Renormalization-group calculation of the critical properties of a free magnetic surface*

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A semi-infinite Ising model is studied by renormalization-group techniques in the position-space formulation due to Niemeijer and van Leeuwen. We show how to set up the calculation of thermodynamic properties (both critical and noncritical) of a sample with a free surface by iteration of a set of recursion relations for spatially inhomogeneous couplings and magnetic fields. Surface and bulk properties are clearly distinguished. The method is illustrated by a calculation (using a two-cell cluster approximation) of the magnetic-surface critical exponent in two dimensions, where exact results are available for comparison.

I. INTRODUCTION

Critical phenomena associated with free magnetic surfaces have been studied recently in the mean-field approximation,[1-5] via phenomenological scaling theories,[3,4,6,7] by series[3,4,6,8,9] and Monte Carlo[6,10] methods, and via renormalization-group techniques in ϵ expansion about four dimensions[11] ($d=4-\epsilon$). Exact solutions for surface properties are available for the spherical model[7,12] and the $d=2$ Ising model.[13,14]

For specificity we consider an Ising model on a hypercubical lattice of unit spacing which is semi-infinite in the z direction ($0 \leq z < \infty$) but infinite in the $(d-1)$ directions parallel to the surface $\vec{r}_{\parallel} = (x, y, \ldots)$ ($-\infty < x, y, \ldots < \infty$). Take magnetic and nearest-neighbor pair interactions which may depend on z but are translationally invariant in the parallel directions, so the Hamiltonian reads,

$$-\beta\mathcal{H} \equiv H = \sum_{z,\vec{r}_{\parallel}} \left(K_0(z) + h(z)\mu(z,\vec{r}_{\parallel}) + K_{\perp}(z)\mu(z,\vec{r}_{\parallel})\mu(z+1,\vec{r}_{\parallel}) + K_{\parallel}(z)\sum_{\vec{\delta}} \mu(z,\vec{r}_{\parallel})\mu(z,\vec{r}_{\parallel}+\vec{\delta}) \right), \tag{1}$$

where $\mu = \pm 1$, $\vec{\delta} = (1,0,\ldots), (0,1,\ldots), \ldots$, and $K_0(z)$ is a spin-independent contribution to the energy, which we shall need later but plays no role here. We confine ourselves to ferromagnetic couplings, $K_{\parallel}, K_{\perp} > 0$. To discuss scaling behavior it is convenient to specialize further, singling out the surface layer $z=0$,

$$\begin{aligned} &h(0) = h + h_1, \quad h(z>0) = h, \quad K_0(z) = K_0, \\ &K_{\parallel}(0) = K(1+D), \quad K_{\parallel}(z>0) = K_{\perp}(z) = K. \end{aligned} \tag{2}$$

The bulk free energy per spin $f_b(K,h)$ depends only on the bulk couplings K and h, whereas the surface free energy per surface spin[15] $f_s(K,D,h,h_1)$ depends in addition on the surface-layer magnetic field h_1 and coupling enhancement D.

For $d>2$ and sufficiently positive surface enhancement D it is known[1,5,16,17] that the surface may become ferromagnetic at a critical temperature T_s higher than the bulk critical temperature T_c. In this situation the bulk free energy f_b is analytic at T_s, while the surface free energy f_s exhibits critical behavior with exponents characteristic of a $(d-1)$-dimensional system. In this paper we shall deal with the "ordinary" situation, where f_s is analytic except at the bulk T_c. Near T_c the bulk free energy then scales in the usual[18,19] way,

$$f_b = t^{2-\alpha}\mathcal{F}_b(h/t^{\Delta}), \quad t = |K - K_c|/K_c. \tag{3}$$

$\mathcal{F}_b$ is the bulk scaling function; α and Δ are bulk critical exponents. However, in the surface free energy, h_1 is a relevant variable (although D is not), so f_s scales as[3,4,6,7]

$$f_s = t^{2-\alpha_s}\mathcal{F}_s(h/t^{\Delta}, h_1/t^{\Delta_1}). \tag{4}$$

The surface specific-heat exponent α_s is related by a scaling argument to bulk exponents, $\alpha_s = \alpha + \nu$, so the only new thermodynamic surface exponent[6] is Δ_1.

