model on a square lattice with homogeneous critical couplings.

B. Smoothly inhomogeneous couplings

We now turn to the case of smoothly inhomogeneous initial couplings that vary as

$$K_i(m)=K_{iB}+A_i m^{-y} , \quad m\gg 1 \tag{3.5}$$

$i=1,2$, where K_{1B} and K_{2B} satisfy the bulk criticality condition (2.9). We calculate the asymptotic behavior of $K_1(\frac{1}{2},n)$ which determines the critical behavior of m_1 and $g_{\parallel}(r)$, from appropriate solutions of the differential flow equations, beginning with the general solution given by Eqs. (2.22).

First, we choose the weight functions $w_1(\rho),\ldots,w_4(\rho)$ in Eqs. (2.22) so that the couplings $K_i(m,n)$ vary as in Eq. (3.5) in the limit $m\to\infty$, n fixed. From our experience with the critical similarity solution (3.1) and with numerical results from the difference equations, we expect that for large fixed n, X and Y increase monotonically from the value 0 at or near $m=0$ to the bulk value $X_B=Y_B$ at $m=\infty$, with the criticality condition $X=Y$ approximately satisfied locally. We shall show that solutions possessing all these properties are obtained with weight functions that have the asymptotic form

$$w_1(\rho)=c\rho^{\sigma+1/2}\exp(-\rho u_B)K_1(\rho v_B) ,$$
$$w_2(\rho)=c\rho^{\sigma+1/2}\exp(-\rho u_B)I_1(\rho v_B) ,$$
$$w_3(\rho)=w_4(\rho)=0 ,$$

for large ρ. The quantities c and σ will be related to the A_i and y of Eq. (3.5). With these substitutions for the weight functions, Eqs. (2.22) take the form

$$m-m_0=uc\int_0^\infty d\rho\,\rho^{\sigma+1/2}e^{-\rho u_B}\times I_1(\rho u)[K_1(\rho v_B)I_0(\rho v)+I_1(\rho v_B)K_0(\rho v)] , \tag{3.6a}$$

$$n=vc\int_0^\infty d\rho\,\rho^{\sigma+1/2}e^{-\rho u_B}\times I_0(\rho u)[K_1(\rho v_B)I_1(\rho v)-I_1(\rho v_B)K_1(\rho v)] . \tag{3.6b}$$

The constant n_0 in Eq. (2.22b) does not contribute in the large-n limit and has been dropped.

The asymptotic behavior of the integrals in Eqs. (3.6) for $m\to\infty$, n fixed, where $u\approx u_B$, and $v\approx v_B$, is entirely determined by the behavior of the integrand for large ρ. We make use of the asymptotic forms

$$I_\nu(x)=(2\pi x)^{-1/2}e^{x}[1+O(x^{-1})] , \tag{3.7a}$$

$$K_\nu(x)=(2x/\pi)^{-1/2}e^{-x}[1+O(x^{-1})] , \tag{3.7b}$$

for $x\gg 1$, and the relation

$$\int_0^\infty d\rho\,\rho^{\sigma-1}e^{-\rho s}=\Gamma(\sigma)s^{-\sigma} \tag{3.8}$$

to evaluate the integrals. Solving for u and v, one obtains

$$u_B-u=\left[\frac{c}{v_B}\left[\frac{u_B}{2\pi}\right]^{1/2}\frac{\Gamma(\sigma)}{m}\right]^{1/\sigma} \quad \text{as } m\to\infty , \tag{3.9a}$$

$$\frac{v-v_B}{u_B-u}=\frac{1}{\sigma}\frac{u_B}{v_B}\frac{n}{m} \quad \text{as } m\to\infty . \tag{3.9b}$$

We now determine the spatial dependence of the couplings K_i for $m\to\infty$, n fixed that follows from Eqs. (3.9) and compare it with Eq. (3.5). Equation (3.9b) implies that $v-v_B\ll u_B-u$ for $m\gg n$. Thus $Q(u,v)$, as defined by Eq. (2.19c), may be replaced by

$$Q(u,v)=[1-\tfrac{1}{4}(v_B-u_B)^2]^{1/2}\mp(u_B-u)^{1/2} . \tag{3.10}$$

The upper and lower signs in Eq. (3.10) correspond to couplings that are weaker than critical ($A_i<0$) and stronger than critical ($A_i>0$), respectively, as discussed below Eqs. (2.20). Inserting Eqs. (3.9a) and (3.10) into Eqs. (2.20) and making use of the criticality condition (2.9) for the bulk couplings, one finds the asymptotic behavior given in Eq. (3.5), where the A_i have a particular ratio $A_1/A_2=2\sinh(2K_{1B})/\cosh(2K_{2B})$. In order to fit the initial condition (3.5), the quantity A defined by

$$A_1=\tfrac{1}{2}A\sinh(2K_{1B}), \quad A_2=\tfrac{1}{4}A\cosh(2K_{2B}) \tag{3.11}$$

and the parameters c and σ in Eqs. (3.6) must satisfy

$$\sigma=1/(2y) , \tag{3.12}$$

$$c=\frac{4\pi^{1/2}|A|^{1/y}}{\Gamma[1/(2y)]\sinh(4K_{2B})} . \tag{3.13}$$

In principle, the differential flow equations can be solved for an arbitrary[14] ratio A_1/A_2. However, in this paper we only consider the particular ratio implied by Eqs. (3.11).

