Nonuniversality, Exponent Asymmetry, and Surface Magnetization in an Inhomogeneous Square Ising Lattice

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(Received 11 July 1983)

A semi-infinite nearest-neighbor square Ising system whose couplings at a distance l from the boundary differ from homogeneity by an amount $\delta K \sim -A/l$ is investigated. On the basis of the Pfaffian method we obtain the critical behavior at the surface of this system. The exponents $\eta_\parallel$, $\nu_\parallel$, β_1, γ_{11}, and δ_{11} display rich nonuniversal behavior as a function of the amplitude A. For A below a critical value, there is exponent asymmetry and a spontaneous surface magnetization when the bulk ($l=\infty$) is critical.

PACS numbers: 75.40.Dy, 05.70.Jk, 75.10.Hk

Instances of fully understood surface critical behavior are rare. They acquire a particular significance in connection with current research in surface physics,[1] especially where it is concerned with such diverse phenomena as wetting, roughening, surface ordering, and polymer adsorption. In this Letter we present a system for which a complete understanding can be gained.

We consider an inhomogeneous ferromagnetic Ising system on a semi-infinite square lattice with Hamiltonian

$$\mathcal{H} = -\sum_{l=1}^{\infty}\sum_{k=-\infty}^{\infty}\left[J_1\sigma_{l,k}\sigma_{l,k+1} + J_2(l)\sigma_{l,k}\sigma_{l+1,k}\right] - h_1\sum_{k=-\infty}^{\infty}\sigma_{1k}. \tag{1}$$

The magnetic field h_1 acts only on the surface spins. The interactions $J_2(l)$ form a layered structure: They depend on the distance l to the boundary. Such inhomogeneous systems have been studied before,[2] in particular when $J_2(l)$ is a random variable. Quantities of interest are the correlation function $g_\parallel(r)$ between two spins a distance r apart on the surface, the surface susceptibility χ_{11}, and the surface magnetization m_1. Instead of random couplings we consider here smoothly varying ones such that

$$J_2(l) - J_2(\infty) \simeq -\bar{A}l^{-p}, \quad l \to \infty, \tag{2}$$

where $p>0$ and the amplitude $\bar{A}$ of the inhomogeneity is a constant. We concentrate on temperatures T near the critical point T_c of a homogeneous bulk system and put $t=(T-T_c)/T_c$.

The equivalent problem on a triangular lattice was recently investigated, for the special case $\bar{A} \geqslant 0$ and $t=h_1=0$, by means of the star-triangle transformation[3] and by renormalization-group arguments.[4,5] These limited studies reveal that the case $p=1$ in Eq. (2) is of special interest: The correlation function exponent $\eta_\parallel$ increases linearly[3] with the amplitude $\bar{A}$. This raises intriguing questions, such as what happens when $\bar{A}$ becomes negative.

We have recently found a complete solution for the surface critical behavior of the model described by Eqs. (1) and (2) with $p=1$. While the method of Ref. 3 can be extended to the general case,[6] our approach here is entirely different. It is an extension of the Pfaffian technique[2,7] to inhomogeneous systems, valid in the limit of smoothly varying couplings. We shall indicate the main steps of the method after discussing our results.

We present here full results, including the critical behavior associated with $t\to 0$, $h_1 \to 0$, for $p=1$, and for general values of the amplitude $\bar{A}$. The system behaves rather spectacularly at criticality. We summarize the critical behavior in Table I. Our notation conforms largely to Ref. 1.

(1) *At criticality.*—In the $\bar{A}$-t-h_1 space the system has the critical line $h_1=t=0$. A useful change of parameter is to put $A = 4\bar{A}/\{k_B T\sinh[2J_2(\infty)/k_B T]\}$. On the critical line, and for $A>-1$, $g_\parallel(r)$ decays to zero as $1/r^{\eta_\parallel(A)}$, with $\eta_\parallel$ linearly dependent on A. This agrees with the expression found[3] for the triangular lattice when $A \geqslant 0$. For $A<-1$, there is a *spontaneous surface magnetization* m_1 at criticality, so that $\eta_\parallel(A)=0$; m_1 vanishes with a square-root singularity as $A \to -1$ from below. For $A<-1$, $g_\parallel(r)$ still decays as a *power law* $1/r^{\eta_\parallel'(A)}$ towards $g_\parallel(\infty)=m_1^2$. For $-2 \leqslant A \leqslant 0$, the boundary susceptibility χ_{11} is infinite. The response $m_1(t=0,h_1)$ of the boundary spins to a small field h_1 has a singular part proportional to $h_1^{1/\delta_{11}}$, where δ_{11} depends continuously on A for $A<1$; when $A \to -1$ from below, δ_{11} diverges. For $A=1$, $m_1(0,h_1)$ has an essential singularity at $h_1=0$, and for $A>1$, the response is analytic.