Derivatives of $f_s(K,D,h,h_1)$ define a host of surface properties.[20] In particular we distinguish the "surface magnetization" $m_s = \partial f_s/\partial h$, the "layer magnetization" $m_1 = \partial f_s/\partial h_1$, and the corresponding susceptibilities $\chi_s = \partial m_s/\partial h$ and $\chi_{1,1} = \partial m_1/\partial h_1$. Critical behavior follows from (4). For example, at $t \to 0$ with $h = h_1 = 0$, $m_s \sim t^{\beta_s}$, with $\beta_s = 2 - \alpha_s - \Delta$; $\chi_s \sim t^{-\gamma_s}$, with $\gamma_s = 2\Delta + \alpha_s - 2$; $m_1 \sim t^{\beta_1}$, with $\beta_1 = 2 - \alpha_s - \Delta_1$; and $\chi_{1,1} \sim t^{-\gamma_{1,1}}$, with $\gamma_{1,1} = 2\Delta_1 + \alpha_s - 2$.

Values of these exponents from the mean-field approximation and for the $d=2$ Ising model are given in Table I. ϵ expansions about $d=4$ were derived by Lubensky and Rubin.[11] Series evaluations are available[3,4,6,8,9] at $d=3$.

Renormalization-group (RG) calculations of bulk properties have been extremely successful.[21-25] So far the only analogous work for surface properties is the series of papers by Lubensky and Rubin,[11] who treat the Landau-Wilson model by ϵ expansion (k-space RG). Direct position-space, Niemeijer–van Leeuwen[22,23] (NvL) surface calculations are also possible. It is our purpose in this paper to demonstrate the feasibility of such calculations. The NvL methods are applied directly to the Ising model in d dimensions ($d=2$ in our calculation). This has the advantages that the vagaries of ϵ expansion are avoided and that one can calculate nonuniversal (and even noncritical) quantities in addition to exponents and critical scaling functions.[23-25] The disadvantage of the NvL method is, of course, that there is no explicit small parameter, so all approximations are to some extent *ad hoc*. This has not prevented very accurate calculations on bulk systems.

In Sec. II we sketch the machinery necessary for extending NvL methods to surface properties. Because the couplings depend on z, it is necessary to develop *spatially inhomogeneous* recursion relations for the couplings. As a consequence the critical fixed-point couplings become z dependent, $K^*(z)$, and the eigenvalue problem associated with linearization about the fixed point becomes infinite dimensional.[26] The added technical difficulties are not great, however, and one can extract exponents (eigenvalues) and scaling fields (eigenvectors) in close parallel with the bulk problem.

To illustrate this we carry out in Sec. III a simple calculation of the surface properties of the $d=2$ Ising model, based on an exceedingly crude NvL recursion relation. This approximation lends itself to essentially analytic calculation and, despite its crudeness, captures the essential *physical* content of the surface critical behavior: The layer field h_1 [Eq. (2)] is a relevant variable, while the surface enhancement D is not. Calculated critical exponents (y's) differ from the exact results shown in Table I by (10–30)%. It is our intention in subsequent work to use better approximate recursion relations to carry out more quantitative (but necessarily more complicated) calculations of surface properties of two- and three-dimensional samples. The general method can handle the surface phases which occur for $d>2$, D large and positive (there is a new, surface fixed point). It also appears applicable to the calculation of interfacial free energies.[27]

TABLE I. Exact and mean-field (MFA) exponents for the $d=2$ Ising model.

	α	ν	Δ	α_s	Δ_1	y_t	y_h	y_{h_1}
MFA[a]	0	$\frac{1}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	$\frac{1}{2}$			
Exact[b] $d=2$	0 (ln)	1	$\frac{15}{8}$	1	$\frac{1}{2}$	1[c]	$\frac{15}{8}$[c]	$\frac{1}{2}$[c]

[a] References 1–5.
[b] Exact results, Refs. 13, 14, and 36.
[c] Obtained by scaling.

II. POSITION-SPACE APPROACH TO SURFACE CRITICAL BEHAVIOR

The principle of the RG method[21,23] is the evaluation of the free energy by iterative elimination of short-wavelength degrees of freedom. The NvL[22,23] technique for performing this elimination is to divide the lattice into cells, each containing b^d spins (degrees of freedom) $\{\mu\}$. b is the (length) scale factor. A single collective (spin) variable $\mu'=\pm 1$ is projected out for each cell via a projection operator $P_{\text{cell}}(\mu'|\{\mu\})$ [with $\sum_{\mu'} P_{\text{cell}}(\mu'|\{\mu\})=1$] and the remaining b^d-1 degrees of freedom are summed out.

