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Renormalization-group approach to the Ising model with a free surface

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We use simple position-space renormalization-group procedures involving only nearest-neighbor interactions to discuss the critical behavior of the ferromagnetically coupled semi-infinite Ising model with a free surface in two and three dimensions. In three dimensions for suitably enhanced surface couplings there are surface transitions and simultaneous surface-bulk transitions as well as the bulk transition. A phase diagram, critical exponents for the various transitions, and some representative magnetization profiles are calculated. Despite their simplicity, the renormalization transformations exhibit complete sets of fixed points for describing the various phase transitions and yield phase diagrams which are a significant improvement over mean-field theory. However, the calculated magnetization profiles show some unphysical features due to the finite cluster size on which the transformations are based.

I. INTRODUCTION

Position-space renormalization-group (RG) methods[1] have been used with remarkable success to calculate the bulk critical properties of Ising-like models. Švrakić and Wortis[2] have shown how the approach can be extended to systems with free surfaces. The Ising model with a free surface has experimental relevance in questions concerning surface critical behavior in magnetic systems and surface segragation phenomena[3] in binary alloys. We refer to Ref. 2 and to recent articles by Binder and Hohenberg[4,5] and Binder and Landau[6] for references to earlier theoretical work on this system based on other calculational methods and to experimental literature.

Švrakić and Wortis (SW)[2] have carried out a simple RG calculation of the bulk and surface critical properties for the semi-infinite ferromagnetically coupled Ising model with dimension $d=2$. In this paper we report results obtained for $d=3,2$ using a similar approach. The $d=3$ phase diagram is more complex than for $d=2$, since in addition to the bulk transition there are surface transitions and simultaneous surface-bulk transitions for suitably enhanced surface couplings. We compute a phase diagram, critical exponents for the various transitions, and some representative magnetization profiles. Our renormalization transformations, which are based on the lowest-order Niemeijer–Van Leeuwen cumulant and cluster expansions[1,7] and involve only nearest-neighbor interactions, are too simple to yield really reliable numerical predictions, but they exhibit a complete set of fixed points describing the various transitions and provide phase diagrams which are a significant improvement over mean-field theory. Renormalization transformations based on small clusters have been extremely successful in predicting the bulk critical properties of the Ising model.[1] Our calculations indicate that position-dependent properties are much more sensitive to this type of approximation. The magnetization profiles we obtain show some unphysical features due to the finite cluster size.

In Sec. II some results obtained using mean-field theory are reported. In Sec. III the renormalization transformations are described. In particular our reasons for considering other weight functions for the surface spins than the majority-rule weight function of Ref. 2 are given. In Sec. IV some numerical results for $d=3,2$ are presented and discussed.

II. MEAN-FIELD THEORY

We will be concerned with the three-dimensional semi-infinite Ising model with ferromagnetic nearest-neighbor interactions on a simple-cubic lattice. The Hamiltonian is given by

$$\mathcal{H}=-\sum_{\langle\alpha\beta\rangle} J_{\alpha\beta}\sigma_\alpha\sigma_\beta-\sum_\alpha H_\alpha\sigma_\alpha\ , \tag{1}$$

where the spin variables σ take the values ±1. Figure 1(a) shows the mean-field phase diagram as obtained by Binder and Hohenberg,[5] Lubensky and Rubin,[8] and others for the case that $J_{\alpha\beta}=J_{\|}$ if spins α and β are both on the surface, and $J_{\alpha\beta}=J_b$, otherwise. The surface enhancement Δ is defined by $J_{\|}=(1+\Delta)J_b$. T_b^c is the bulk critical temperature. Phase P is paramagnetic, whereas phase BF (bulk-ferromagnetic) has a bulk spon-

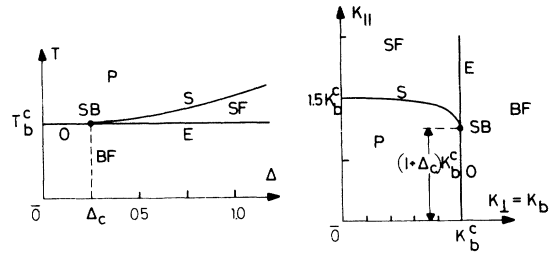

FIG. 1. Mean-field phase diagram for the Ising model with enhanced surface coupling $J_\parallel = (1+\Delta)J_b$. P, BF, and SF refer to the paramagnetic, bulk-ferromagnetic, and surface-ferromagnetic phases. O, E, and S represent lines of ordinary, extraordinary and surface transitions. SB denotes the multicritical point of the surface-bulk transition. $K_\parallel = J_\parallel/k_BT$, $K_b = J_b/k_BT$. $\bar{0}$ denotes the origin.

taneous magnetization. For Δ greater than a critical enhancement Δ_c, there is an additional phase SF (surface-ferromagnetic) with $T > T_b^c$ in which the system has a spontaneous magnetization at the surface which decays exponentially to zero bulk magnetization with increasing distance from the surface. Lubensky and Rubin[8] refer to the transitions along lines O, E, and S as the ordinary, extraordinary, and surface transitions, respectively. At the multicritical point[6] SB a simultaneous surface-bulk transition takes place (the $\lambda = \infty$ transition in the continuum approach of Lubensky and Rubin). For $T < T_b^c$ the surface magnetization is less, equal, or greater than the bulk magnetization for $\Delta < \Delta_c$, $\Delta = \Delta_c$, $\Delta > \Delta_c$, respectively. We refer to Refs. 5 and 8 for the mean-field critical exponents for the various transitions. In mean-field theory $\Delta_c = \frac{1}{4}$, and the branch of surface transitions approaches point SB as $T - T_b^c \sim (\Delta - \Delta_c)^2$.

