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Surface critical behavior of the smoothly inhomogeneous Ising model

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We consider a semi-infinite two-dimensional Ising model with nearest-neighbor coupling constants that deviate from the bulk coupling by Am^{-y} for large m, m being the distance from the edge. The case $A<0$ of couplings which are weaker near the surface has been discussed by Hilhorst and van Leeuwen. We report exact results for the boundary magnetization and boundary pair-correlation function when $A>0$. At the bulk critical temperature there is a rich variety of critical behavior in the A-y plane with both paramagnetic and ferromagnetic surface phases. Some of our results can be derived and generalized with simple scaling arguments.

In a recent Letter Hilhorst and van Leeuwen[1] reported exact results for the Ising model on a semi-infinite triangular lattice with nearest-neighbor couplings $K_1(m)$, $K_2(m)$ (see Fig. 1) which depend on the distance m from the edge. Far from the surface the couplings vary as[2]

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

They give A_i a convenient ratio, setting

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

and consider the case $A<0$ of couplings which are *weaker* near the surface. The following behavior for the pair-correlation function $g(r)$ of the surface spins at the bulk critical temperature is found. For $y>1$, $g(r)$ decays as $r^{-\eta_\parallel}$, $\eta_\parallel=1$, just as in the homogeneous semi-infinite[3] case $A=0$. For $y=1$ the exponent $\eta_\parallel$ is nonuniversal and varies with A. For $y<1$ there is an anomalous exponential decay rather than an algebraic decay.

Burkhardt[4] and Cordery[5] subsequently pointed out that these results are compatible with a local scaling picture applicable to any semi-infinite system with a divergent bulk correlation length with critical exponent ν. In a rescaling or renormalization operation in which the lattice constant is multiplied by a factor b, the quantity A transforms as

$$A'=b^{(1-\nu y)/\nu}A \quad . \tag{3}$$

Thus the inhomogeneity is a "relevant" parameter[6] which modifies the surface critical behavior for $y<\nu^{-1}$ but not for $y>\nu^{-1}$. Burkhardt and Guim[7] have shown that the Gaussian model with $A<0$ exhibits the same variety of surface critical behavior as the Ising model, with crossover at $y=\nu^{-1}=2$ in accordance with the scaling prediction.

In this Rapid Communication we consider an Ising model described by Eqs. (1) and (2) with $A>0$, i.e., the couplings are *stronger* than the bulk coupling (but never infinite) nearer the surface. From the scaling theory one expects the surface critical behavior for $y>1$ and $A>0$ to be essentially the same as for $A=0$, since the inhomogeneity is "irrelevant." We were particularly interested in learning whether or not there is a spontaneous boundary magnetization at the bulk critical temperature for $y<1$. The enhancement of the coupling constants over the bulk coupling favors a magnetization, whereas the one-dimensional surface has an opposing tendency.

Our results for $A>0$ were obtained with the method of Hilhorst and van Leeuwen[1] with modifications noted below. Blöte and Hilhorst[8] have independently applied a Pfaffian method to the same problem. Before outlining our calculational procedure, we summarize the results:

(1) For $y>1$ and $A>0$ there is no spontaneous surface magnetization at the bulk critical temperature, and the correlation function of surface spins falls off as $r^{-\eta_\parallel}$, $\eta_\parallel=1$, just as in the homogeneous semi-infinite[3] case.

(2) For $y=1$ there is a spontaneous surface magnetization m_1 at the bulk critical temperature for $A>A_c=\frac{1}{2}\sinh 2K_{2B}$. As A approaches A_c from above, m_1 vanishes[9] as $(A-A_c)^{1/2}$. For $A<A_c$ and $A>A_c$ the correlation function falls off algebraically with the nonuniversal exponent

$$\eta_\parallel=|1-A/A_c| \quad . \tag{4}$$

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

(3) When $y<1$ there is a spontaneous surface magnetization at the bulk critical temperature for all $A>0$. As A approaches zero, it vanishes as $A^{1/[2(1-y)]}$. The correlation