We briefly sketch the RG development for the *homogeneous* bulk system for subsequent comparison with the layered system (1): The original bulk partition function is

$$Z[K_0,K_\alpha,h_\alpha]=\mathrm{Tr}_\mu e^{H[K_0,K_\alpha,h_\alpha,\{\mu\}]}, \tag{5}$$

where $H=-\beta\mathcal{H}$ is the bulk Hamiltonian, which depends on the values of the generic bulk couplings[28] K_α (even) and h_α (odd). The constant K_0 multiplies the spin-independent part of H [Eqs. (1) and (2)] and is usually taken to vanish initially. The projection operation defines a new reduced Hamiltonian (for the cell variables μ') of the same functional form H but with new, renormalized couplings

$$e^{H[K_0',K_\alpha',h_\alpha',\{\mu'\}]}=\mathrm{Tr}_\mu \prod_{\text{cells}} P_{\text{cell}}(\mu'|\{\mu\}) \times e^{H[K_0,K_\alpha,h_\alpha,\{\mu\}]}. \tag{6}$$

The projection property of P_{cell} guarantees that

$$Z[K_0',K_\alpha',h_\alpha']=Z[K_0,K_\alpha,h_\alpha]. \tag{7}$$

The number of cells is b^{-d} of the original number of spins N, so, invoking the thermodynamic limit

$$f_b\equiv\lim_{N\to\infty} N^{-1}\ln Z[K_0,K_\alpha,h_\alpha],$$

one finds the important bulk free energy relation

$$f_b[K_0,K_\alpha,h_\alpha]=b^{-d}f_b[K_0',K_\alpha',h_\alpha']. \tag{8}$$

Equation (6) defines[29] "recursion relations" connecting the old and new couplings

$$K'_\alpha = K'_\alpha[K_\beta, h_\beta], \quad h'_\alpha = h'_\alpha[K_\beta, h_\beta], \tag{9}$$

and

$$K'_0 = b^d K_0 + R[K_\beta, h_\beta]. \tag{10}$$

Once recursion relations are known, the calculation proceeds in a now-canonical manner: Fixed points are defined by $K^*_\alpha = K'_\alpha[K^*_\beta, h^*_\beta]$, $h^*_\alpha = h'_\alpha[K^*_\beta, h^*_\beta]$. The ordinary critical fixed point occurs at $h^*_\alpha = 0$, so the linear recursion matrix defined by linearization about the fixed point splits into even and odd parts

$$T^{\text{even}}_{\alpha\beta} \equiv \left.\frac{\partial K'_\alpha}{\partial K_\beta}\right|_{K^*, h^*}, \quad T^{\text{odd}}_{\alpha\beta} \equiv \left.\frac{\partial h'_\alpha}{\partial h_\beta}\right|_{K^*, h^*}. \tag{11}$$

The eigenvalues of T are written $\Lambda = b^y$. At the ordinary critical fixed point T^{even} and T^{odd} each have a single "relevant" eigenvalue ($y > 0$), which we denote y_t ("thermal") and y_h ("magnetic"), respectively. Corresponding eigenvectors are predominantly along the nearest-neighbor-coupling and magnetic field axes. This information in conjunction with (8) leads[22,23] to the bulk scaling relation (3) with $2 - \alpha = d/y_t$ and $\Delta = y_h/y_t$. Finally, the bulk free energy (not restricted to the critical region) may be calculated[23,25] by direct iteration of (8)–(10),

$$f_b[K_0, K_\alpha, h_\alpha] = \lim_{n\to\infty} K_0^{(n)} = K_0 + \sum_{n=0}^{\infty} b^{-d(n+1)} R[K_\beta^{(n)}, h_\beta^{(n)}]. \tag{12}$$

Generalization of (5)–(12) to the semi-infinite sample (1) is quite straightforward: Eqs. (5)–(7) continue to hold, subject to the reminder that couplings are no longer spatially homogeneous but now depend on distance from the $z = 0$ surface, i.e., $K_0(z), K_\alpha(z), h_\alpha(z)$. Under the reasonable proviso that all couplings go to uniform bulk values at distances from the surface greater than some finite[30] z_s [i.e., for $z > z_s, K_0(z) = K_0, K_\alpha(z) = K_\alpha, h_\alpha(z) = h_\alpha$], the bulk thermodynamic limit goes through unchanged and f_b is strictly independent of the surface couplings ($z < z_s$). There remains, however, a surface free energy, which is picked out by the limit[15]

$$f_s[K_0(z), K_\alpha(z), h_\alpha(z)] = \lim_{N,S\to\infty} S^{-1}\{\ln Z[K_0(z), K_\alpha(z), h_\alpha(z)] - N f_b[K_0, K_\alpha, h_\alpha]\} \tag{13}$$

(S is the number of surface spins) and depends on both surface and bulk couplings. Because the number of surface *cells* is $b^{-(d-1)}$ of the number of surface *spins*, the surface analog of (8) is

$$f_s[K_0(z), K_\alpha(z), h_\alpha(z)] = b^{-(d-1)} f_s[K'_0(z), K'_\alpha(z), h'_\alpha(z)]. \tag{14}$$

