Orientation Dependence of Surface Critical Phenomena in Antiferromagnets: Exact Results in Two Dimensions

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For an Ising antiferromagnet, we analyze *exact* expressions for the one- and two-point correlation functions for spins on the edge of a square lattice with a magnetic field applied to the surface sites. Two different edge orientations, with respect to the crystal axes, are treated. At bulk criticality, we confirm that the surface universality class depends on the edge orientation and show the importance of having the bulk phase in a pure state. For the two-point function, we find a singularity in the correlation length due to depinning effects which we argue is also present in higher dimensions.

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Since the seminal work of McCoy and Wu [1], it has been realized that surfaces in uniaxial magnets and their analogs can display novel phase transitions and critical phenomena. A key idea for *bulk* critical phenomena is that of distinct universality classes. The relevance of universality classes for surface critical behavior has become increasingly apparent over the past 20 years or so [2,3]. Thus we now have the picture that surface criticality depends on the bulk universality class, on relevant surface modifications (such as fields and coupling strengths) and, most recently, on the orientation of the surface with respect to the crystal axes. Note that several surface universality classes may be compatible with a single bulk one. The first theoretical work on orientation dependence was by Schmid [4], who carried out Monte Carlo simulations and mean-field calculations on the Ising *antiferromagnet* with a free surface on the bcc lattice. This system has an experimental realization in the $A2$-$B2$ disorder transition in FeAl [5]. The theoretical work has been considerably advanced more recently [6], particularly in a numerical transfer matrix and conformal theoretic treatment of a planar case. In this Letter, we report results of an *exact* calculation which amplifies these points further, giving explicit expressions for one- and two-point functions which are directly relevant but not given in Ref. [1]. We also interpret our results using the droplet model [7,8] which, in turn, suggests novel behavior in three dimensions.

For systems consisting of Ising spins $\sigma_{\mathbf{i}} = \pm 1$ placed on sites $\mathbf{i}$ of a d-dimensional lattice with a surface Σ and a *surface* magnetic field h_1 applied to all sites in Σ, the surface critical phenomenon is manifested in surface quantities, examples of which are defined as follows. If $\mathbf{j} \in \Sigma$, the surface magnetization, m_1, is defined by $m_1 := \langle \sigma_{\mathbf{j}} \rangle$ (where $\langle \cdot \rangle$ is the ensemble average). As the temperature, T, passes through the *bulk* critical temperature, $T_c = T_c(d)$, in zero *bulk* magnetic field, m_1 has leading singular behavior $m_1^{\text{sing}} \sim |t|^{\beta_1}$ as $t := (T - T_c)/T_c \to 0$ defining the *surface* critical exponent β_1. Another surface exponent of interest is $\eta_\parallel$, describing the decay of critical pair-spin correlations parallel to Σ. Thus, for both $\mathbf{0}, \mathbf{r} \in \Sigma$, $\langle \sigma_{\mathbf{0}} \sigma_{\mathbf{r}} \rangle^T \sim r^{-(d-2+\eta_\parallel)}$ as $r \to \infty$ at the *bulk* critical point (throughout, the superscript T denotes truncation by subtracting away $\langle \sigma_{\mathbf{0}} \rangle \langle \sigma_{\mathbf{r}} \rangle$ from $\langle \sigma_{\mathbf{0}} \sigma_{\mathbf{r}} \rangle$).

For a given bulk universality class, the values of the surface exponents, β_1, $\eta_\parallel$, etc., depend on the *surface* universality class. In this Letter we encounter just two surface universality classes: the *ordinary transition* and the *normal transition*. If the spins in the bulk are coupled *ferromagnetically* the ordinary transition characterizes the case where $h_1 = 0$ with surface couplings de-enhanced so that the surface does not (locally) break the symmetry of the order parameter and the surface stays disordered whenever the bulk is disordered. On the other hand, the normal transition occurs when $h_1 \neq 0$ which breaks the symmetry of the order parameter and gives a magnetized surface even when the bulk is disordered (for $T > T_c$, zero bulk field). This situation changes considerably when the bulk couplings are *antiferromagnetic* and the orientation of Σ, relative to the lattice axes, is allowed to vary; a $d = 2$ version of this case is the subject of this Letter.