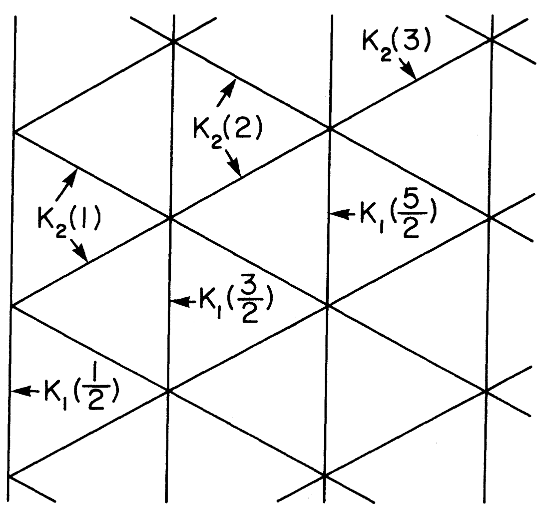

FIG. 1. Semi-infinite Ising model. The vertical bonds parallel to the edge are designated by $K_1(m)$, $m=\frac{1}{2},\frac{3}{2},\ldots$, and the diagonal bonds by $K_2(m)$, $m=1,2,\ldots$.

function exhibits an anomalous exponential decay of the form

$$g(r) \sim \exp[-(r/\tilde{\xi})^{1-y}] \;, \tag{5}$$

$$\tilde{\xi} = \left[\frac{1-y}{2|A|}\right]^{1/(1-y)} \left[\frac{2A_c\Gamma(1/2y)}{\pi^{1/2}\Gamma(1/2y+\frac{1}{2})}\right]^{y/(1-y)} \;. \tag{6}$$

We note that Eqs. (4), (5), and (6) hold[1] for $A<0$ as well as $A>0$.

These results were calculated using the method described in Ref. 1. One uses a mapping based on the star-triangle transformation to generate a sequence $(n=0,1,2,\ldots)$ of Ising models with coupling constants $K_1(m,n)$, $K_2(m,n)$ (see Fig. 1) from the original model $(n=0)$. The surface magnetization and boundary correlation function transform according to

$$m_1(n) = \{1-\exp[-4K_1(\tfrac{1}{2},n+1)]\}^{1/2} m_1(n+1) \;, \tag{7}$$

$$g(r,n) = \tfrac{1}{4}\{1-\exp[-4K_1(\tfrac{1}{2},n+1)]\} \times [g(r+1,n+1)+2g(r,n+1)+g(r-1,n+1)] \;. \tag{8}$$

The correlation function $g(r,n)=\langle\sigma(r)\sigma(0)\rangle-\langle\sigma\rangle^2$ satisfies the boundary condition $g(0,n)=1-m_1^2(n)$. It follows[1] that $m_1=m_1(0)$ and $g(r)=g(r,0)$ are given by

$$m_1 = \lim_{n\to\infty} [f(n)]^{1/2} m_1(n) \;, \tag{9}$$

$$g(r) = \sum_{n=1}^{\infty} 2^{-2n}\frac{r}{n}\begin{pmatrix}2n\\ n+r\end{pmatrix} f(n)[1-m_1^2(n)] \;, \tag{10}$$

$$f(n) = \prod_{j=1}^{n} \{1-\exp[-4K_1(\tfrac{1}{2},j)]\} \;. \tag{11}$$

The quantity $\exp[-4K_1(\frac{1}{2},n)]$ approaches zero as n tends toward infinity. All of our results for the critical behavior listed above follow from the asymptotic form of $\exp[-4K_1(\frac{1}{2},n)]$ for large n. As in Ref. 1 we calculate the asymptotic form replacing the difference equations which relate the nth and $(n+1)$st sets of coupling constants by differential equations. We also introduce variables u, v where

$$\sinh 2K_1 = \frac{v^2-u^2}{4uv}Q, \quad \sinh 2K_2 = \frac{1}{v}Q \;, \tag{12}$$

$$Q = [1-\tfrac{1}{4}(v-u)^2]^{1/2} \mp [1-\tfrac{1}{4}(v+u)^2]^{1/2} \;. \tag{13}$$

The upper sign is used for supercritical couplings and the lower sign for subcritical couplings. Both the supercritical and subcritical domains map onto $u+v<2$. The bulk criticality condition corresponds to $u+v=2$. With these substitutions the differential flow equations for the coupling constants may be put in the form

$$v\frac{\partial m}{\partial u} = u\frac{\partial n}{\partial v}, \quad v\frac{\partial m}{\partial v} = u\frac{\partial n}{\partial u} \;. \tag{14}$$