We now consider the inhomogeneous analog of the recursion relations (9) and (10). The key physical point here is that [despite the global appearance of (6)] the renormalized couplings are determined in a spatially local way, e.g., the renormalized magnetic field $(h'_a \mu'_a)$ belonging to a *specific* cell a depends appreciably only on the original couplings (K, h) within some *microscopic* distance z_0, i.e., only on couplings associated with the cell a and its nearby neighbors. We shall refer to z_0 as the "localization length." Its existence is attested to by the striking success of NvL calculations[22-25,31] based on small-cell clusters. This locality property is a feature of the recursion relations and in no way depends, for example, on the physical coherence length being small. Thus,

$$\begin{aligned} K'_\alpha(z') &= K'_\alpha[z', K_\beta(z), h_\beta(z)], \\ h'_\alpha(z') &= h'_\alpha[z', K_\beta(z), h_\beta(z)], \end{aligned} \tag{15}$$

and

$$K'_0(z') = b^{(d-1)} \sum_{n=0}^{b-1} K_0(bz' + n) + R[z', K_\beta(z), h_\beta(z)]. \tag{16}$$

Because of the spatial locality, the renormalized couplings at z' depend appreciably only on original couplings with $|z - bz'| \lesssim z_0$. When $bz' \gg z_0$ (deep in the bulk), the *form* of this dependence is independent of z'; however, for $bz' \lesssim z_0$ the proximity of the surface modifies the recursion relations and leads to *explicit* z' dependence, as indicated in (15) and (16). A simple example of such recursion relations is given in Sec. III.

Fixed-point *functions* are defined from (15), $K^*_\alpha(z') = K'_\alpha[z', K^*_\beta(z), h^*_\beta(z)]$, $h^*_\alpha(z') = h'_\alpha[z', K^*_\beta(z), h^*_\beta(z)]$. The ordinary critical fixed point has $h^*_\alpha(z) = 0$; however, $K^*_\alpha(z)$ will in general be z dependent, going to K^*_α (bulk) for large z but differing noticeably from its bulk value when z is less than the localization length z_0. The linear recursion matrix

$$\begin{aligned} T^{\text{even}}_{\alpha\beta}(z', z) &\equiv \left.\frac{\partial K'_\alpha(z')}{\partial K_\beta(z)}\right|_{K^*, h^*}, \\ T^{\text{odd}}_{\alpha\beta}(z', z) &\equiv \left.\frac{\partial h'_\alpha(z')}{\partial h_\beta(z)}\right|_{K^*, h^*} \end{aligned} \tag{17}$$

now depends on z and z'. When z and bz' are both much greater than z_0, then T depends only on $(z - bz')$; otherwise, there may be separate dependence on z and z'. Furthermore, when $|z - bz'| \gg z_0$, then $T = 0$. The schematic form of T (topological indices α, β will henceforth be suppressed)

is shown in Fig. 1.

Denote by $e(z)$ the right eigenvectors of $T(z',z)$. Because the nonzero[32] elements of $T(z',z)$ are above the diagonal for sufficiently large z, there are a finite number $n_s \sim z_0/(b-1)$ of eigenvectors which vanish in the bulk [$e(z)=0$ for $z>n_s$]. We shall refer to these as "surface" eigenvectors. They are associated with "surface" eigenvalues. The remaining eigenvectors (and eigenvalues) are not normalizable to unity and belong to the bulk. At the ordinary critical fixed point[33] T^{even} and T^{odd} each have one relevant ($y>0$) bulk eigenvector with eigenvalue $\Lambda^{\text{even}}=b^{y_t}$ and $\Lambda^{\text{odd}}=b^{y_h}$, respectively, agreeing precisely with the exponents defined after (11) for the corresponding *pure bulk* problem. These eigenvectors have the generic form[34] $e(z)=1$ for $z>n_s$, $e(z)=$ finite for $z\leq n_s$. Since these relevant bulk eigenvectors are not normalizable, the couplings in any finite number of surface layers (e.g., z_s) do not contribute finitely to the bulk scaling fields and so disappear from the bulk free energy (3), (8), and (12). Any relevant *surface* eigenvectors *will* contribute to the *surface* free energy (4) and (14). It is consistent with present evidence that T^{odd} has exactly one relevant surface eigenvector and T^{even} has none. We denote this relevant odd surface eigenvalue exponent y_{h_1}. The corresponding scaling field couples finitely to odd surface layer interactions [e.g., h_1 in Eq. (2)]. Combining this information with (14), one obtains