Having matched Eqs. (3.6) with the initial conditions (3.5) in the limit $m\to\infty$, n fixed, we now determine the asymptotic behavior for $n\to\infty$, m fixed. From our experience with the critical similarity solution and with computer results from the difference equations, we expect that u and $\delta v=2-v$ fulfill the conditions u, $\delta v\ll 1$. Under these circumstances the second term in the integrand in Eqs. (3.6a) and (3.6b) is negligible in comparison with the first. Using the asymptotic forms (3.7) for $I_0(\rho v)$ and $I_1(\rho v)$, and substituting $\sigma=(2y)^{-1}$, we obtain

$$m-m_0=\frac{uc}{2\sqrt{2v_B}}\int_0^\infty d\rho\,\rho^{(1-y)/(2y)}I_1(\rho u)e^{-\rho\delta v}\,, \tag{3.14a}$$

$$n=\frac{c}{\sqrt{2v_B}}\int_0^\infty d\rho\,\rho^{(1-y)/(2y)}I_0(\rho u)e^{-\rho\delta v}\,. \tag{3.14b}$$

We discuss the cases $y>1$, $y=1$, and $y<1$ separately.

1. $y>1$

From Eqs. (3.7), one sees that the asymptotic behavior of the integrals in Eqs. (3.14) is determined by the asymptotic forms of $I_1(\rho u)$ and $I_0(\rho u)$ for $\rho u \gg 1$ if $0<\delta v-u \ll u$. Evaluating the integrals using these limiting forms and solving for u and v, one obtains

$$\delta v-u=\left[\left[\frac{c\Gamma[1/(2y)]}{2\sqrt{2\pi v_B}}\right]^2\frac{1}{(m-m_0)n}\right]^y\,,$$
$$u=\frac{2(m-m_0)}{n}\,. \tag{3.15}$$

The inequality $0<\delta v-u\ll u$ is clearly fulfilled in the limit m fixed, $n\to\infty$ for $y>1$, but not for $y<1$. Calculating X and Y from u and v using Eqs. (2.19), we find $X(m,n)=Y(m,n)=(m-m_0)/n$ for either sign of A. [Recall that the upper and lower signs in Eq. (2.19c) correspond to $A<0$ and $A>0$, respectively, as discussed below Eqs. (2.20).] The surface boundary condition (2.16a) clearly requires $m_0=0$. Thus for $y>1$ in the limit $n\to\infty$, m fixed,

$$X(m,n)=Y(m,n)=m/n\,. \tag{3.16}$$

Equation (3.16) is identical with the critical similarity solution (3.1) for $m<n$. Since Eqs. (2.14) and (2.15) determine the surface magnetization m_1 and the correlation function $g_{\parallel}(r)$ of the surface spins from $X(\frac{1}{2},n)$, there is ordinary[2] critical behavior for $y>1$. At the bulk critical temperature, $m_1=0$ for either sign of A, and $g_{\parallel}(r)$ falls off as $r^{-\eta_{\parallel}}$, $\eta_{\parallel}=1$, just as in the homogeneous semi-infinite[1] case $A=0$.

2. $y=1$

For $y=1$ it is no longer permissible to use the asymptotic forms for $I_0(\rho u)$ and $I_1(\rho u)$ with $\rho u\gg 1$ in evaluating the integrals in Eqs. (3.14). Making use of exact results for the integrals[15] and solving for u and δv, one finds

$$u=2\left[(m-m_0)\left[\frac{c}{\sqrt{2v_B}}+m-m_0\right]\right]^{1/2}n^{-1}\,, \tag{3.17a}$$

$$\delta v=\left[\frac{c}{\sqrt{2v_B}}+2(m-m_0)\right]n^{-1}\,. \tag{3.17b}$$

Calculating X and Y from u and v using Eqs. (2.19), with the upper and lower signs corresponding to $A<0$ and $A>0$, respectively, we obtain

$$X(m,n)=\frac{2(m-m_0)+|A|/A_c}{2n}\,,\quad Y(m,n)=\frac{m-m_0}{n}\,,\qquad A<0 \tag{3.18a}$$

$$X(m,n)=\frac{m-m_0}{n}\,,\quad Y(m,n)=\frac{2(m-m_0)+|A|/A_c}{2n}\,,\qquad A>0\,. \tag{3.18b}$$

Here,

$$\frac{c}{\sqrt{2v_B}}=\frac{1}{2}\frac{|A|}{A_c}\,,\quad A_c=\tfrac{1}{2}\sinh(2K_{2B})\,, \tag{3.19}$$

in accordance with Eq. (3.13).