Hilhorst and van Leeuwen[1] solve Eqs. (14) for $A<0$ with the surface boundary condition $K_2(0,n)=0$ suggested by Fig. 1 and by computer iterations of the transformation equations for the coupling constants. Instead, we require that the solution to Eqs. (14) satisfy the transformation law for the edge coupling,

$$K_1(\tfrac{1}{2},n+1) = K_1(\tfrac{1}{2},n) + \tfrac{1}{2}\ln\cosh 2K_2(1,n) \;, \tag{15}$$

which differs from the transformation equations for interior couplings, from which Eqs. (14) follow. For $A<0$ both procedures lead to identical results. However, for $y=1$, $A>A_c$ and $y<1$, $A>0$ our analytical results imply that $K_2(m,n)$ no longer extrapolates to zero at $m=0$. Computer iterations of the difference equations appear to confirm this.

Following Ref. 1, we consider solutions of Eqs. (12)–(15) of the form

$$m-m_0 = u\int_0^\infty d\rho\, w(\rho)e^{-\rho u_B} I_1(\rho u)[K_1(\rho v_B)I_0(\rho v)+I_1(\rho v_B)K_0(\rho v)] \;, \tag{16}$$

$$n = v\int_0^\infty d\rho\, w(\rho)e^{-\rho u_B} I_0(\rho u)[K_1(\rho v_B)I_1(\rho v)-I_1(\rho v_B)K_1(\rho v)] \;. \tag{17}$$

Here I_μ and K_μ denote modified Bessel functions. A constant m_0 to be fixed by the boundary condition Eq. (15) has been included in Eq. (16). For $A>0$ we find that a weight function $w(\rho)\propto\rho^{(1/y+1)/2}$ for large ρ yields coupling constants with the m^{-y} dependence of Eqs. (1) and (2) for $m \gg n$, just as for $A<0$.

We now discuss the large-n behavior of the surface coupling $K_1(\frac{1}{2},n)$ in different regions of the A-y plane. Our conclusions are summarized in Table I. Proceeding as in Ref. 1, one finds that for $y>1$ and $m \ll n$ Eqs. (16) and (17) imply

$$\exp(-4K_1) = \sinh^2 2K_2 = \frac{m-m_0}{n} \;. \tag{18}$$

The boundary condition Eq. (15) requires $m_0=0$.

For $y=1$ and $m \ll n$ we find

$$\exp(-4K_1) = \frac{m-m_0}{n}, \quad \sinh^2 2K_2 = \frac{2(m-m_0)+A/A_c}{2n} \;. \tag{19}$$

TABLE I. Asymptotic form of $\exp[-4K_1(\frac{1}{2},n)]$ in the large-n limit. For completeness we have also included the results of Ref. 1 for $A<0$. $\tilde{\xi}$ is defined in Eq. (6). c_1 and c_2 are constants (Ref. 10).

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

For $A < A_c$ the boundary condition requires $m_0 = \frac{1}{2}A/A_c$. For $A > A_c$ we set $m_0 = \frac{1}{2}$. Then $\exp[-4K_1(\frac{1}{2},n)]$ vanishes to order n^{-1}. However, it does not vanish identically, but instead approaches zero faster than n^{-1}. Inserting $\sinh^2 2K_2$ from Eq. (19) with $m_0 = \frac{1}{2}$ into Eq. (15), one finds that

$$\exp[-4K_1(\tfrac{1}{2},n)] = c_1 n^{-(1+A/A_c)/2} ,$$

where c_1 is a constant.[10] Computer iterations of the difference equations confirm this n dependence.

This correction to the leading $O(n^{-1})$ behavior is not contained in Eqs. (16) and (17) but follows if extra terms of the form

$$m - m_0 = \cdots + u \int_0^\infty d\rho\, w_1(\rho) e^{-2\rho} K_1(\rho u) I_0(\rho v) \quad , \tag{20}$$

$$n = \cdots - v \int_0^\infty d\rho\, w_1(\rho) e^{-2\rho} K_0(\rho u) I_1(\rho v) \quad , \tag{21}$$

are included, with a weight function

$$w_1(\rho) \propto c_1 \rho^{1/2 + (1 - A/A_c)/2}$$

for large ρ. The additional terms do not alter the m^{-y} dependence of K_1, K_2 for $m >> n$ given in Eqs. (1) and (2).