$$f_s(t,h,h_1)=b^{-(d-1)}f_s(b^{y_t}t,b^{y_h}h,b^{y_{h_1}}h_1), \tag{18}$$

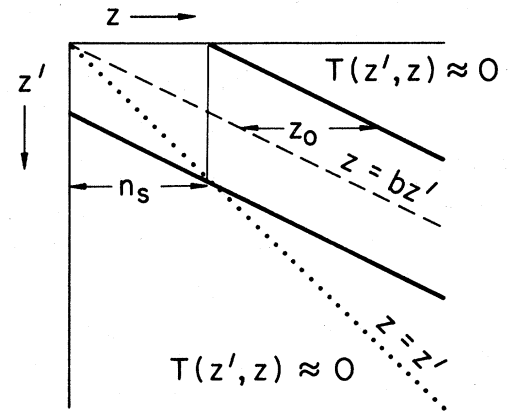

FIG. 1. Schematic form of the linear recursion matrix $T(z',z)$. T is infinite dimensional but is essentially zero outside of the diagonal region $|z-bz'|\sim z_0$. At the upper left T depends separately on z and z' because of the changed form of near-surface recursion relations. For $z\gg z_0$ (the localization length) T depends only on $(z-bz')$. The fact that nonzero elements are above the diagonal for $z>n_s$ divides the spectrum into surface and bulk parts.

where we follow the usual convention in denoting the even bulk, odd bulk, and odd surface scaling fields by t, h, and h_1, respectively. The scaling relation (4) follows from (18), with $2-\alpha_s=(d-1)/y_t$ ($\alpha_s=\alpha+\nu$) and $\Delta_1=y_{h_1}/y_t$. An explicit representation for the surface free energy (*not* restricted to the critical region) follows from (12)–(14) and (16):

$$f_s[K_0(z),K_\alpha(z),h_\alpha(z)]=\sum_{z=0}^{\infty}[K_0(z)-K_0]+\sum_{n=0}^{\infty}b^{-(d-1)(n+1)}\sum_{z'=0}^{\infty}\{R[z',K_\beta^{(n)}(z),h_\beta^{(n)}(z)]-R[K_\beta^{(n)},h_\beta^{(n)}]\}. \tag{19}$$

Equation (18) is the surface analog of (12). All couplings go to bulk values for large z; therefore, the layer sums converge and the free energy per surface spin is well defined.

III. SURFACE PROPERTIES FROM THE TWO-CELL CLUSTER APPROXIMATION

We describe in this section an exceedingly crude position-space renormalization-group calculation of some surface critical properties of the $d=2$ Ising model on the simple quadratic lattice. The lattice is divided into cells of four spins each ($b=2$), as pictured in Fig. 2. We assign the cell spin μ' according to "majority rule" by the projection

$$P_{\text{cell}}(\mu'|\{\mu\})=\frac{1}{2}\left[1+\mu'\,\text{sgn}\left(\sum_{i=1}^{4}\mu_i\right)\right], \tag{20}$$

$$\text{sgn}x=\begin{cases}1, & x>0,\\ 0, & x=0,\\ -1, & x<0,\end{cases}$$

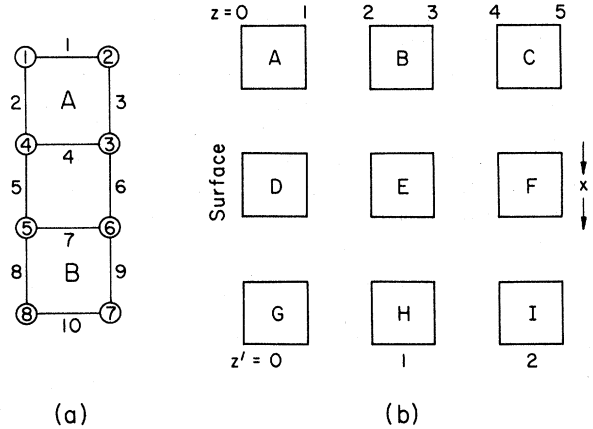

FIG. 2. Spin groupings for the two-cell cluster calculation on the simple quadratic Ising model. (a) The basic two-cell cluster for the transformations (21) and (22). (b) Spin cells for the semi-infinite lattice.