The surface boundary condition (2.16a) requires $m_0=0$ for $A<0$ and $m_0=\frac{1}{2}(A/A_c)$ for $0<A<A_c$. In both cases,

$$X(\tfrac{1}{2},n)=\tfrac{1}{2}(1-A/A_c)n^{-1}\,,\quad A<A_c\,. \tag{3.20}$$

Inserting these results into Eqs. (2.14) and (2.15), one finds that $m_1=0$ and that $g_{\parallel}(r)$ decays as $r^{-\eta_{\parallel}}$ for large r, with a *nonuniversal* exponent

$$\eta_{\parallel}(A)=1-A/A_c\,,\quad A<A_c \tag{3.21}$$

that varies continuously with A. For $A=0$, the result $\eta_{\parallel}=1$ for homogeneous couplings is recovered. [In Eq. (4) of Ref. 4 for $\eta_{\parallel}(A)$, a factor 2 is missing; our Eqs. (3.19) and (3.21) give the correct result.]

At $A=A_c$, $X(\frac{1}{2},n)$ as defined by Eq. (3.20) vanishes. However, it does not vanish identically, but instead approaches zero faster than n^{-1}. We will show below that $X(\frac{1}{2},n)=(n\ln n)^{-1}$ for large n. However, before considering the special point $A=A_c$ in detail, we discuss the case $A>A_c$.

For $A>A_c$ we set $m_0=\frac{1}{2}$ in Eqs. (3.18), so that $X(\frac{1}{2},n)$ vanishes to order n^{-1}. Substituting $Y(1,n)=\frac{1}{2}(1+A/A_c)n^{-1}$ from Eq. (3.18b) into the surface boundary condition (2.16a), we see that

$$X(\tfrac{1}{2},n)=c_1 n^{-(1+A/A_c)/2}\,, \tag{3.22}$$

where c_1 is an undetermined constant. Inserting this result into Eq. (2.14), one finds that $m_1\neq 0$ for $A>A_c$, i.e., there is a spontaneous surface magnetization at the bulk critical temperature. In Appendix C we show that m_1 vanishes as $(A-A_c)^{1/2}$ as A approaches A_c from above. Equations (2.15) imply that $g_{\parallel}(r)$ decays as $r^{-\eta_{\parallel}}$ for $A>A_c$, with the nonuniversal exponent $\eta_{\parallel}=A/A_c-1$. This result and Eq. (3.21) may be combined into the single formula

$$\eta_{\parallel}(A)=|1-A/A_c|\,,\quad y=1\,. \tag{3.23}$$

The correction to the order n^{-1} behavior given in Eq. (3.22) is not implied by Eqs. (3.6) but follows from Eqs. (2.22) with the same $w_1(\rho)$ and $w_2(\rho)$ as discussed above, with $w_4(\rho)=0$, and with

$$w_3(\rho)\propto\rho^{1/2+(1-A/A_c)/2}e^{-2\rho} \tag{3.24}$$

for large ρ. This choice for $w_3(\rho)$ does not alter the $A_i m^{-y}$ dependence of K_1 and K_2 for $m\to\infty$, n fixed.

The constant c_1 in Eq. (3.22) is fixed by the proportionality constant in Eq. (3.24). The amplitudes of m_1 and $g_{\parallel}(r)$ depend on the value of c_1, but the critical exponents that we calculate do not.

We now return to the case $A = A_c$, where the choice

$$w_3(\rho) \propto \rho^{1/2} (\ln\rho)^{-2} \exp(-2\rho)$$

for large ρ yields a consistent solution that satisfies the boundary condition (2.16a). In the region m fixed, $n \to \infty$, one obtains

$$X(m,n) = \frac{m-\frac{1}{2}}{n} + \frac{c_0}{n \ln n}, \quad Y(m,n) = \frac{m}{n} + \frac{c_0}{n \ln n}. \tag{3.25}$$

The constant c_0 is fixed by the proportionality constant in $w_3(\rho)$. The value of m_0 has been chosen so that the contribution to $X(m,n)$ of order n^{-1} in Eq. (3.25) vanishes at $m = \frac{1}{2}$. The boundary condition (2.16a) implies $c_0 = 1$. Thus

$$X(\tfrac{1}{2}, n) = (n \ln n)^{-1}, \quad A = A_c. \tag{3.26}$$

Upon substituting Eq. (3.26) into Eqs. (2.14) and (2.15), one sees that $m_1 = 0$ and that $g_{\parallel}(r)$ decays as $(\ln r)^{-1}$ at the bulk critical temperature.

3. $y < 1$

The integrals in Eqs. (3.14) may be evaluated using the small argument expansions

$$I_0(\rho u) = 1 + O((\rho u)^2), \tag{3.27a}$$

$$I_1(\rho u) = \tfrac{1}{2}\rho u [1 + O((\rho u)^2)], \tag{3.27b}$$

for $u/\delta v \ll 1$. Keeping only the first term in the expansion and solving for u and v, one obtains

$$\frac{u^2}{\delta v} = \frac{8y}{1+y} \frac{m - m_0}{n}, \quad \delta v = a n^{-2y/(1+y)}, \tag{3.28}$$

where

$$a = \{c(2v_B)^{-1/2} \Gamma[\tfrac{1}{2} + 1/(2y)]\}^{2y/(1+y)}. \tag{3.29}$$

The inequality $u/\delta v \ll 1$ is fulfilled in the limit m fixed, $n \to \infty$ if $y < 1$. Calculating X and Y from u and v using Eqs. (2.19), with the upper and lower signs corresponding to $A < 0$ and $A > 0$, respectively, we find

$$X(m,n) = a n^{-2y/(1+y)}, \quad Y(m,n) = \frac{2y}{1+y} \frac{m - m_0}{n}, \quad A < 0 \tag{3.30a}$$

$$X(m,n) = \frac{2y}{1+y} \frac{m - m_0}{n}, \quad Y(m,n) = a n^{-2y/(1+y)}, \quad A > 0. \tag{3.30b}$$