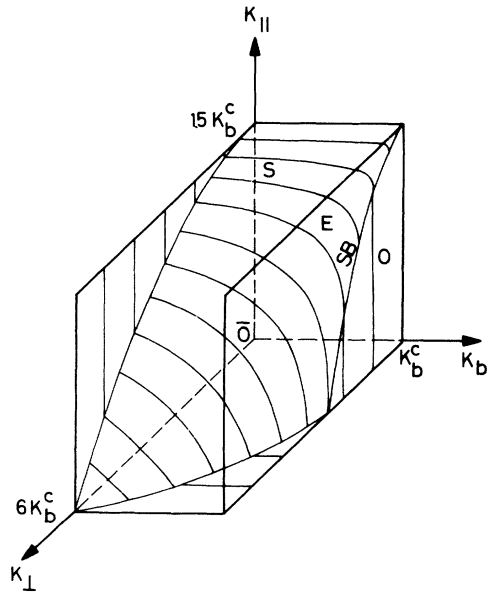

FIG. 2. Mean-field phase diagram in the variables $K_\parallel$, $K_\perp$, K_b. S denotes the critical surface for surface transitions. The line of surface-bulk transitions SB divides the plane of bulk transitions $K_b = K_b^c$ into surfaces O and E of ordinary and extraordinary transitions. $\bar{0}$ denotes the origin.

Figure 1(b) shows the mean-field phase diagram in the variables $K_\parallel = J_\parallel/k_BT$, $K_b = J_b/k_BT$. Note that the critical enhancement Δ_c is simply related to the coordinates $(K_\parallel, K_b) = (1+\Delta_c, 1)K_b^c$ of point SB.

The renormalization transformations we use involve three independent spin couplings $\vec{K} = (K_\parallel, K_\perp, K_b)$, where $K_\parallel$ is the coupling between nearest-neighbor surface spins, $K_\perp$ is the coupling between a spin in the surface layer and its nearest neighbor in the next layer, and all other nearest-neighbor couplings equal K_b. For comparison with the RG results we have calculated the mean-field phase diagram in the variables $\vec{K}$ with a procedure similar to that of Ref. 5. The mean-field equations for the layer magnetization m_i have the form

$$m_1 = \tanh(4K_\parallel m_1 + K_\perp m_2 + h_1)\,, \tag{2a}$$

$$m_2 = \tanh(K_\perp m_1 + 4K_b m_2 + K_b m_3 + h_2)\,, \tag{2b}$$

$$m_i = \tanh[K_b(m_{i-1} + 4m_i + m_{i+1}) + h_i]\,, \quad i > 2\,, \tag{2c}$$

where h_i denotes the field acting on each spin in layer i. The phase diagram obtained from Eqs. (2) is shown in Fig. 2. It is similar to Fig. 1(b) except that there are surfaces of ordinary, extraordinary, and surface transitions and a line of surface-bulk transitions. A larger variety of magnetization profiles is also possible than before. The bulk transition occurs for $K_b = K_b^c = \frac{1}{6}$. The critical surface for surface transitions satisfies

$$(1 - 4K_\parallel)[1 - (4 + e^{-1/\xi(K_b)})K_b] - K_\perp^2 = 0\,, \tag{3}$$

where the bulk correlation length ξ is given by

$$e^{-1/\xi(K_b)} = (1/2K_b)\{1 - 4K_b - [(1-2K_b)(1-6K_b)]^{1/2}\}. \tag{4}$$

This surface intersects the $K_\parallel$ axis at $K_\parallel = \frac{1}{4}$. Inserting $K_b = \frac{1}{6}$ into Eqs. (3) and (4), one sees that the line of surface-bulk transitions is given by

$$4K_\parallel + 6K_\perp^2 - 1 = 0\,. \tag{5}$$

Some qualitative shortcomings of the mean-field phase diagram are readily apparent. The critical surface S should intersect the planes $K_\perp = 0$ and $K_b = 0$ in Fig. 2 in straight horizontal lines $K_\parallel = \text{constant}$, since the surface layer has exactly the same critical coupling as a planar Ising model if $K_\perp = 0$ or $K_b = 0$. Although the first intersection is

horizontal, the second is not. That the critical surface goes to $K_{\parallel}=0$ as $K_{\perp}$ is increased is also an unphysical consequence of the mean-field approximation. According to mean-field theory a surface transition can always be produced by making $K_{\perp}$ sufficiently large, regardless of how weak the surface and bulk couplings are. However, the exact critical surface approaches a nonzero $K_{\parallel}$ as $K_{\perp}$ is increased with K_b held constant. In the limit $K_{\perp}\to\infty$ a spin in the surface layer is always in the same state as its nearest neighbor in the next layer, and the system is exactly equivalent to a system with one less layer and new couplings $K'_{\parallel}=K_{\parallel}+K_b$, $K'_{\perp}=K'_b=K_b$. In summary the exact critical surface for surface transitions $K_{\parallel}(K_{\perp},K_b)$ should satisfy the relations

$$K_{\parallel}(0,K_b)=K_{\parallel}(0,0)\,, \tag{6a}$$

$$K_{\parallel}(K_{\perp},0)=K_{\parallel}(0,0)\,, \tag{6b}$$

$$K_{\parallel}(\infty,K_b)=K_{\parallel}(K_b,K_b)-K_b\,, \tag{6c}$$

the second two of which are violated in mean-field theory.