which allocates to $\mu' = +1(-1)$ all site-spin configurations with net positive (negative) moment and splits the configurations with net zero moment evenly between $\mu' = \pm 1$. Our recursion relations will be built from the recursion relations for the isolated two-cell cluster[35] shown in Fig. 2(a). Only magnetic fields and nearest-neighbor interactions can be generated in such a cluster, so there is no proliferation of further-neighbor and many-site interactions. The Hamiltonian for the two-cell cluster of Fig. 2(a) involves 26 independent variables: ten nearest-neighbor bonds $\{K_i\}_{i=1}^{10}$, eight magnetic fields $\{h_i\}_{i=1}^{8}$, and eight constant terms $\{K_{0i}\}_{i=1}^{8}$. Application of (6) yields a new coupling K'_{AB}, two new magnetic fields h'_A and h'_B, and a new constant term $(K'_{0A}+K'_{0B})$, according to cumbersome but straightforward formulas of the form

$$K'_{AB} = f_K(K_1, \ldots, K_{10}; h_1, \ldots, h_8) \tag{21}$$

and

$$h'_A = f_h(K_1, \ldots, K_{10}; h_1, \ldots, h_8). \tag{22}$$

In dealing with the bulk system,[22-25] one would at this point set $K_i = K, i = 1, \ldots, 10; h_i = h, i = 1, \ldots, 8$. The bulk critical fixed point is at $h = 0$ and

$$K^* = f_K(\{K^*\}; \{0\}), \quad \text{giving } K^*_{\text{bulk}} = 0.5689, \tag{23}$$

some 29% higher than Onsager's exact value[36] $K_{\text{Onsager}} = 0.440\,69\ldots$. The linear recursion matrices T^{even} and T^{odd} [Eq. (11)] reduce to single entries

TABLE II. Independent fixed-point derivatives of the transformations f_K and f_h [(21) and (22)]. Subscripts refer to labeling of Fig. 2(a). All derivatives are evaluated at the fixed point (23).

$a_1 = \frac{\partial f_K}{\partial K_1} = 0.0228$	$c_1 = \frac{\partial f_h}{\partial h_1} = 0.7472$
$a_2 = \frac{\partial f_K}{\partial K_2} = 0.1421$	$c_2 = \frac{\partial f_h}{\partial h_4} = 0.6748$
$a_3 = \frac{\partial f_K}{\partial K_4} = 0.2096$	$c_3 = \frac{\partial f_h}{\partial h_5} = 0.2112$
$a_4 = \frac{\partial f_K}{\partial K_5} = 0.4108$	$c_4 = \frac{\partial f_h}{\partial h_8} = -0.0015$

$$T^{\text{even}} = \left.\frac{\partial f_K}{\partial K}\right|_{K^*, h^*} = 2a_1 + 4a_2 + 2a_3 + 2a_4$$
$$= \Lambda^{\text{even}}_{\text{bulk}} = b^{y_t} = 1.8549, \tag{24}$$

$$T^{\text{odd}} = \left.\frac{\partial f_h}{\partial h}\right|_{K^*, h^*} = 2(c_1 + c_2 + c_3 + c_4)$$
$$= \Lambda^{\text{odd}}_{\text{bulk}} = b^{y_h} = 3.2634. \tag{25}$$

Table II defines notation for the derivatives. The corresponding bulk exponents, $y_t = 0.8913, y_h = 1.7064$, are to be compared with the exact values in Table I.

Inhomogeneous recursion relations for the pair couplings in the surface problem can be derived directly from (21):

$$\begin{aligned} K'_{\parallel}(z') = f_K(&K_\perp(2z'), K_\parallel(2z'), K_\parallel(2z'+1), K_\perp(2z'), K_\parallel(2z'), K_\parallel(2z'+1), K_\perp(2z'), K_\parallel(2z'), K_\parallel(2z'+1), K_\perp(2z'); \\ &h(2z'), h(2z'+1), h(2z'+1), h(2z'), h(2z'), h(2z'+1), h(2z'+1), h(2z')), \\ K'_\perp(z') = f_K(&K_\parallel(2z'), K_\perp(2z'), K_\perp(2z'), K_\parallel(2z'+1), K_\perp(2z'+1), K_\perp(2z'+1), K_\parallel(2z'+2), K_\perp(2z'+2), K_\perp(2z'+2), \\ &K_\parallel(2z'+3); h(2z'), h(2z'), h(2z'+1), h(2z'+1), h(2z'+2), h(2z'+2), h(2z'+3), h(2z'+3)). \end{aligned} \tag{26}$$

Note that the form differs for parallel orientation [e.g., EH in Fig. 2(b)] and perpendicular orientation [e.g., EF in Fig. 2(b)]. It is less clear how to formulate a recursion relation for the magnetic fields: The cell field at E in Fig. 2(b) may with equal logic be determined by applying (22) to the four two-cell clusters, ED, EF, EB, and EH. We make the symmetrical but *ad hoc* choice of averaging these four possibilities and write for the magnetic recursion relation

$$h'(z') = \tfrac{1}{4}[f_h(-\hat{z}) + f_h(+\hat{z}) + f_h(-\hat{x}) + f_h(+\hat{x})], \quad z' > 0 \tag{27}$$