Applying the surface boundary condition (2.16a) to Eq. (3.30a), one finds that $m_0 = 0$ for $A < 0$. For $A > 0$ we satisfy the boundary condition as in the case $y = 1$, $A > A_c$ considered above. We set $m_0 = \frac{1}{2}$ in Eq. (3.30b), so that $X(\frac{1}{2}, n)$ vanishes to order n^{-1}, and then use Eq. (2.16a) to generate $X(\frac{1}{2}, n)$, taking $Y(1,n)$ from Eq. (3.30b). The resulting expressions are

$$X(\tfrac{1}{2}, n) = \begin{cases} a n^{-2y/(1+y)}, & A < 0 \\ c_2 \exp\left[-\dfrac{1+y}{1-y} a n^{(1-y)/(1+y)}\right], & A > 0 \end{cases} \tag{3.31}$$

where c_2 is a constant.

Substituting Eqs. (3.31) into Eqs. (2.14) and (2.15), one finds the following results for m_1 and $g_{\parallel}(r)$. For $A < 0$, $m_1 = 0$ at the bulk critical temperature, as expected. For $A > 0$, $m_1 \neq 0$. In Appendix C we show that m_1 vanishes as $A^{1/[2(1-y)]}$ as A approaches 0 from above. For either sign of A, $g_{\parallel}(r)$ exhibits an anomalous exponential decay of the form

$$g_{\parallel}(r) \sim \exp[-(r/\xi_{\parallel})^{1-y}] \tag{3.32}$$

at the bulk critical temperature. Written in terms of A with the help of Eqs. (3.13) and (3.29), the correlation length

$$\xi_{\parallel}^{1-y} = \tfrac{1}{2}(1-y) a^{-(1+y)/2}$$

is given by

$$\xi_{\parallel} = \left[\frac{1-y}{2|A|}\right]^{1/(1-y)} \left[\frac{\sinh(2K_{2B})\Gamma[1/(2y)]}{\pi^{1/2}\Gamma[\frac{1}{2} + 1/(2y)]}\right]^{y/(1-y)}. \tag{3.33}$$

In the limit $y \to 0$, the inhomogeneous semi-infinite system with couplings $K_i(m) = K_{iB} + A_i m^{-y}$ and bulk critical couplings reduces to a homogeneous semi-infinite system with noncritical couplings. In this limit the anomalous exponential decay reduces to an ordinary exponential decay with characteristic length $\xi_{\parallel} = (2|A|)^{-1}$, in agreement[16] with Ref. 1.

One can readily verify that our solutions X and Y to the differential flow equations (2.16) for $m \gg n$ and $m \ll n$ also satisfy the original difference equations (2.8) in the large-n limit. Lack of an explicit solution for intermediate m prevents us from checking this for all m. However, all evidence suggests that X and Y vary increas-

TABLE I. Asymptotic forms of $X(\frac{1}{2}, n)$ in the large-n limit. The quantities A_c and $\xi_{\parallel}$ are defined in Sec. IV. c_1 and c_2 are constants on which the critical properties summarized in Table II do not depend.

y	A	$X(\frac{1}{2}, n)$
$y > 1$	A arbitrary	$(2n)^{-1}$
$y = 1$	$A < A_c$	$\frac{1}{2}(1 - A/A_c) n^{-1}$
	$A = A_c$	$(n \ln n)^{-1}$
	$A > A_c$	$c_1 n^{-(1+A/A_c)/2}$
$y < 1$	$A < 0$	$a n^{-2y/(1+y)}$
	$A > 0$	$c_2 \exp\left[-\frac{1+y}{1-y} a n^{(1-y)/(1+y)}\right]$
		Here, $a = \left[\frac{1-y}{2\xi_{\parallel}^{1-y}}\right]^{2/(1+y)}$

TABLE II. Critical behavior of the boundary magnetization m_1 and of the boundary pair correlation function $g_{\parallel}(r)$ of the inhomogeneous semi-infinite Ising model on a triangular lattice at the bulk critical temperature. The results shown here are discussed in Sec. IV.

y	A	m_1	$g_{\parallel}(r)$
$y>1$	A arbitrary	0	$r^{-\eta_{\parallel}}$, $\eta_{\parallel}=1$
$y=1$	$A>A_c$	$(A-A_c)^{1/2}$, $A\searrow A_c$	$r^{-\eta_{\parallel}}$, $\eta_{\parallel}=\lvert 1-A/A_c\rvert$
	$A<A_c$	0	
	$A=A_c$	0	$(\ln r)^{-1}$
$y<1$	$A<0$	0	$\exp[-(r/\xi_{\parallel})^{1-y}]$,
	$A>0$	$A^{1/[2(1-y)]}$, $A\searrow 0$	$\xi_{\parallel}\sim\lvert A\rvert^{-1/(1-y)}$

ingly slowly with m and n as n increases, and that the asymptotic behavior for large n of the solutions to the difference and differential equations is indeed the same. Our results for the large-n behavior of $X(\frac{1}{2},n)$ and for the critical behavior of m_1 and $g_{\parallel}(r)$ are summarized in Tables I and II, respectively.