We consider an Ising model on a square lattice with *antiferromagnetic* couplings (in units of $k_B T$) K_1 (respectively, K_2) along bonds in the $(0, 1)$ [respectively, $(1, 0)$] direction, as shown in Fig. 1(a). Edges are formed by cleaving the lattice in either the $(1, 1)$ or $(1, 0)$ direction; a uniform surface field h_1 (in units of $k_B T$) is applied to the surface sites in either case. Henceforth, we refer *only* to the equivalent *ferromagnets* obtained by reversing all the spins on one of the sublattices (white dots, say) in Fig. 1(a) leading to the ferromagnetic lattices shown in Fig. 1(b) for the $(1, 1)$ edge, with a *uniform* surface field, and Fig. 1(c) for the $(1, 0)$ edge, with a *staggered* surface field. These lattices are wrapped onto a cylinder of circumference M (assumed to be even) and height N with the edge field applied to the bottom edge. We shall always set the bulk field to zero. Clearly, the behavior of the one-point function, or

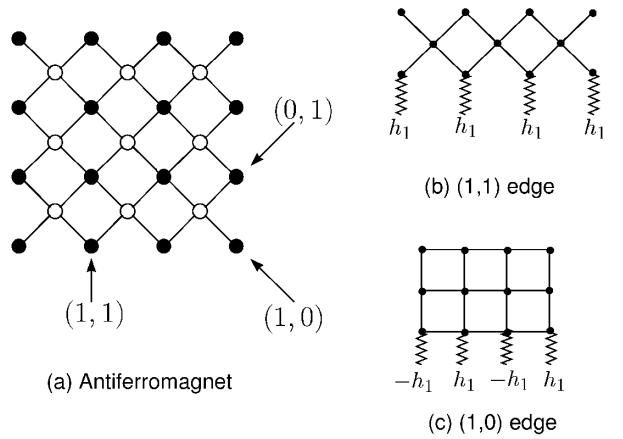

FIG. 1. (a) shows the antiferromagnet with edge orientations indicated and the equivalent ferromagnets are shown in (b) for the $(1, 1)$ edge, with a *uniform* surface field, and (c) for the $(1, 0)$ edge, with a *staggered* surface field.

spin expectation at each lattice site, will depend on the bulk state for $T < T_c(2)$, since we then have two coexistent pure phases with magnetization $\pm m^*$. The bulk can take any intermediate value in $[-m^*, m^*]$, selected by a suitable choice of boundary condition at the top edge. We determine the one-point and two-point functions and show explicitly that the appropriate universality classes do depend on the orientation of the edge as might be anticipated by the fact that the uniform field breaks up-down symmetry whereas the staggered field does not.

If $\mathbf{n} = (1, 0), (1, 1)$ denotes the edge direction, standard transfer matrix theory gives the results

$$\langle \sigma_{1,1}\sigma_{1+s,1}\rangle(\mathbf{n}) = Z(\mathbf{n})^{-1}\langle +|V(\mathbf{n})^N \sigma_1^x \sigma_{1+s}^x|\mathbf{n}\rangle, \quad (1)$$

where

$$|(1,0)\rangle = V_2^{1/2} V_1(h_1^*)\,|+-\rangle, \qquad |(1,1)\rangle = V_1(h_1^*)\,|+\rangle, \quad (2)$$

and the partition functions, $Z(\mathbf{n})$, are obtained by evaluating the matrix elements on the right-hand side of (1) with both spin operators replaced by 1. Also σ_j^α ($\alpha = x, y, z$) is the α-component Pauli operator acting on site j ($1 \le j \le M$). The end state $|+\rangle$ (respectively, $|-\rangle$) denotes the state where *all* the spins are up (respectively, down) in the x direction and $|+-\rangle$ is the state where the spins are staggered (alternately up and down) in the x direction with $|-+\rangle$ being this state shifted by one lattice spacing. The one-point function, or surface magnetization, is given similarly by deleting σ_1^x in (1). The transfer matrix $V(1,0) = V_2^{1/2} V_1 V_2^{1/2}$, where