TABLE I. Critical behavior of the inhomogeneous, two-dimensional Ising model described in the text. These results apply in the limits $t \to 0$, $h_1 \to 0$, and $r \to \infty$. They describe the singular part of the critical behavior only: In some cases, this is so weak that the regular part dominates. The exponent δ_{11} is only given for $A < 1$; for $A > 1$, $m_1(0,h_1)$ is analytic at $h_1 = 0$. For $A < -1$, $\beta_1^{(0)} = 0$ describes that the spontaneous surface magnetization $m_1(t,0)$ does not vanish when $t \uparrow 0$, and $\beta_1^{(1)}$ describes how this limit is approached: $m_1(t,0) - m_1(0,0) \sim (-t)^{\beta_1^{(1)}}$. For the amplitudes we put $\xi_\pm = (\frac{1}{2}\gamma/q)\hat{\xi}_\pm$.

	$t < 0$	$t = 0$	$t > 0$

$A \leqslant -1$	$\gamma_{11}' = 2 + A$
	$\nu_{//}' = 1$
	$\xi_- = 1$
	$\beta_1^{(0)} = 0$
	$\beta_1^{(1)} = -1 - A$
		$\eta_{//} = 0$
		$\eta_{//}' = -1 - A$
		$\delta_{11} = \frac{1}{-1-A}$
			$\gamma_{11} = \frac{1-A}{2}$
			$\nu_{//} = \frac{1-A}{2}$

$A = -1$	$m_1(t,0) \sim \{\log(-t^{-1})\}^{\frac{1}{2}}$	$g_{//}(r) \sim 1/\log r$ $m_1(0,h_1) \sim (\log h_1^{-1})^{-\frac{1}{2}}$	$\xi_{//} \sim \frac{(\log t^{-1})^{\frac{1}{2}}}{t}$
$-1 \leqslant A \leqslant 0$	$\gamma_{11}' = -A$ $\nu_{//}' = 1$ $\xi_- = 1$ $\beta_1 = \frac{1+A}{2}$	$\eta_{//} = 1+A$ $\delta_{11} = \frac{1-A}{1+A}$	$\gamma_{11} = -A$ $\nu_{//} = 1$ $\xi_+ = \frac{2+A}{2\sqrt{1+A}}$
$A = 0$	$\chi_{11}(t,0) \sim \log(-t^{-1})$	$m_1(0,h_1) = h_1 \log h_1^{-1}$	$\chi_{11}(t,0) \sim \log t^{-1}$
$A \geqslant 0$	$\gamma_{11}' = -A$ $\nu_{//}' = 1$ $\xi_- = \frac{2+A}{2\sqrt{1+A}}$ $\beta_1 = \frac{1+A}{2}$	$\eta_{//} = 1+A$ $\delta_{11} = \frac{1-A}{1+A}$ $(A < 1)$	$\gamma_{11} = -A$ $\nu_{//} = 1$ $\xi_+ = 1$
	$m_1(0,0) \sim (-A-1)^{\frac{1}{2}}$ as $A \uparrow -1$ $\chi_{11}(0,0) \sim (-A-2)^{-1}$ as $A \uparrow -2$ $\chi_{11}(0,0) \sim A^{-1}$ as $A \downarrow 0$		

(2) *Approach of criticality.*—For $t > 0$ $(t < 0)$ we write the correlation length as $\xi_\parallel(t) = \hat{\xi}_+ t^{-\nu_\parallel}$ $[\xi_\parallel(t) = \hat{\xi}_-(-t)^{-\nu_\parallel'}]$. In homogeneous systems one usually finds[1] that $\xi_\parallel$ is equal to the bulk correlation length ξ_b. However, in this system, the equality no longer holds: $\xi_\parallel$ may differ from ξ_b, either in its amplitude or even in its exponent. The surface susceptibility χ_{11} behaves as $t^{-\gamma_{11}}$ when $t \to 0$ from above, and γ_{11} depends on A. There is an *exponent asymmetry:* $\nu_\parallel$ and γ_{11} differ from $\nu_\parallel'$ and γ_{11}' if $A < -1$. For $t < 0$ there is a spontaneous surface magnetization m_1, decreasing as $|t|^{\beta_1}$ towards its value at $t = 0$, which is nonzero if $A < -1$. For $A < -1$, the spontaneous surface mag-