IV. CONCLUSIONS

We briefly list our main findings, which are summarized in Table II, and compare them with the predictions of the scaling or renormalization-group approach reviewed in Appendix A.

The results pertain to the two-dimensional semi-infinite Ising model on a triangular lattice, with inhomogeneous coupling constants $K_1(m)$ and $K_2(m)$ (see Fig. 1) that approach the bulk couplings K_{iB} at large distances m from the surface as

$$K_i(m)=K_{iB}+A_i m^{-y}\ ,\quad m\gg 1\ . \tag{4.1}$$

The A_i have a particular ratio[14] implied by

$$A_1=\tfrac{1}{2}A\sinh(2K_{1B})\ ,\quad A_2=\tfrac{1}{4}A\cosh(2K_{2B})\ . \tag{4.2}$$

At bulk criticality, i.e., when $\exp(-2K_{1B})=\sinh(2K_{2B})$, we find the following critical behavior for the spontaneous surface magnetization m_1 and the pair correlation function $g_{\parallel}(r)$ of the surface spins:

(1) For $y>1$, $m_1=0$, and $g_{\parallel}(r)$ decays as $r^{-\eta_{\parallel}}$, $\eta_{\parallel}=1$. This value of $\eta_{\parallel}$ is the same as in the homogeneous semi-infinite[1] case $A=0$.

(2) For $y=1$, $m_1\neq 0$ if $A>A_c=\frac{1}{2}\sinh(2K_{2B})$. As A approaches A_c from above, m_1 vanishes as $(A-A_c)^{1/2}$. The critical exponent $\eta_{\parallel}$ which characterizes the behavior of $g_{\parallel}(r)$ for large r is nonuniversal, varying with A according to

$$\eta_{\parallel}(A)=\lvert 1-A/A_c\rvert\ . \tag{4.3}$$

At $A=A_c$, where $\eta_{\parallel}$ vanishes, $g_{\parallel}(r)$ decays as $(\ln r)^{-1}$.

(3) For $y<1$, $m_1\neq 0$ for $A>0$. As A approaches zero from above, m_1 vanishes as $A^{1/[2(1-y)]}$. For either sign of A, $g_{\parallel}(r)$ decays according to the anomalous exponential form

$$g_{\parallel}(r)\sim\exp[-(r/\xi_{\parallel})^{1-y}]\ , \tag{4.4}$$

$$\xi_{\parallel}=\left[\frac{1-y}{2\lvert A\rvert}\right]^{1/(1-y)}\left[\frac{\sinh(2K_{2B})\Gamma[1/(2y)]}{\pi^{1/2}\Gamma[\frac{1}{2}+1/(2y)]}\right]^{y/(1-y)}\ . \tag{4.5}$$

The crossover in critical behavior at $y=1$, with ordinary critical behavior for $y>1$, anomalous behavior for $y<1$, and nonuniversality at $y=1$, is entirely consistent with the scaling or renormalization-group approach of Appendix A. According to this approach the inhomogeneity of the coupling constants is "irrelevant" for $y>\nu^{-1}$, "relevant" for $y<\nu^{-1}$, and "marginal" for $y=\nu^{-1}$ in any semi-infinite system with bulk exponent ν. For the two-dimensional Ising[1] model, $\nu=1$.

In Appendix A it was argued that for $y<\nu^{-1}$, m_1 vanishes as

$$m_1\sim A^{\beta_1/(1-\nu y)} \tag{4.6}$$

as A approaches zero from above. Here β_1 is the conventional exponent[2] associated with the ordinary semi-infinite transition. For the two-dimensional semi-infinite Ising[1] model, $\beta_1=\frac{1}{2}$, $\nu=1$, and Eq. (4.6) reduces to the result $m_1\sim A^{1/[2(1-y)]}$ obtained with the star-triangle method in Appendix C. The scaling prediction

$$\xi_{\parallel}\sim\lvert A\rvert^{-\nu/(1-\nu y)} \tag{4.7}$$

derived in Appendix A for the characteristic length at the bulk critical temperature when $y<1$ is also consistent with the exact Ising result given in Eq. (4.5). The predictions of the scaling theory have also been verified[17] for the semi-infinite Gaussian model with inhomogeneous coupling constants that vary as in Eq. (4.1). In the marginal case $y=\nu^{-1}=2$, the critical exponent $\eta_{\parallel}$ is again nonuniversal.