III. THE RENORMALIZATION TRANSFORMATION

To construct a renormalization transformation we apply the method of Niemeijer and van Leeuwen[1,7] in the manner outlined in Ref. 2. As in Fig. 3(a) the simple cubic lattice is divided into cubic cells of eight site spins, to each of which a single cell spin is assigned. For all cells other than the layer of surface cells we use the majority-rule (MR)[9] weight function in assigning cell spins. For reasons discussed below, we have considered two modified weight functions for the surface cell as well as the MR weight function used in Ref. 2.

Nienhuis and Nauenberg[1,10] have derived formulas for calculating the bulk spontaneous magnetization with the RG approach. They show that a nonzero spontaneous magnetization implies a magnetic eigenoperator of the low-temperature fixed point with eigenvalue $y_h=d$, where d is the dimension of the system. To calculate the spontaneous magnetization it is advisable to choose the weight function relating the cell and site spins so that the ferromagnetic ground state is mapped upon itself. Then there is a corresponding low-temperature fixed point at $\vec{K}=\infty$, and the existence of the eigenvalue $y_h=d$ is guaranteed, even in an approximate calculation.

Since we are interested in surface transitions, which are basically two-dimensional, as well as bulk transitions, it is desirable to choose the surface weight function in such a way that any state in which all the surface spins are parallel is mapped onto a similar state. This allows for low-temperature surface fixed points with infinite surface couplings but other couplings finite and the magnetic eigenvalue[2] $y_{h_1}=d-1$ consistent with a spontaneous surface magnetization. The usual MR weight function[9] does not map a configuration with all the surface site spins parallel onto a configuration with all surface cell spins parallel and in the same direction since half of the weight of the configuration shown in Fig. 3(b) (and of the configuration with all spins reversed) is assigned to cell spin up and half to cell spin down. However, the following two modified surface weight functions (and others as well) do have this property:

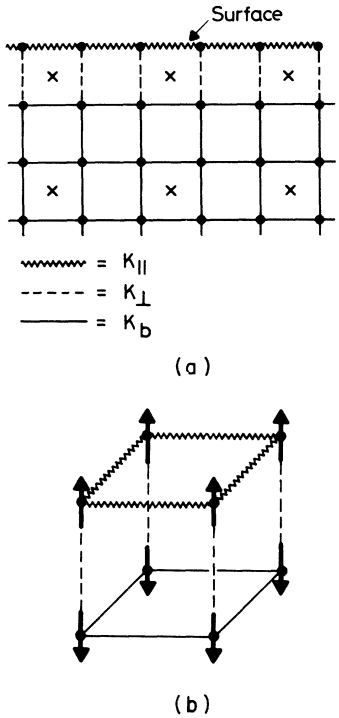

FIG. 3. (a) The rescaling procedure illustrated for $d=2$. The dots represent site spins and the crosses cell spins. For $d=2$ there are four site spins per square cell and for $d=3$ eight site spins per cubic cell. (b) The majority-rule weight function divides the weight of the illustrated configuration equally between cell-spin up and cell-spin down. Weight functions $M1$ and $M2$ assign cell-spin up to the configuration.

Weight function $M1$. $M1$ is the same as for MR except that the configuration of Fig. 3(b) is assigned to cell-spin up and the spin-reversed configuration to cell-spin down.

Weight function $M2$. The cell spin for the eight-site surface cell is determined by applying the MR to the four surface-site spins except if the sum of the four spins is zero. In this case the MR is applied to all eight site spins.

$M1$ represents perhaps the minimum modification to MR necessary for low-temperature surface

fixed points at $K_{\parallel}=\infty$ with the other couplings finite. If all couplings except $K_{\parallel}$ are zero and one sums over the site spins in the second layer, $M2$ reduces to the two-dimensional majority rule for square cells of four site spins, although it is not unique in this respect. We will see that the critical surface calculated with $M2$ satisfies Eq. (6b) exactly, whereas this is not the case with MR and $M1$.

In the lowest-order cumulant expansion[1,7] in which the interactions between cells are treated as first-order perturbations or in the two-cell cluster approximation of SW, the recursion relations in zero magnetic field have the form

$$K_{\parallel}'=f_{\parallel}(K_{\parallel},K_{\perp},K_b)\,, \tag{7a}$$

$$K_{\perp}'=f_{\perp}(K_{\parallel},K_{\perp},K_b)\,, \tag{7b}$$

$$K_b'=f_b(K_b)\,. \tag{7c}$$

Note that the bulk coupling transforms independently of $K_{\parallel}$ and $K_{\perp}$. Lengthy but straightforward explicit expressions for the functions f in Eqs. (7) can be constructed following Refs. 1, 2, and 7.