$$V_1 = \prod_{j=1}^{M} \exp(-K_1^* \sigma_j^z), \qquad V_2 = \prod_{j=1}^{M} \exp(K_2 \sigma_j^x \sigma_{j+1}^x), \quad (3)$$

with cyclic boundary conditions on the cylinder of circumference M and $e^{-2K_1^*} = \tanh K_1$. The transfer operator $V(1,1)$ is not well known. For the present purpose, the eigenvalues are not needed; the eigenvectors can be obtained from the star-triangle relation. A prototypical Yang-Baxter idea [9] shows that $V(1,1)$ commutes with the Hamiltonian for a 1-dimensional Ising model in a transverse field, the handling of which is straightforward. For both $\mathbf{n}$, $V_1(h_1^*)$ is given by V_1 in (3) with h_1^* ($= -\frac{1}{2}\ln\tanh h_1$) replacing K_1^*. The formula (1) is appropriate for a bulk + magnetized state which is selected by the upper boundary state $\langle +|$. Strictly, we should take $M \to \infty$, followed by $N \to \infty$ to approach the thermodynamic limit so as to select the + magnetized state. The physically relevant factor in this argument is that for $T < T_c(2)$, the maximum eigenvalue of $V(\mathbf{n})$ is *asymptotically* (but not strictly) degenerate as $M \to \infty$. Taking $N \to \infty$ first means that only the maximum term is included. We have evaluated (1) for finite N and M; the prolixity of this makes publication elsewhere advisable—in this case the full spectrum of $V(1,1)$ is needed [10]. The finite-M results we give below tend to the physically correct thermodynamic limit as $M \to \infty$. Let the asymptotically degenerate eigenvectors be $|\Phi_\pm\rangle$: then we have

$$\langle \sigma_{1,1}\sigma_{1,1+s}\rangle(\mathbf{n}) = \hat{Z}(\mathbf{n})^{-1} \sum_{\varepsilon=+,-} \langle \Phi_\varepsilon|\sigma_1^x \sigma_{1+s}^x|\mathbf{n}\rangle. \quad (4)$$

To finish setting the problem up, we note that $|+\rangle$ and $|+-\rangle$ can be obtained from the asymptotically degenerate eigenvectors $|\Phi_\pm\rangle$ of $V(1,0)$ by taking $K_1^* \to 0$, with $K_2 > 0$ and $K_2 < 0$, respectively. In this case, the degeneracy becomes exact and $|\Phi_\pm\rangle \to |\Phi_\pm^0\rangle$ (respectively, $|\Phi_\pm^-\rangle$) for $K_2 > 0$ (respectively, $K_2 < 0$); $|\pm\rangle$ and $|\pm\mp\rangle$ become linear combinations of the appropriate vectors. In the former case, the coefficients have been evaluated elsewhere [11]. Analogous procedures apply in the latter case, giving

$$\begin{aligned} \sqrt{2}\,|\pm\rangle &= |\Phi_+^0\rangle \pm |\Phi_-^0\rangle, \\ \sqrt{2}\,|\pm\mp\rangle &= |\Phi_+^-\rangle \pm |\Phi_-^-\rangle, \end{aligned} \quad (5)$$

where, for $i = 0, -$,

$$|\Phi_\pm^i\rangle = Q_\pm^i \prod_{\omega>0}^{<\pi} [\cos\theta^i(\omega) + i\sin\theta^i(\omega) F_{-\omega}^\dagger F_\omega^\dagger]|0\rangle \quad (6)$$

with $\exp iM\omega = \mp 1$, $\theta^0(\omega)$ [respectively, $\theta^-(\omega)$] $= (\pi + \omega)/2$ (respectively, $\omega/2$) modπ and F_ω, $F_\omega^\dagger$ are (discrete) Fourier transforms of Fermi operators f_j, $f_j^\dagger$ acting on sites $1 \le j \le M$. Also, $|0\rangle$ is the F_ω vacuum, $Q_+^i = 1$ always and Q_-^0 (respectively, Q_-^-) $= F_0^\dagger$ (respectively, $F_\pi^\dagger$). The appropriateness of the $F_\pi^\dagger$ factor is intuitively clear, since under the unit translation operator $\hat{T}$, $|+-\rangle \to |-+\rangle$ [as seen from (5) noting $\hat{T}|\Phi_-^-\rangle = e^{i\pi}|\Phi_-^-\rangle$]. Had we taken free boundary conditions at the top, bringing in $\langle 0|$ rather than $\langle +|$ at the left in (1), the term $\varepsilon = -$ in (4) would be absent. This factor is quite crucial in getting the surface universality class behavior correct for the one- and two-point functions.