Enhanced couplings in conjunction with infinite-range bulk correlations produce the nonzero boundary magnetization at the bulk critical temperature in the Ising results for $y=1, A>A_c$ and $y<1, A>0$. Above the critical temperature, the bulk correlation length is finite, and m_1 vanishes. Thus the surface magnetization is discontinuous at $T=T_c$, whereas the bulk magnetization is continuous.

In this paper we have only considered surface critical phenomena at the bulk critical temperature. With an approach based on Pfaffians, Blöte and Hilhorst[6] have recently obtained results for $T\neq T_c$ in the marginal case $y=1$. We refer to Ref. 6 for a detailed discussion of the rich critical behavior. The star-triangle method of this paper can also be used for temperatures $T\neq T_c$. Work on this and other applications of the method is in progress.

APPENDIX A: SCALING THEORY

Our exact Ising results are compatible with a simple scaling theory[7,8] that is applicable to any smoothly inhomogeneous semi-infinite system with a divergent bulk correlation length. In this theory the short-range coupling constants $K(m)$ are assumed to transform locally[18] as the system is renormalized. More specifically, we argue that for $K(m)$ which vary sufficiently slowly with m, the renormalization transformation has the form

$$K'(m/b)=R(K(m)) , \quad m \gg 1 \tag{A1}$$

far from the surface. Here, b is the factor by which lengths are rescaled, and the function R is the same as in the renormalization transformation

$$K_B'=R(K_B) \tag{A2}$$

for homogeneous bulk couplings.

Linearizing Eq. (A1) around the bulk fixed point K_B^* gives[18]

$$K'(m/b)-K_B^*=b^{y_t}[K(m)-K_B^*] , \tag{A3}$$

where $y_t=\nu^{-1}$ is the thermal scaling index of the homogeneous bulk system and ν is the conventional critical exponent associated with the bulk correlation length. Upon substituting $K'(m)-K_B^*=A'm^{-y}$ and $K(m)-K_B^*=Am^{-y}$ into Eq. (A3), one finds that the parameter A transforms according to

$$A'=b^{y_t-y}A . \tag{A4}$$

From Eq. (A4) one sees that the inhomogeneity of the couplings is "relevant"[18,19] and modifies the surface critical behavior for $y<y_t=\nu^{-1}$, but is "irrelevant" for $y>y_t$ and "marginal" for $y=y_t$.

At the bulk critical temperature the correlation function of the surface spins transforms as

$$g_{\parallel}(r,A)=b^{-2(d-1-y_{h_1})}g_{\parallel}(r/b,b^{y_t-y}A) , \tag{A5}$$

in accordance with Eq. (A4) and standard scaling analyses.[18,19] The scaling index y_{h_1} is the conventional index[2] associated with a surface magnetic field in the homogeneous semi-infinite case $A=0$. Since the scale factor b is arbitrary, Eq. (A5) implies

$$g_{\parallel}(r,A)=r^{-2(d-1-y_{h_1})}F_y(r^{y_t-y}A) . \tag{A6}$$

From Eq. (A6) one again sees that if $y>y_t$, the correlation function exhibits ordinary critical behavior, falling off as $r^{-(d-2+\eta_{\parallel})}$, $\eta_{\parallel}=d-2y_{h_1}$, just as in the homogeneous semi-infinite case $A=0$. For $y<y_t$ the asymptotic behavior depends on the form of the scaling function $F_y(x)$ for large $x=[r/\xi_{\parallel}(A)]^{y_t-y}$, where

$$\xi_{\parallel}(A)\sim|A|^{-1/(y_t-y)}=|A|^{-\nu/(1-\nu y)} . \tag{A7}$$

The quantity $\xi_{\parallel}(A)$ is a finite characteristic length at the bulk critical temperature. When $y=0$, $\xi_{\parallel}(A)$ is proportional to the usual bulk correlation length.

An ordinary exponential decay $\exp(-r/\xi_{\parallel})$ in the spatially homogeneous case $y=0$ corresponds to

$$F_y(x)\sim\exp(-x^{1/y_t}) \tag{A8}$$

for large x and $y=0$. If we conjecture that Eq. (A8) holds for all $y<y_t$, not just $y=0$, we are led to an anomalous exponential decay of the form

$$g_{\parallel}(r,A)\sim\exp\{-[r/\xi_{\parallel}(A)]^{1-y/y_t}\} . \tag{A9}$$

The exact results of Eqs. (4.4) and (4.5) for the Ising model ($y_t=1$) and corresponding results[17] for the inhomogeneous semi-infinite Gaussian model ($y_t=2$) are consistent with Eqs. (A7) and (A9).

In analogy with Eq. (A5), the spontaneous surface magnetization at the bulk critical temperature transforms as

$$m_1(A)=b^{-(d-1-y_{h_1})}m_1(b^{y_t-y}A) . \tag{A10}$$

Since b is arbitrary, Eq. (A10) implies that m_1 vanishes as

$$m_1\sim A^{(d-1-y_{h_1})/(y_t-y)}=A^{\beta_1/(1-\nu y)} \tag{A11}$$

for $y<y_t$ as A approaches zero from above. In Eq. (A11), $\beta_1=(d-1-y_{h_1})/y_t$ is the conventional exponent[2] associated with the ordinary transition in the homogeneous case $A=0$.