To compute magnetic critical exponents and the spontaneous magnetization, it is necessary to introduce infinitesimal fields h_i coupling to the spins in layer i. In the same approximations leading to Eqs. (7a)–(7c) the fields transform as

$$h_i'=\sum_j \frac{\partial h_i'(\vec{\mathrm{K}})}{\partial h_j}\,h_j\,, \tag{8}$$

where $\partial h_i'/\partial h_j$ has the form[11] shown in Table I. A recursion relation for the magnetization per spin m_i in layer i may be obtained by differentiating the transformation law for the extensive free energy $F_N(\vec{\mathrm{K}},\vec{\mathrm{h}})=F_{N'}(\vec{\mathrm{K}}',\vec{\mathrm{h}}')$ with respect to h_i and dividing by the number of spins per layer.

$$m_i(\vec{\mathrm{K}})=\sum_j T_{ij}(\vec{\mathrm{K}})m_j(\vec{\mathrm{K}}') \tag{9a}$$

$$T_{ij}(\vec{\mathrm{K}})=b^{-(d-1)}\frac{\partial h_j'(\vec{\mathrm{K}})}{\partial h_i}\,. \tag{9b}$$

The quantity $b^{-(d-1)}=\frac{1}{4}$, where $b=2$ is the length-rescaling factor, is the factor by which the number of spins per layer is reduced.

TABLE I. Matrix T_{ij}. Elements A_i, B_i, C_i depend on $K_{\parallel}$, $K_{\perp}$, K_b, whereas A, B, C only depend on K_b.

$$T_{ij}=\tfrac{1}{4}\frac{\partial h'_j}{\partial h_i}=\begin{bmatrix} C_1 & A_1 & 0 & 0 & 0 & \cdots \\ C_2 & B_2 & 0 & 0 & 0 & \cdots \\ B_3 & C_3 & A & 0 & 0 & \cdots \\ A_4 & C_4 & B & 0 & 0 & \cdots \\ 0 & B & C & A & 0 & \cdots \\ 0 & A & C & B & 0 & \cdots \\ 0 & 0 & B & C & A & \cdots \\ 0 & 0 & A & C & B & \cdots \\ 0 & 0 & 0 & B & C & \cdots \\ 0 & 0 & 0 & A & C & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \end{bmatrix}_{ij}$$

IV. RESULTS

A. $d=3$

Figure 4 shows the phase diagram and seven associated fixed points of Eqs. (7a)–(7c) obtained with a cluster calculation as in Ref. 2 but with weight function $M2$ for the surface spins. The critical surface for bulk transitions is the plane $K_b=K_b^*$. A point in the plane remains in the plane under application of the renormalization transformation. Points with $K_b<0$ and $K_b>0$ are mapped toward $K_b=0$ and $K_b=\infty$ by the transformation respectively.

The paramagnetic phase P with $K_b<K_b^*$, the bulk ferromagnetic phase BF with $K_b>K_b^*$, and the surface ferromagnetic phase SF with $K_b<K_b^*$ are

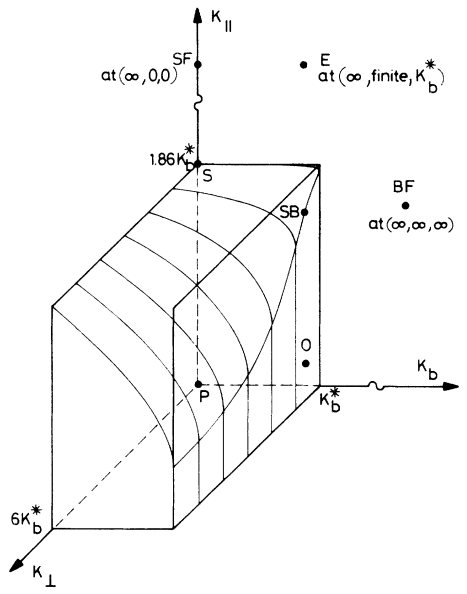

FIG. 4. RG phase diagram calculated with the cluster approximation and weight function $M2$ for the surface spins. The paramagnetic, bulk-ferromagnetic, and surface-ferromagnetic phases are mapped onto fixed points P, BF, and SF, respectively. The critical surfaces for the ordinary, extraordinary, and surface transitions are mapped onto fixed points O, E, and S, and the critical line of surface-bulk transitions is mapped onto fixed point SB.

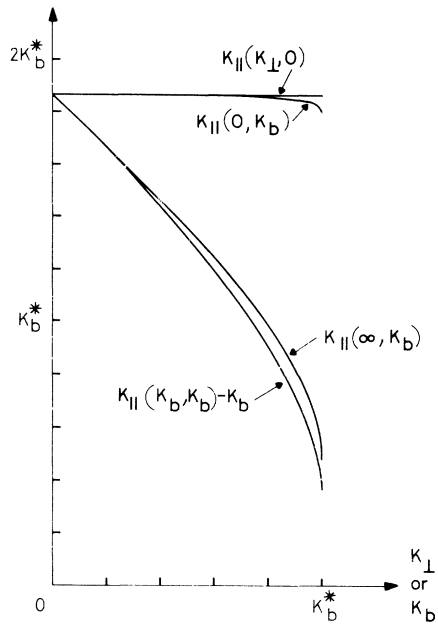

FIG. 5. RG results for the critical surface of surface transitions $K_{\parallel}(K_{\perp},K_b)$ obtained with the cluster approximation and weight function $M2$. The properties of an exact solution, Eqs. (6a)–(6c) are satisfied to a good approximation. In an exact solution the two upper curves would be replaced by a single horizontal line, and the lower two curves would coincide.

mapped onto the completely attractive fixed points P, BF, and SF, respectively. The critical surface for surface transitions is mapped onto fixed point S, which has a single repulsive eigenvector parallel to the $K_{\parallel}$ axis. The critical surfaces for the surface and bulk transitions intersect along the critical line of surface-bulk transitions. The line of surface-bulk transitions is mapped onto the fixed point SB, which with one repulsive eigenvector in the plane $K_b = K_b^*$ and one out of the plane has the topology of a multicritical[6] fixed point. The line of surface-bulk transitions divides the plane $K_b = K_b^*$ into critical surfaces for the ordinary and extraordinary transitions, which are mapped onto fixed points O and E, respectively. Both of these fixed points are completely attractive in the plane but are unstable, as is every point in the plane, with respect to perturbations away from the plane.