netization jumps discontinuously to zero as soon as $t > 0$. It is evident from the results shown in Table I that the scaling relations[1] $\nu_{\parallel}(1-\eta_{\parallel}) = \gamma_{11}$ and $\nu_{\parallel}'(1-\eta_{\parallel}') = \gamma_{11}'$ are satisfied. We remark that $\eta_{\parallel}$ and $\nu_{\parallel}$ apply to $g_{\parallel}(r)$, and that $\eta_{\parallel}'$ and $\nu_{\parallel}'$ apply to $g(r) - g(\infty)$.

These results apply to a large class of systems. Firstly, on physical grounds, it is plausible that changing the couplings in a finite number of surface layers will not change the exponents associated with large-r behavior of $g_{\parallel}(r)$. Secondly, putting $J_2(l) - J_\infty(l) \sim -\overline{A}/(l + l_0 - 1)$ in Eq. (2), with $l_0 > 0$ and finite, amounts to introducing a specific combination of higher powers of $1/l$ into the asymptotic behavior of $J_2(l)$. This is equivalent to studying a system described by Eq. (2), but having its surface at $l = l_0$, instead of at $l = 1$. From the analysis below it can be seen that this choice does not affect the exponents obtained. Further, a simple argument[4,5] shows not only that the amplitude A is marginal under renormalization, but also that contributions of the form l^{-p} with $p > 1$ are irrelevant. Apparently, there exist universality classes of inhomogeneous systems, each characterized by the value of the amplitude A, with exponents as given above. The critical surface exponents are determined by the long tail of the inhomogeneous part of the couplings, deep in the bulk. This justifies the mathematical analysis below, which is based on a smooth variation of the couplings $J_2(l)$. We shall now show how the above results can be obtained.

For $h_1 = 0$ in Eq. (1) we make use of a result due to McCoy and Wu,[2] which expresses $g_{\parallel}(r)$ in the form

$$g_{\parallel}(r) = \frac{1}{2\pi i} \int_{-\pi}^{\pi} d\theta\, e^{-ir\theta}/x_1(\theta). \tag{3}$$

The quantity $x_1(\theta)$ depends on all parameters of the problem. It is determined by the recursion relation

$$x_{l-1} = a + b^2 x_l/[a x_l + z_2^2(l)] \tag{4}$$

with the boundary condition that x_∞ be the stable fixed point of Eq. (4). Furthermore,

$$a(\theta) = -2z_1 \sin\theta\, |1 + z_1 e^{i\theta}|^{-2}, \qquad b(\theta) = (1 - z_1^2)|1 + z_1 e^{i\theta}|^{-2}, \tag{5}$$

$z_1 = \tanh[J_1/k_B T]$ and $z_2(l) = \tanh[J_2(l)/k_B T]$. We set $z_2 \equiv z_2(\infty)$. When $T = T_c$, $z_2 = (1 - z_1)$; a pair (z_1, z_2) satisfying this relation is denoted by (z_{1c}, z_{2c}). The recursion is trivial for the homogeneous lattice, $A = 0$. The case $A \neq 0$ is more involved. We therefore use the fact that the large-r behavior of $g_{\parallel}(r)$ follows from the small-θ behavior of $x_1(\theta)$. Further simplification is obtained by taking T close to T_c, i.e., $|t| \ll 1$. Finally, we assume that $|\overline{A}/l| \ll 1$. We expand Eq. (4) in these three small quantities. To lowest order,

$$y_{l-1} = \psi + (1 + \beta t) y_l/(\psi y_l + 1 - \zeta t - A/l), \tag{6}$$

where $y_l = x_l/z_{2c}$, $\psi = -q\theta$, $q = 2z_{1c}/\{z_{2c}(1 + z_{1c})^2\}$, $\beta = 4J_1/k_B T_c$, and $\zeta = (2 - 2z_{2c} k_B T_c)$. From Eq. (6) we see that $y_{l-1} - y_l$ is of the order of the quantities that were assumed small. We therefore consider l as a continuous variable and replace Eq. (6) by the differential equation