One can readily derive approximate renormalization transformations that satisfy the locality condition (A1) and thus correctly predict the relevance, marginality, and irrelevance of the inhomogeneity in the coupling constants for $y<y_t$, $y=y_t$, and $y>y_t$, respectively. One such transformation, based on the Migdal-Kadanoff method, is applied to the two-dimensional Ising model in Ref. 20. The approximation also yields a nonuniversal exponent $\eta_{\parallel}$ in the marginal case $y=y_t$ and a nonvanishing surface magnetization at bulk criticality for A greater than a threshold value A_c, in qualitative agreement with the exact results.

APPENDIX B: DERIVATION OF EQ. (2.13b)

In this section we derive Eq. (2.13b), which determines the correlation function $g_{\parallel}(r,0)$ of the initial system, from the sequence of $X(\frac{1}{2},n)$.

Iterating Eq. (2.12b) n times, one obtains an expression of the form

$$g_{\parallel}(r,0)=\tfrac{1}{4}\sum_{j=1}^{n}P(1,j-1\,|\,r,0)f(j)g_{\parallel}(0,j) + \sum_{s=1}^{\infty}P(s,n\,|\,r,0)f(n)g_{\parallel}(s,n) , \quad r\geq 1 \tag{B1}$$

where $f(n)$ is defined by Eq. (2.13c). The first sum gives the contributions of all the $g_{\parallel}(0,j)$ produced in the n iterations. The second sum only involves correlation functions $g_{\parallel}(s,n)$ with spin separation $s\geq 1$. The coefficients $P(s,n\,|\,r,0)$, which are determined below, vanish for $|r-s|>n$.

From Eqs. (2.12b) and (B1) it follows that the $P(s,n\,|\,r,0)$ satisfy the difference equations

$$P(s,n+1\,|\,r,0)=\tfrac{1}{4}[P(s+1,n\,|\,r,0)+2P(s,n\,|\,r,0) + P(s-1,n\,|\,r,0)] , \quad s\geq 1 \tag{B2}$$

with boundary conditions

$$P(s,0\,|\,r,0)=\delta_{rs} , \quad P(0,n\,|\,r,0)=0 . \tag{B3}$$

Equations (B2) and (B3) have an obvious interpretation in terms of a random walk. For $s \geq 1$, $P(s,n \mid r,0)$ represents the probability that a particle with initial coordinate r (a positive integer) is at s after n steps in which the particle changes its coordinate by $+1,0,-1$ with probabilities $\frac{1}{4},\frac{1}{2},\frac{1}{4}$, respectively, and sticks if it reaches the origin. The solution to this problem is[21]

$$P(s,n \mid r,0)=\frac{1}{4^n}\left[\begin{bmatrix}2n\\ n+r-s\end{bmatrix}-\begin{bmatrix}2n\\ n+r+s\end{bmatrix}\right]. \tag{B4}$$

The first term on the right-hand side is the solution to the random-walk problem on an infinite line without sticking at the origin. The second term, which corresponds to an "image" particle with initial coordinate $-r$ instead of r, ensures that the boundary condition (B3) at the origin is satisfied.

We now take the limit $n \to \infty$ in Eq. (B1). Since $f(n)$ and $g_{\parallel}(s,n)$ are bounded, and $\sum_{s=1}^{\infty} P(s,n \mid r,0)$ vanishes[22] in the limit $n \to \infty$, only the first sum on the right-hand side of Eq. (B1) survives, and we obtain

$$g_{\parallel}(r,0)=\tfrac{1}{4}\sum_{n=1}^{\infty} P(1,n-1 \mid r,0) f(n) g_{\parallel}(0,n) . \tag{B5}$$

Substituting from Eq. (B4) and making use of elementary properties of the binomial coefficients, we write Eq. (B5) as

$$g_{\parallel}(r,0)=\sum_{n=1}^{\infty} 4^{-n}\frac{r}{n}\begin{bmatrix}2n\\ n+r\end{bmatrix} f(n) g_{\parallel}(0,n) . \tag{B6}$$

Upon substituting $g_{\parallel}(0,n)=1-m_1^2(n)$ into Eq. (B6), one obtains Eq. (2.13b).

APPENDIX C: CRITICAL BEHAVIOR OF m_1

In this appendix we show that the spontaneous surface magnetization vanishes as

$$m_1 \sim (A-A_c)^{1/2} , \quad y=1 , \quad A \searrow A_c \tag{C1}$$

$$m_1 \sim A^{1/[2(1-y)]} , \quad y<1 , \quad A \searrow 0 . \tag{C2}$$

From Eq. (2.14) one sees that m_1 vanishes when the integral

$$I(A,y)=\int_{n_0}^{\infty} dn\, X(\tfrac{1}{2},n) \tag{C3}$$

diverges positively. First, we study the divergence in the case $y=1$, $A \to A_c$. According to Table I, $X(\frac{1}{2},n)$ varies as

$$X(\tfrac{1}{2},n)=\begin{cases} c_1 n^{-(1+A/A_c)/2} , & A>A_c \\ (n \ln n)^{-1} , & A=A_c \end{cases} \tag{C4}$$

for large n. From these asymptotic forms it is clear that $I(A,y)$ is indeed finite for $A>A_c$ and infinite for $A=A_c$.