We have calculated the phase diagram and the fixed points with surface weight functions MR, $M1$, and $M2$ and with the first-order cumulant approximation[1,7] as well as the two-cell cluster approximation of Ref. 2. The general appearance of the phase diagram is the same in all the calculations. In the RG results the exact conditions Eqs. (6a)–(6c) are all satisfied to a good approximation, as shown in Figs. 4 and 5. In the calculations with $M2$ Eq. (6b) is satisfied exactly. With the other weight functions $K_{\parallel}(K_{\perp},0)$ decreases monotonically by less than 10% as $K_{\perp}$ goes from 0 to ∞. The RG phase diagram represents a considerable improvement over the mean-field phase diagram of Fig. 2 as far as the behavior for large $K_{\perp}$ is concerned.

Table II shows the location of the various fixed points in some of the cases we considered.[12] In Table III the RG results for several critical couplings and fixed-point values are compared with exact values or best estimates. The $K_{\parallel}$ coordinate of fixed-point S and the K_b coordinate of O, SB, or E yield values for the bulk critical couplings $K_c^{d=2}$, $K_c^{d=3}$ of the Ising model. The relevant eigenvalues y_t and y_h (we follow the notation of Ref. 2) of these fixed points determine the usual bulk critical exponents. Δ_c, the critical enhancement for the case $J_{\perp} = J_b$, can readily be determined from the intersection of the phase diagram with the plane $K_{\perp} = K_b$, as indicated in Fig. 1b. The eigenvalue y_{h_1} describes the instability of a fixed point with respect to a surface magnetic field.[2]

We refer to Ref. 2 for a detailed discussion of the relationship between the eigenvalues y and the singularities of the free energy. For the ordinary transition the singular part of the surface free energy is found to have the form

TABLE II. Coordinates $(K_{\parallel},K_{\perp},K_b)$ of the various fixed points. MR, $M1$, and $M2$ denote the weight function of the surface cells.

		Cluster, MR	Cluster, $M1$	Cluster, $M2$	Cumulant, $M2$
P	Paramag. phase	(0, 0, 0)	(0, 0, 0)	(0, 0, 0)	(0, 0, 0)
BF	Bulk ferromag. phase	(∞,∞,∞)	(∞,∞,∞)	(∞,∞,∞)	(∞,∞,∞)
SF	Surface ferromag. phase	(1.20, 0, 0)	$(\infty, 0, 0)$	$(\infty, 0, 0)$	$(\infty, 0, 0)$
S	Surface transition	(0.854, 0, 0)	(0.665, 0, 0)	(0.569, 0, 0)	(0.519, 0, 0)
O	Ordinary transition	(0.305, 0.305, 0.305)	(0.262, 0.293, 0.305)	(0.0937, 0.186, 0.305)	(0.0925, 0.186, 0.298)
SB	Surface-bulk transition	(0.340, 0.306, 0.305)	(0.381, 0.290, 0.305)	(0.481, 0.176, 0.305)	(0.446, 0.175, 0.298)
E	Extraordinary transition	(1.95, 0.332, 0.305)	$(\infty, 0.228, 0.305)$	$(\infty, 0.228, 0.305)$	$(\infty, 0, 0.298)$
E'	Extra fixed point of cluster $M1$, cluster $M2$	...	$(\infty, 0, 0.305)$	$(\infty, 0, 0.305)$	...

TABLE III. Critical couplings and relevant eigenvalues of the various transitions for $d=3$. MR, $M1$, and $M2$ denote the weight function of the surface cell.

	Cluster, MR	Cluster, $M1$	Cluster, $M2$	Cumulant, $M2$	Exact value or best estimate
$K_c^{d=3}$	0.305	0.305	0.305	0.298	0.222
$K_c^{d=2}$	0.854	0.665	0.569	0.519	0.441
Δ_c	0.114	0.215	0.357	0.307	0.6 ± 0.1 [a]
$y_t^{d=3}$	1.21	1.21	1.21	1.25	1.56 ± 0.04
$y_h^{d=3}$	2.19	2.19	2 19	2.79	2.50 ± 0.02
$y_t^{d=2}$	0.462	0.972	0.891	1.01	1
$y_h^{d=2}$	1.84	1.73	1.66	2.15	1.875
$y_{h_1}^{O}$	1.13	1.04	0.791	0.557	1.0 ± 0.2 [b]
$y_{t_1}^{SB}$	0.082 [c]	0.28 [c]	0.72 [c]	0.79 [c]	...
$y_{h_1}^{SB}$	1.21	1.33	1.56	1.97	...
$y_{h_1}^{E}$	1.98	2	2	2	...