$$dy(l)/dl = \psi[y^2(l) - 1] - (A/l + \gamma t) y(l) \tag{7}$$

with $\gamma = \beta + \zeta$. Higher powers of small quantities have been neglected. The proper boundary condition is easily found to be $y(\infty) = (\gamma t + \xi)/2\psi$, where $\xi = (\gamma^2 t^2 + 4q^2\theta^2)^{1/2}$. To solve Eq. (7), we introduce

$$u(\xi l) = \exp[-\int_1^l \{\psi y(l') - A/(2l') - \gamma t/2\} dl'].$$

Then it reduces to a linear second-order differential equation, namely

$$d^2u(z)/dz^2 = [\tfrac{1}{4} - \kappa/z - (\tfrac{1}{4} - \mu^2)/z^2] u(z) \tag{8}$$

with $\kappa = -\frac{1}{2}A\gamma t/\xi$ and $\mu = \frac{1}{2}(1 - A)$. The solution in agreement with the boundary condition is, up to an irrelevant factor, $u(z) = W_{\kappa,\mu}(z)$ where $W_{\kappa,\mu}(z)$ is the Whittaker function.[8] Upon putting $l = 1$ and making a few substitutions we obtain $x_1(\theta)$, which, with Eq. (3), gives

$$g_{\parallel}(r) = \frac{q}{\pi i z_{2c}} \int_{-\pi}^{\pi} d\theta\, \theta e^{-ir\theta} \times \frac{\Gamma^- \xi^{2\mu} M^+ + \Gamma^+ M^-}{\Gamma^- \xi^{2\mu}[\alpha M^+ + \beta^+ M'^+] + \Gamma^+[\alpha M^- + \beta^- M'^-]} \tag{9}$$

where $\Gamma^\pm = \Gamma(\pm 2\mu)/\Gamma(\frac{1}{2} \pm \mu - \kappa)$, $\alpha = (\xi - \gamma t)\{1 + (1 - 2\mu)/\xi\}$, $\beta^\pm = 1 \pm 2\mu + (2\mu - 1)\gamma t/\xi$, $M^\pm = M(\frac{1}{2} \pm \mu - \kappa, 1 \pm 2\mu, \xi)$, and $M'^\pm = M(-\frac{1}{2} \pm \mu - \kappa, 1 \pm 2\mu, \xi)$; and M denotes the Kummer function.[8]

Further analysis for $t = 0$ comprises expansion of the fraction in Eq. (9) in powers of θ, and evaluation of the leading terms and singular corrections for small θ. For special values of A, two terms may merge into a logarithm. The Fourier transformation Eq. (9) then gives $g_{\parallel}(r)$ for large r. For $t \neq 0$, $g_{\parallel}(r)$ is found from the singularities of the integrand of Eq. (9) in the complex θ plane. These singularities lie on the imaginary axis: branch cuts due to the square root in the definition of ξ, and poles for zeros of the denominator of the integrand in Eq. (9), associated with nonpositive integral arguments of Γ functions.

In order to derive the singular part of the boundary magnetization $m_1(t=0, h_1)$ for small h_1 and of the susceptibility $\chi_{11}(t, h_1=0)$ for small $|t|$, we make use of an expression for m_1 given by McCoy and Wu[2]. In our case, it reduces to

$$m_1(h_1) \simeq h_1 + \frac{h_1}{2\pi}\int_{-\pi}^{\pi} \frac{d\theta}{h_1^{\,2} + c x_1(\theta)} \tag{10}$$

with $c = -2\sin\theta|1+e^{i\theta}|^{-2}$. The zero-field boundary susceptibility follows by differentiation:

$$\chi_{11} = 1 - \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta \{c\bar{x}_1(\theta)\}^{-1} \tag{11}$$

where

$$\bar{x}_1^{-1}(\theta) = x_1^{-1}(\theta) - \theta^{-1}\lim_{\theta\to 0} \theta/x_1(\theta).$$

Upon using the solution $x_1(\theta)$ in Eqs. (10) and (11), and analyzing the small-θ behavior of the integrands in Eqs. (9)–(11), one derives the critical properties shown in Table I.

More details, especially about the mathematical part of this work, will be published elsewhere.

We acknowledge stimulating discussions on this subject with J. M. J. van Leeuwen, and with T. W. Burkhardt, who has also communicated some of his results to us prior to publication.

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