Noting that $|+\rangle$ and $|+-\rangle$ are eigenvectors of σ_j^x, we move the σ_1^x and σ_{1+s}^x through the appropriate operators in $|(1,0)\rangle$ and $|(1,1)\rangle$, getting factors $\exp 2h_1^* \sigma_j^z$ for $j = 1$ and $j = 1 + s$ [and an overall factor of $(-1)^s$ for the $(1,0)$ edge coming from $\sigma_{1+s}^x|+-\rangle$]. These in turn can be expressed in terms of bilinear forms in f_j and $f_j^\dagger$: $\exp 2h_1^* \sigma_j^z = A_j^\dagger A_j$, where $A_j = e^{-h_1^*} f_j^\dagger + e^{h_1^*} f_j$. Thus (4) can be evaluated by Wick's theorem. We now describe the salient features in the results for both edge types in turn.

(1, 0) Edge.—First consider the one-point function $m_1(s) = \langle \sigma_{1+s,1} \rangle$. Since the A_j are linear in the fermions, the $\varepsilon = +$ term in (4) is evaluated as a contraction. From translational invariance of the end states, it is clear that there can be no s dependence in this $\varepsilon = +$ contraction and thus, due to the overall prefactor of $(-1)^s$, this term gives rise to an "antiferromagnetic" contribution to $m_1(s)$. The analogous translational argument for the $\varepsilon = -$ term shows that, since the right state $|\Phi_-^-\rangle$ changes sign under translation, an additional $e^{i\pi s}$ factor comes out of the contractions which cancels with the overall $(-1)^s$ factor leading to a "ferromagnetic" contribution to $m_1(s)$. Its evaluation proceeds again by Wick's theorem, except now we must contract both the F_0 and the $F_\pi^\dagger$, each with a different A-type operator. Then finally, we have to estimate the ratio of the $-$ and $+$ "vacuum" expectations to get the final result. The conclusion for the $(1,0)$ boundary is that

$$m_1(s) = m_{\rm f} + (-1)^s m_{\rm af}\,, \tag{7}$$

where $m_{\rm f} \sim |t|^{1/2}$ and $m_{\rm af}^{\rm sing} \sim t^2 \ln|t|$ so that the ferromagnetic term produces the dominant scaling behavior corresponding to $\beta_1 = 1/2$, i.e., that of the *ordinary* transition. However, we stress that this ferromagnetic term would be *absent* when there is zero bulk magnetization [which includes the case for $T < T_{\rm c}(2)$ with the top of the cylinder having a *free* edge]; in that case, the ferromagnetic term vanishes identically simply because the bulk state has no projection on the $-$ spectrum. Note also that the antiferromagnetic term, which is nontrivial for $T > T_{\rm c}$, as well as $T < T_{\rm c}$, gives rise to a curious correction-to-scaling contribution behaving as $t^2 \ln|t|$, which has the same form as the leading singularity in the *bulk* free-energy density and also the *leading* singularity of m_1 for a *normal* surface. Such a correction-to-scaling term is *not* present when the ordinary transition is realized by having a free ($h_1 = 0$) boundary; here all the correction terms behave as $|t|^{n+\frac{1}{2}}$, where $n \geq 1$ is an integer.