[a] Reference 5.
[b] Estimated from Ref. 5 using Eq. (12b).
[c] The last significant figure shown is uncertain by ± 2.

$$f_s^O(t,h,\tilde{h}_1) = t^{(d-1)/y_t}\mathcal{F}_O\left(\frac{h}{t^{y_h/y_t}}, \frac{\tilde{h}_1}{t^{y_{h_1}^O/y_t}}\right), \tag{10}$$

where t is the relevant reduced termperature variable and h is the bulk magnetic field. y_t and y_h represent the relevant bulk eigenvalues for $d=3$. The relevant surface field $\tilde{h}_1$ is a function of h_1, h_2 and h in our approximation.

At the multicritical[6] fixed point SB there is an additional relevant eigenvector in the plane $K_b = K_b^*$ with eigenvalue $y_{t_1}^{SB}$ corresponding to perturbations in $K_\parallel$ and $K_\perp$ away from the line of surface-bulk transitions. Denoting the corresponding relevant variable by t_1 one finds the following form for the singular part of the surface free energy:

$$f_s^{SB}(t,t_1,h,\tilde{h}_1) = t^{(d-1)/y_t}\mathcal{F}_{SB}\left(\frac{t_1}{t^{y_{t_1}^{SB}/y_t}}, \frac{h}{t^{y_h/y_t}}, \frac{\tilde{h}_1}{t^{y_{h_1}^{SB}/y_t}}\right). \tag{11}$$

Formulas which express the critical exponents in terms of the y's and numerous scaling relations between the critical exponents follow from Eqs. (10) and (11). For example, using the definitions

$$C_s \sim \frac{\partial^2 f_s}{\partial t^2} \sim t^{-\alpha_s}, \quad m_1 \sim \frac{\partial f_s}{\partial h_1} \sim t^{\beta_1}, \quad m_s \sim \frac{\partial f_s}{\partial h} \sim t^{\beta_s},$$

$$\chi_{11} \sim \frac{\partial^2 f_s}{\partial h_1^2} \sim t^{-\gamma_{11}}, \quad \chi_1 \sim \frac{\partial^2 f_s}{\partial h_1 \partial h} \sim t^{-\gamma_1}, \quad \chi_s \sim \frac{\partial^2 f_s}{\partial h^2} \sim t^{-\gamma_s}$$

and expressions[1,2] for the bulk exponents in terms of y_t and y_h, and remembering that $\tilde{h}_1$ depends on both h_1 and h, we deduce such relations from Eqs. (10) and (11) as

$$\alpha_s^{O,SB} = 2 - (d-1)/y_t^{d=3}, \tag{12a}$$

$$\beta_1^{O,SB} = (d - 1 - y_{h_1}^{O,SB})/y_t^{d=3}, \tag{12b}$$

$$\gamma_{11}^{O,SB} = (2y_{h_1}^{O,SB} - d + 1)/y_t^{d=3}, \tag{12c}$$

and

$$\alpha_s^{O,SB} = \alpha + \nu, \tag{13a}$$

$$\beta_s^{O,SB} = \min(\beta_1^{O,SB}, \beta - \nu) = \beta - \nu, \tag{13b}$$

$$\gamma_1^{O,SB} = \gamma_{11}^{O,SB} + \beta_1^{O,SB} - \beta_s^{O,SB}, \tag{13c}$$

$$\gamma_s^{O,SB} = \max(\gamma_{11}^{O,SB}, \gamma + \nu) = \gamma + \nu. \tag{13d}$$

In Eqs. (13a)–(13d) the exponents α, β, γ, and ν represent the bulk critical exponents for $d=3$. All the scaling laws for the ordinary transition which follow from Eq. (10) are consistent with phenomenological scaling theories.[5,13,14] For the case of the SB transition Eqs. (13b)–(13d) contradict the exponent relations $\beta_s^{SB} = \beta^{d=2} - \nu^{d=3}$ and $\gamma_1^{SB} = \gamma_{11}^{SB} = \gamma^{d=2}$, $\gamma_s^{SB} = \gamma^{d=2} + \nu^{d=3}$ proposed in Refs. 5 and 6 on the basis of a high temperature series analysis. Additional series and Monte Carlo results would be useful in clarifying this discrepancy. In a RG analysis such as ours an exact scaling relation between the surface-bulk exponents and the bulk exponents for $d=2$ and 3 is not impossible but would be surprising, since the surface-bulk exponents and the $d=2$ bulk exponents are determined by quite different fixed points SB and S, respectively. Using standard arguments[6,15] one can show that the critical surface for surface transitions has the asymptotic form $t_1 \sim t^{\Phi}$ on ap-

proaching the line of surface-bulk transitions $t_1 = t = 0$, where the crossover exponent ϕ is given by

$$\phi = y_{t_1}^{SB}/y_t^{d=3}. \tag{14}$$

This behavior is consistent with the infinite slope $\partial K_{\|}/\partial K_b$ of the critical surface of surface transitions as K_b approaches K_b^*, which is evident in Figs. 1, 2, and 4. In mean-field theory $\phi = \frac{1}{2}$, as mentioned in Sec. II. At the surface-bulk transition, the surface magnetization is characterized by exponents β_1^{SB} and $\hat{\beta}_1^{SB} = \beta_1^{SB}/\phi$, depending on whether the line of surface-bulk transitions is approached along a t or t_1-like direction,[6,15] respectively.