in which the notation gives the direction of the appropriate two-cell axis. Equation (27) determines $h'(z')$ in terms of $K_\parallel(z)$ and $h(z)$, $2z' - 2 \leq z \leq 2z' + 3$, and $K_\perp(z)$, $2z' - 2 \leq z \leq 2z' + 2$. Equation (27) must be modified at the surface $z' = 0$, because the two-cell cluster in the $-\hat{z}$ direction is truncated. To allow for this, we simply set $K_5 = K_6 = 0$ [Fig. 2(a)] in (22) and call the result[37] $f_h^0 \equiv f_h(\ldots, K_5 = 0, K_6 = 0, \ldots)$. Then,

$$h'(z') = \tfrac{1}{4}[f_h^0(-\hat{z}) + f_h(+\hat{z}) + f_h(-\hat{x}) + f_h(+\hat{x})], \quad z' = 0. \tag{28}$$

Equations (26)–(28) are our realization of the general recursion relations (15). The difference between (27) and (28) is an example of the explicit z' dependence discussed after (16). The absence of a similar explicit z' dependence in (26) is a failure of our crude two-cell approximation. From the calculational point of view, however, this fail-

TABLE III. Surface and near-surface entries in the linear recursion matrices defined by (17) and (26)–(28). (a) T^{even}; (b) T^{odd}. $s = c_1 + c_2 + c_3 + c_4$; $c_0 = 0.7409$ and is explained in the text. Otherwise, notation follows Table II. The upper-left-hand matrix elements determine surface eigenvalues and eigenvectors (see text).

(a) $T^{\text{even}}(z', z)$

	$K_{\parallel}(0)$	$K_{\perp}(0)$	$K_{\parallel}(1)$	$K_{\perp}(1)$	$K_{\parallel}(2)$	$K_{\perp}(2)$	$K_{\parallel}(3)$	$K_{\perp}(3)$
$K'_{\parallel}(0)$	$2a_2 + a_4$	$2(a_1 + a_3)$	$2a_2 + a_4$	0	0	0	0	0
$K'_{\perp}(0)$	a_1	$2a_2$	a_3	$2a_4$	a_3	$2a_2$	a_1	0
$K'_{\parallel}(1)$	0	0	0	0	0	0	$2a_2 + a_4$	$2(a_1 + a_3)$
$K'_{\perp}(1)$	0	0	0	0	0	0	a_1	$2a_2$

(b) $T^{\text{odd}}(z', z)$

	$h(0)$	$h(1)$	$h(2)$	$h(3)$	$h(4)$	$h(5)$
$h'(0)$	$\frac{1}{2}(c_0 + c_1 + s)$	$\frac{1}{2}(c_0 + c_2 + s)$	$\frac{1}{2}c_3$	$\frac{1}{2}c_4$	0	0
$h'(1)$	$\frac{1}{2}c_4$	$\frac{1}{2}c_3$	$\frac{1}{2}(c_1 + c_2 + s)$	$\frac{1}{2}(c_1 + c_2 + s)$	$\frac{1}{2}c_3$	$\frac{1}{2}c_4$
$h'(2)$	0	0	$\frac{1}{2}c_4$	$\frac{1}{2}c_3$	$\frac{1}{2}(c_1 + c_2 + s)$	$\frac{1}{2}(c_1 + c_2 + s)$
$h'(3)$	0	0	0	0	$\frac{1}{2}c_4$	$\frac{1}{2}c_3$

ure has the great merit that it makes trivial the determination of the critical fixed point: The recursion relations (26) feel no *explicit* surface; $h^*(z) = 0$ solves (27) and (28) by symmetry. So, there is a critical fixed point[38] of the *full* recursion relations (26)–(28) at [see (23)],

$$K_{\parallel}^*(z) = K_{\perp}^*(z) = K_{\text{bulk}}^*, \quad h^*(z) = 0. \tag{29}$$

The fact that $K_{\parallel}^*(z)$, $K_{\perp}^*(z) \to K_{\text{bulk}}^*$, as $z \to \infty$ is quite general; the lack of z dependence near the *surface* is a consequence of the artificial simplicity of (26).