The same type of analysis obtains for the two-point function for the $(1,0)$ edge; by careful consideration, the connected two-point function can be extracted and shown to vanish for infinite separation, as it should. For this to happen, the $\varepsilon = -$ term in (4) plays an essential role, leading to the correct *clustering* property appropriate for a *pure* phase. Thus we have

$$\langle \sigma_{1,1} \sigma_{1+s,1} \rangle^T = C_{\rm f}(s) + (-1)^s C_{\rm af}(s)\,, \tag{8}$$

where in the scaling regime, for $t \to 0^\pm$,

$$C_{\rm f}(s) \sim \tau F_\pm(\tau s) + O(|t|^{3/2})\,, \tag{9}$$

$C_{\rm af}(s) = O(|t|^{3/2})$ with $\tau = (\xi_0^+)^{-1}|t|$ and ξ_0^+ is the supercritical amplitude of the *bulk* correlation length ξ. The leading part, in a scaling sense, is pure monotone in s, which supports the point of view that, since the bulk state is plus magnetized, this permeates to the boundary and so the energy of typical configurations has a "weak" h_1 dependence because of its alternating character along the edge. The asymptotic behavior is $F_\pm(x) \sim e^{-x}/x^{3/2}$ as $x \to \infty$. Also, $F_\pm(x) \sim 1/x$ as $x \to 0$, implying that $\eta_\parallel = 1$ as for the ordinary transition. The idea that coarse graining to the level of about ξ eliminates the surface field when ξ is large suggests that, in the $(1,0)$ case, the two-point function should behave as though it is in a *free* edge [with the same scaling functions $F_\pm(x)$]. This is easily confirmed by an exact calculation as given originally by McCoy and Wu [1]. Second, the truncated two-point function in the edge is described in the droplet model of uniaxial correlations [7] by a solid-on-solid (SOS) path connecting the two spin locations as extrema, with fluctuations controlled by the surface tension—strictly, lattice anisotropy of the surface tension outside the scaling region would require surface stiffness [12]. Such a picture invites generalizations to $d = 3$ with SOS lattice tubes [8] to be explained below.

(1, 1) Edge.—We now continue with the $(1,1)$ edge behavior. For $t \to 0^\pm$ (in the scaling region)

$$\langle \sigma_{1,1} \sigma_{1+s,1} \rangle^T \sim \tau F_\pm(\tau s; y)\,, \tag{10}$$

where $\tau = (\xi_0^+)^{-1}|t|$, $\Delta_1^{\rm ord} = 1/2$ is the surface gap exponent for the $d = 2$ *ordinary* transition, $y = \sqrt{2}\, h_1 \tau^{-\Delta_1^{\rm ord}}$ is the scaled surface field, and

$$F_\pm(x; y) = J_\pm(x, y) \int_0^\infty du \times e^{-xu} \frac{A(u) f_\pm(u, y)}{B_\pm(u, y)} + G_\pm(x, y)\,, \tag{11}$$

where $A(u) = \sqrt{u(2+u)}$, $f_+(u, y) = (1+u)^2$, $f_-(u, y) = [1 + u - y(2 - y^2)^{1/2}]^2$,

$$B_\pm(u, y) = (1+u)[(1+u)^2 + y^4 \pm 2y^2]\,, \tag{12}$$

and

$$G_\pm(x, y) = \left(\frac{y e^{-x}}{\pi}\right)^2 \int_0^\infty du_1 \int_0^\infty du_2 \times \frac{e^{-x(u_1+u_2)} A(u_1) A(u_2) (u_1 - u_2)^2}{B_\pm(u_1, y) B_\pm(u_2, y)}\,. \tag{13}$$

Finally, $J_+(x, y) = 2e^{-x}/\pi(2 + y^2)$ and

$$J_-(x, y) = \frac{2(1 - y^2)\Theta(1 - y) e^{-x[1 + y(2-y^2)^{1/2}]}}{\pi(2 - y^2)}\,, \tag{14}$$

where $\Theta(\cdot)$ is the Heaviside function. Thus, for $T < T_{\rm c}(2)$, we see that a new dominant length scale (dependent