As mentioned in Sec. III and discussed more explicitly below, the eigenvalue $y_{h_1}^E = d - 1$ is consistent[10] with a nonzero surface magnetization at the extraordinary transition, i.e. $\beta_1^E = 0$. Calculating the leading corrections to the constant value on approaching the transition temperature involves other details of the renormalization transformation besides the eigenvalues and eigenvectors, and we have not carried out a complete analysis. However, our transformations appear to be consistent with the mean-field result of Ref. 8, according to which the magnetization at the surface and its first temperature derivative are continuous at the extraordinary transition temperature. Intuitively, one would expect a fairly smooth temperature dependence of the surface magnetization and nondivergent[16] susceptibilities χ_{11} and χ_1, as found in mean-field theory, in an exact solution. Since the surface transition takes place at a higher temperature, the extraordinary transition takes place in an effective field extending roughly a bulk correlation length into the sample, which weakens the singularities in the surface free energy.

Since the RG bulk critical couplings and eigenvalues in Table III show sizeable deviations from the accepted values and depend rather sensitively on the choice of weight function, the numerical predictions for the surface quantities should not be taken too seriously. All the values of Δ_c we calculate are smaller than the series estimate[5] of 0.6 ± 0.1. It is encouraging that our values of $y_{h_1}^O$ are not wildly inconsistent with the value 1.0 ± 0.2 obtained using Eq. (12b) from estimates of β_1^O reviewed in Ref. 5. We have already mentioned a discrepancy between Refs. 5 and 6, and our scaling-law analysis in the case of $y_{h_1}^{SB}$. We know of no series estimates of $y_{t_1}^{SB}$. Determining the exponents of the surface-bulk transition experimentally would be very difficult since precise adjustment of the ratios of the coupling constants would be required.

Magnetization profiles may be calculated with an iterated form of Eq. (9a)

$$m_i(\vec{K}^{(0)}) = \sum_j [T(\vec{K}^{(0)})T(\vec{K}^{(1)}) \cdots T(\vec{K}^{(n)})]_{ij} m_j(\vec{K}^{(n+1)}) \tag{15}$$

The number of iterations n is chosen large enough so that $m_i(\vec{K}^{(n+1)})$ may be replaced by its fixed-point value $m_i(\vec{K}^{(\infty)}) = m_i(\vec{K}^*)$ to a high degree of numerical accuracy. The fixed point magnetization satisfies Eq. (9a) in the form

$$m_i(\vec{K}^*) = \sum_j T_{ij}(\vec{K}^*) m_j(\vec{K}^*). \tag{16}$$

From Eq. (16) it is clear that $T_{ij}(\vec{K}^*)$ must have eigenvalue 1 if the fixed point $\vec{K}^*$ is associated with a nonzero magnetization.

At fixed points BF, SF, and E one expects a nonzero magnetization. With our RG transformations T_{ij}^* does indeed have eigenvalue 1 at fixed point BF, where all the couplings are infinite, and the eigenvector has the expected form $m_i^* = 1$ for all i, corresponding to a completely saturated magnetization. With weight functions $M1$ and $M2$ the fixed points SF and E have coordinate $K_{\|}^* = \infty$, and $y_{h_1} = d - 1$. Using Eq. (9b) and the definition of y_{h_1} as the largest magnetic surface eigenvalue, one sees that the maximum surface eigenvalue of T_{ij}^* is $b^{y_{h_1}-(d-1)} = 2^{y_{h_1}-2}$. Thus with weight functions $M1$ and $M2$ T_{ij}^* does have the surface eigenvalue 1 at fixed points SF and E necessary for a nonzero surface magnetization.[17] With weight function MR a difficulty referred to in the previous section is encountered: Fixed points SF and E have finite rather than infinite values of $K_{\|}^*$, and y_{h_1} is slightly less than 2. Thus, the maximum surface eigenvalue of T_{ij}^* is slightly less than 1, and straightforward application of Eqs. (15) and (16) leads to the unphysical result of a zero surface magnetization in the SF phase or on the E critical surface. For this reason, we prefer weight functions $M1$ and $M2$ for approximate calculation. The results of an exact calculation would, of course, be independent of the choice of the weight function.

Typical magnetization profiles for enhanced and weakened surface couplings, calculated using Eq. (15) and the cluster approximation,[18] are shown in Figs. 6(a)–6(b). The temperature is just below the bulk critical temperature. For the SF phase and weight functions $M1$, $M2$ typical profiles are similar to Fig. 6(a) except that the bulk magnetization is zero.

A disconcerting unphysical feature of the profiles is the presence of plateaus of $2, 4, 8, 16, \ldots$ layers, which are clearly associated with the rescaling procedure. The plateaus arise in repeated multiplications with the matrix T_{ij} in Eq. (15) because the elements A_i, A, B_i, B (see Table I) are much smaller than the elements C_i, C. In the li-

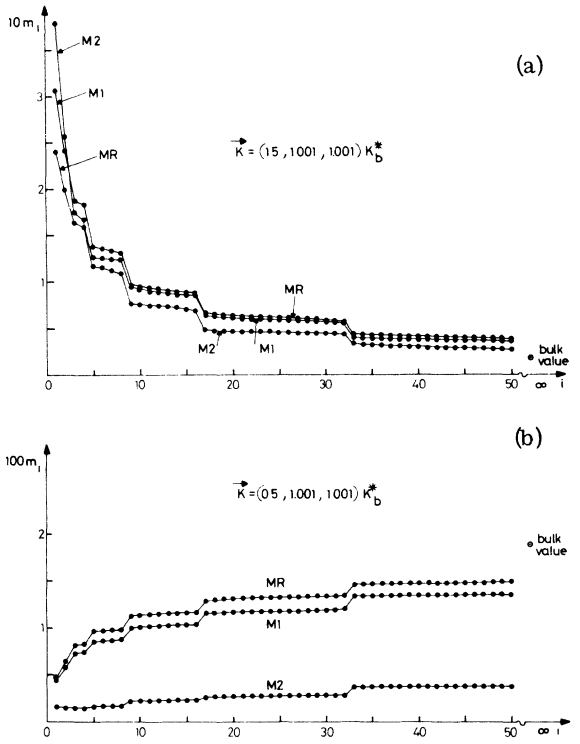

FIG. 6. Magnetization profiles for enhanced and weakened surface couplings calculated with the cluster approximation and weight functions MR, $M1$, and $M2$. The magnetizations of the first 50 layers and the asymptotic bulk value are shown. K_b^* denotes the bulk critical coupling.