For $y=1$, $A=A_c$ we find that the choice $w_1(\rho) \propto \rho^{1/2}(\ln\rho)^{-2}$ for large ρ yields a consistent solution satisfying the boundary conditions. For $m << n$ one obtains

$$\exp(-4K_1) = \frac{m - \frac{1}{2}}{n} + \frac{c_0}{n \ln n}, \quad \sinh^2 2K_2 = \frac{m}{n} + \frac{c_0}{n \ln n} \quad . \tag{22}$$

The quantity c_0 is a proportionality constant in $w_1(\rho)$. m_0 has been chosen so that the coefficient of the n^{-1} term in $\exp(-4K_1)$ vanishes at $m = \frac{1}{2}$. The boundary condition Eq. (15) implies $c_0 = 1$.

Finally for $y < 1$, $A > 0$, and $m << n$ Eqs. (16) and (17) yield

$$\exp(-4K_1) = \frac{2y}{1+y} \frac{m - m_0}{n}, \quad \sinh^2 2K_2 = \frac{\alpha}{n^{2y/(1+y)}} \quad , \tag{23}$$

where

$$\alpha = [\tfrac{1}{2}(1-y)\tilde{\xi}^{-(1-y)}]^{2/(1+y)}$$

with $\tilde{\xi}$ defined in Eq. (6). Again we satisfy the boundary condition by setting $m_0 = \frac{1}{2}$ in Eq. (23) and using Eq. (15) to generate $\exp[-4K_1(\frac{1}{2},n)]$. The result is recorded in Table I.

Our results for the asymptotic form of $\exp[-4K_1(\frac{1}{2},n)]$ for large n are summarized in Table I. All of our conclusions concerning the critical behavior listed above follow from Table I and Eqs. (9)–(11) in a fairly straightforward manner. We plan to publish a more detailed account of our work in the future.

The local scaling picture[4,5] which leads to Eq. (3) suggests that other critical systems with couplings described by Eq. (1) exhibit the same variety of critical behavior in the A-y plane as the Ising model, with marginal behavior at $y = \nu^{-1}$. The characteristic length $\tilde{\xi}(A)$ at the bulk critical temperature for $y < \nu^{-1}$ is expected to diverge as

$$\tilde{\xi}(A) \sim |A|^{-\nu/(1-\nu y)} \tag{24}$$

as A vanishes. This follows from Eq. (3) and the requirement that $\tilde{\xi}(A)$ transform[6] according to $\tilde{\xi}(A') = b^{-1}\tilde{\xi}(A)$. An assumption beyond scaling that suggests generalizing Eq. (5) to

$$g(r) \sim \exp[-(r/\tilde{\xi})^{1-\nu y}]$$

is discussed in Ref. 4(b). These predictions are consistent with exact results[7] we have obtained for the Gaussian model $(\nu = \frac{1}{2})$.

A final generalization we obtain from scaling is the prediction that the surface magnetization vanish as

$$m_1 \sim A^{\beta_1/(1-\nu y)} \tag{25}$$

for $y < \nu^{-1}$ as A approaches zero from above. Here β_1 is the conventional exponent associated with the "ordinary" transition[11] in the homogeneous case $A=0$. Equation (25) follows from Eq. (3) and the scaling ansatz $m_1(A') = b^{\beta_1/\nu} m_1(A)$, which is analogous to the ansatz for the correlation function considered in Ref. 4(b). For the two-dimensional Ising[3] model, $\beta_1 = \frac{1}{2}$ and $\nu = 1$, and Eq. (25) reduces to the result we calculated from the information in Table I.

The exact results that have been obtained for the Ising model and the information which follows from scaling have led to a fairly complete picture of surface critical behavior in critical systems with smoothly inhomogeneous couplings.

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[2]Our quantities A_1, A_2, A differ by a sign from the corresponding quantities in Ref. 1. Otherwise we follow the notation of Ref. 1.

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[8]H. W. J. Blöte and H. J. Hilhorst (unpublished).

[9]We learned of this result from the authors of Ref. 8 and have confirmed it with the methods of this paper.

[10]The amplitudes of m_1 and $g(r)$ depend on the value of c_1, but the critical exponents and other results listed at the beginning of this paper do not. The same is true of the constant c_2 in Table I.

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