For A very close but not equal to A_c we argue that $X(\frac{1}{2},n)$ varies as $(n \ln n)^{-1}$ for moderately large n but crosses over to $c_1 n^{-(1+A/A_c)/2}$ when the two asymptotic forms become comparable. The crossover, which occurs when $\ln n \approx k/(A-A_c)$, k being a constant, provides an effective upper cutoff in the integral $I(A,y)$. Thus the leading singular behavior as $A \to A_c$ is given by

$$I(A,y) \to \int_{n_0}^{\exp[k/(A-A_c)]} \frac{dn}{n \ln n} \to -\ln(A-A_c) . \tag{C5}$$

Substituting Eq. (C5) into Eq. (2.14), one obtains $m_1 \sim (A-A_c)^{1/2}$ as in Eq. (C1).

In an alternate approach which leads to the same results, we utilize the interpolation formula

$$X(\tfrac{1}{2},n)=(n \ln n + c_1^{-1} n^{(1+A/A_c)/2})^{-1} , \tag{C6}$$

which reproduces the large-n behavior in Eq. (C4) for both $A>A_c$ and $A=A_c$. Substituting Eq. (C6) into Eq. (C3) and changing the integration variable to $x=\ln n$ gives

$$I(A,y)=\int_{x_0}^{\infty} dx (x+c_1^{-1}e^{\epsilon x})^{-1} , \quad \epsilon=\tfrac{1}{2}(A/A_c-1) . \tag{C7}$$

This integral has upper and lower bounds $I_>$ and $I_<$ given by

$$I_>(A,y)=\int_{x_0}^{\infty} dx \left[x+\frac{(\epsilon x)^s}{c_1 s!}\right]^{-1} , \tag{C8a}$$

$$I_<(A,y)=\int_{x_0}^{\infty} dx\, e^{-\epsilon x}(x+c_1^{-1})^{-1} , \tag{C8b}$$

which are more amenable to analytical integration than the integral of (C7). Both bounds lead to the result of Eq. (C5), $I(A,y) \to -\ln(A-A_c)$. We emphasize that there is no arbitrariness in the coefficient of the logarithm.

Equation (C2) may be established in the same manner as Eq. (C1), expect that the asymptotic forms

$$X(\tfrac{1}{2},n)=\begin{cases} c_2 \exp\left[-\dfrac{1+y}{1-y} a n^{(1-y)/(1+y)}\right] , & A>0 \\ (2n)^{-1} , & A=0 \end{cases} \tag{C9}$$

for $y<1$, with $a \sim |A|^{2/(1+y)}$, as given in Table I, replace Eqs. (C4).

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$$A_1/A_2=2\sinh(2K_{1B})/\cosh(2K_{2B})$$

can be generalized to arbitrary A_1,A_2. One makes a decomposition in terms of eigenperturbations $u_i^{(1)}(m),u_i^{(2)}(m)$ of the form

$$A_i m^{-y}=Au_i^{(1)}(m)+Bu_i^{(2)}(m) ,$$

where

$$u_i^{(1)}(m)=(-\tfrac{1}{2}\sinh(2K_{1B}) , \tfrac{1}{4}\cosh(2K_{2B}))m^{-y}$$

and

$$u_i^{(2)}(m)=(-\exp(-2K_{1B}), \cosh(2K_{2B}))m^{-y} .$$

The eigenperturbation $u_i^{(2)}(m)$ leaves the criticality condition $\exp(-2K_1)=\sinh(2K_2)$ satisfied locally and is "irrelevant" (see Appendix A and Ref. 20). Thus the surface critical behavior is determined by the terms $Au_i^{(1)}(m)$, which have the particular ratio considered in this paper. Since $|A_i m^{-y}| \ll K_{iB}$ for any A_i if m is sufficiently large, no nonlinear corrections are expected in the scaling theory. Expressing the coefficient A in the above expansion in terms of A_1 and A_2, one obtains

$$A=4[A_1+A_2\tanh(2K_{2B})] .$$

This is the appropriate generalization of Eqs. (3.11) or (4.2) to arbitrary A_1 and A_2. All of the Ising results summarized in Sec. IV are expected to hold for arbitrary A_1,A_2 if the quantity A is defined by this relation.

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$$Q(n,r)=\sum_{s=1}^{\infty} P(s,n\mid r,0)$$

as

$$Q(n,r)=4^{-n}\sum_{k=n-r+1}^{n+r}\binom{2n}{k} .$$

Since $\binom{2n}{k}\le\binom{2n}{n}$,

$$Q(n,r)\le(2r-1)4^{-n}\binom{2n}{n} .$$

Evaluating $\binom{2n}{n}$ with Stirling's approximation, we obtain $Q(n,r)\le(2r-1)(\pi n)^{-1/2}$ for $n\gg 1$. Clearly, $Q(n,r)$ vanishes in the limit $n\to\infty$, r fixed. This proof is due to Per Hemmer, whom we thank for useful discussions.