on h_1) emerges for $y < 1$. This was also observed by McCoy and Wu, but they did not give the scaling function or offer an interpretation of this. The scaling functions, $F_{\pm}(x; y)$, express the *full* crossover from the *ordinary transition,* $y = 0$, to the *normal transition,* $y = \infty$. So, $\lim_{y\to 0} F_{\pm}(x; y) = F_{\pm}^{\mathrm{ord}}(x)$, where $F_{\pm}^{\mathrm{ord}}(x)$ is essentially the same as $F_{\pm}(x)$ in (9), corresponding to $\eta_{\parallel} = \eta_{\parallel}^{\mathrm{ord}} = 1$ (ordinary transition). In addition, $F_{\pm}(x; y) \sim y^{-6} F_{\pm}^{\mathrm{nor}}(x)$ as $y \to \infty$, where $F_{\pm}^{\mathrm{nor}}(x) \sim x^{-4}$ as $x \to 0$ giving $\eta_{\parallel} = \eta_{\parallel}^{\mathrm{nor}} = 4$ (normal transition). This ordinary-normal crossover is analytic in y for $T > T_c$ but is singular at $y = 1$ for $T < T_c$. Note that this singularity in the two-point function has *no* thermodynamic consequences for the surface susceptibility obtained as a fluctuation sum. But, as we indicate below, that part of the inverse correlation length extracted from $J_{-}(x, y)$ has singular behavior at $y = 1$ and gives the incremental free energy associated with a pinning-depinning transition at $y = 1$. This is best seen qualitatively (but it can be established analytically) in the *droplet picture*.

Here the truncated two-point function for the $(1, 1)$ edge is a sum over SOS *loops* [7] separating regions of opposite magnetization with the spin locations as apices. We have *loops* because $h_1 > 0$ in this application. The loop consists of an *upper* and a *lower* path. The lower one behaves like an interface at a wall with a binding potential supplied by h_1. Thus we have a pinning-depinning, or wetting, scenario. The upper interface cannot cross the lower one, and when the lower one is pinned, behaves essentially as a free interface confined to a half-plane, and therefore wanders away from it. These ideas reproduce the behavior of $F_{-}(x, y)$ for x large.

The droplet idea can be extended to $d = 3$ by noting that the natural objects which separate regions of opposite magnetization are tubes [8]. In both the staggered and uniform field case, there is an energetic binding of the tube to the substrate where fewer, or weaker, bonds get broken. Preliminary results can be obtained by treating the tube as an SOS string connecting the locations of the spins at surface sites $\mathbf{0}$ and $\mathbf{r}$. The string motion decouples into a free part parallel to the substrate plane and a perpendicular one which manifests pinning-depinning behavior at a temperature $T_p < T_c(3)$; we expect $T_p = T_p(h_1)$ for the uniform surface field, whereas T_p will be independent of (or only weakly dependent on) h_1 for the staggered field and T_p should be orientation dependent. We find that $\langle \sigma_{\mathbf{0}} \sigma_{\mathbf{r}} \rangle^T \approx K(r) e^{-\kappa_1 r}$ as $r \to \infty$, where $K(r) \sim r^{-1/2}$ for all $T < T_p$ and $K(r) \sim r^{-2}$ for all $T_p \le T < T_c(3)$. Furthermore, if κ_b is the *bulk* inverse correlation length then $\kappa_1 = \kappa_b$ for all $T_p \le T < T_c$ but $\kappa_1 < \kappa_b$ for $T < T_p$ [where $\kappa_1 = \kappa_1(h_1)$ for the uniform surface field case] with $\kappa_1 \nearrow \kappa_b$ as $T \nearrow T_p$ in a manner similar to $d = 2$. Clearly, such phenomena should be sought both experimentally and in Monte Carlo simulation. Generalizations to $d \ge 3$ are straightforward; in this case one finds that $K(r)$ has the behavior $K(r) \sim r^{-(d-2)/2}$ for $T < T_p$ and $K(r) \sim r^{-(d+1)/2}$ for $T_p \le T < T_c(d)$.

In this Letter, we have analyzed the orientation dependence of surface critical phenomena in two-dimensional uniaxial antiferromagnets. Key features are the dependence of surface exponents on the bulk state, the explicit character of crossover functions between *normal* and *ordinary* behavior, and the occurence of pinning-depinning and associated h_1 dependence of surface correlation lengths and changes in the algebraic prefactors. Related pinning-depinning phenomena are also predicted for three dimensions. Also, the inverse correlation length displayed by the surface pair correlation function has the same singular behavior as the incremental free energy associated with pinning of an interface for $d = 2$, or of a polymer for $d \ge 3$.

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