Linear recursion matrices for the recursion relations (26)–(28) at the fixed point (29) are defined by (17). The first few elements of these infinite matrices are shown in Table III. Notation follows Table II, with the addition that $c_0 = (\partial f_h^0 / \partial h_i)_{K^*, h^*} = 0.7409$ enters the top row of T^{odd} because of the special form (28) of the magnetic recursion relation at the surface [$h'(0)$]. With this exception the rows belonging to each $K'_{\parallel}(z')$, $K'_{\perp}(z')$, and $h'(z')$ look the same for $z' = 0, 1, 2, \ldots$, only translated successively to the right. Note that the rows of T^{even} all sum to $\Lambda_{\text{bulk}}^{\text{even}}$ (24), while (except again for $z' = 0$) those of T^{odd} sum to $\Lambda_{\text{bulk}}^{\text{odd}}$ (25). One easily verifies that the relevant bulk eigenvectors are

$$e_{\text{bulk}}^{\text{even}}(z) = 1, \quad z \geq 0 \text{ (belonging to } y_t),$$

$$e_{\text{bulk}}^{\text{odd}}(z) = \begin{cases} 0.956, & z = 0 \\ & \text{(belonging to } y_h) \\ 1, & z > 0 \end{cases} \tag{30}$$

[y_t and y_h are given in (24) and (25)]. The upper left-hand 2×2 submatrix $[K_{\parallel}(0), K_{\perp}(0)]$ of T^{even} and the corresponding 3×3 submatrix $[h(0), h(1), h(2)]$ of T^{odd} (see Table III) determine surface eigenvalues and surface eigenvectors (normalizable). Both the even (thermal) surface eigenvalues turn out to be irrelevant ($y = -0.4751, -1.9442$). Of the three odd (magnetic) surface eigenvalues two are irrelevant but one is relevant and has an eigenvector which couples very strongly into the surface field[39] $h(z = 0)$:

$$y_{h_1} = 0.6408, \quad e_{h_1} = \begin{cases} 1.00, & z = 0 \\ -5.16 \times 10^{-4}, & z = 1 \\ 0, & z > 1. \end{cases} \tag{31}$$

Our calculated magnetic surface exponent y_{h_1} is 28% above the exact value (Table I); however, our very crude approximation has proved adequate to reproduce correctly the qualitative features discussed in Secs. I and II. Better recursion relations for $K_{\parallel}$ and $K_{\perp}$ would lead to fixed-point couplings $K_{\parallel}^*(z)$ and $K_{\perp}^*(z)$ somewhat weaker at the surface than in the bulk. Such a change reduces the entries in the first few rows of T^{odd} and would certainly improve the accuracy of y_{h_1}.

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[15]More formally, one may define bulk and surface free energies in terms of a stack of n $(d-1)$-dimensional layers. This system has two free surfaces, so in the thermodynamic limit $(N\to\infty, n\to\infty)$ the total free energy goes as $N[f_b+(2/n)f_s]$. See Refs. 3 and 6.

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[26]We are stressing here the dimensionality associated with the infinite number of inequivalent layers. Even the bulk problem has (in principle) an infinite number of topologically different couplings.

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[28]K_α includes nearest- and further-neighbor pair couplings, etc.; h_α includes the usual magnetic field, plus three-spin couplings, etc. Although further-neighbor and many-spin interactions are included, they do not play a special role in what follows and will not be stressed in the notation.

[29]In practice a truncating approximation is necessary in order to make Eq. (5) tractable. See Refs. 22–25.

[30]This assumption is sufficient but not necessary. What is at issue is the existence of bulk and surface thermodynamic limits.

[31]Even in small- (NvL) cluster approximations it is striking how weakly a particular renormalized local coupling depends on original couplings outside its *immediate* neighborhood. See, e.g., the entries a_1 and c_4 in Table II.

[32]Strictly speaking the elements of the *exact* $T(z',z)$ are all nonzero; however, for $|z-bz'|>z_0$ their magnitudes fall off very rapidly. Strict vanishing *does* occur in finite-cluster approximations.

[33]In contrast to the ordinary critical transition (which is "driven" by the bulk) the *surface transition* (Refs. 1, 5, 16, 17) is controlled by a fixed point for which $K^*_{\text{bulk}}=0$, and $K^*(z)$ is only appreciable in the first few layers. One anticipates that at this "surface" fixed point there will be one even (thermal) and one odd (magnetic) eigenvalue, just characteristic of the bulk $(d-1)$-dimensional system.

[34]Recall that the topological indices α, β are being suppressed. The bulk eigenvector will still have topological dependence beyond $z=n_s$.

[35]In bulk calculations accuracy is often improved by using periodic boundary conditions, thus currently incorporating the coordination number of the lattice (which is important at low temperatures). However, periodicity seriously violates locality relations in small clusters and we choose *not* to use it.

[36]L. Onsager, Phys. Rev. 65, 117 (1944).

[37]This has the effect of rendering h'_A in (22) dependent *only* on the couplings and fields of cell A.

[38]One must verify numerically that there are no *other* critical fixed points of (26)–(28) in addition to (29).

[39]It is likely that the negative (but very small!) coupling into $h(z=1)$ is spurious. In a better approximation both $e_{h1}(z=1)$ and c_4 would presumably prove to be small but positive.