mit in which only the elements C_i, C are nonzero, all the layer magnetizations within a plateau are identical.

Renormalization transformations which include only the short-range interactions between small clusters of block spins have been remarkably successful in calculations of bulk critical properties.[1] This suggests that short-range interactions would turn out to be the dominant interactions in an exact calculation of the fixed point associated with a bulk transition. An important question is whether approximations based on small clusters can also be used to calculate magnetization profiles and other spatially inhomogeneous quantities[19] realistically or whether such quantities will always bear an unphysical imprint of the small cluster.

A plausible ansatz for the magnetization profile just below the bulk transition temperature has the form

$$m_i = t^{\beta} J(i/\xi), \tag{17a}$$

$$J(x) \to \text{constant}, \quad x \gg 1, \tag{17b}$$

$$J(x) \to x^{(\beta_1-\beta)/\nu}, \quad x \ll 1, \tag{17c}$$

The limiting forms insure the crossover from surface exponent β_1 to bulk exponent β at a distance of the order of a bulk correlation length from the surface. The ansatz is consistent[20] with the scaling law $\beta_s^{O,SB} = \beta - \nu$, Eq. (13b), which our RG analysis predicts at both the ordinary and surface-bulk transitions. In mean-field theory[8] $J(i/\xi)$ approaches its large-argument limit with corrections which decay exponentially with characteristic length ξ.

The small number of nonzero elements of the matrix T_{ij} in Table I stems from the fact that only nearest-neighbor interactions between the cell spins are included. A matrix with this form is consistent with the plateau structure discussed above. However, for i well away from the surface and m_i slowly varying, the transformation law for the magnetization [Eq. (9a)] is compatible[21] with any ansatz of the form of Eq. (17a). We have addressed the question whether for suitable choices of A, B, and C the matrix can be made consistent with an asymptotic exponential decay with characteristic length ξ. Substituting exponential profiles for $m_i(\vec{K})$ and $m_i(\vec{K}')$ into Eq. (9a), one finds that the following conditions must be satisfied

$$\xi(K_b') = \tfrac{1}{2}\xi(K_b), \tag{18a}$$

$$Q = e^{-1/\xi(K_b)} = \frac{A(K_b) + C(K_b)Q^2 + B(K_b)Q^4}{B(K_b) + C(K_b)Q^2 + A(K_b)Q^4}. \tag{18b}$$

Equation (18b) determines ξ as a function of K_b. For a nonlinear weight function,[1] the function $\xi(K_b)$ obtained by solving Eq. (18b) and the transformation law Eq. (7c) for K_b will not be consistent with (18a) in general. For a linear weight function[1,22,23] Eq. (18a) is satisfied automatically. However, it still is not true that a physically reasonable exponential profile is consistent with arbitrary functions A, B, C of K_b; for example, that ξ be zero at $K_b = 0$ or $K_b = \infty$ and that ξ diverge as the critical value of K_b is approached restrict the K_b dependence of A, B, C. An additional problem with linear transformations is that a variable parameter in the transformation[1,22,23] must be adjusted differently at the critical fixed point and at the ferromagnetic fixed point. No single choice of the parameter is consistent with both a nonzero value of $d - 2 + \eta$ and a nonzero magnetization. The discussion of Eq. (18a) and (18b) can be generalized to larger clusters and to exponential functions modulated by a power law with similar conclusions about the difficulty of describing the magnetization profile correctly with a finite-cluster RG transformation.

To gain further insight into the problem of calculating the magnetization profile with an approximate renormalization transformation, we have found it useful to consider a one-dimensional Ising chain with a single magnetic field applied to spin

TABLE IV. Critical coupling and relevant eigenvalues for $d=2$. MR, $M1$, and $M2$ denote the weight function of the surface cell.

	Cluster, MR	Cluster, $M1=M2$	Exact value
Fixed-point O	(0.569, 0.569, 0.569)	(0.408, 0.465, 0.569)	
$K_c^{d=2}$	0.569	0.569	0.441
$y_t^{d=2}$	0.891	0.891	1
$y_h^{d=2}$	1.71	1.71	1.875
$y_{h_1}^{d=2}$	0.641	0.609	0.500[a]

[a] Reference 29.

1 at the end of the chain. The exact profile, which is exponential, is given by $m_i=(\tanh h_1)(\tanh K)^{i-1}$. This result can readily be reproduced with an exact decimation transformation,[24,25] which, as is well known, introduces no new couplings in addition to the nearest neighbor coupling. The associated matrix T_{ij} has a simple structure with no more than three nonzero elements per row. With the majority-rule weight function and two site spins per cell, neither the cumulant nor the cluster expansion[1,7] of Niemeijer and van Leeuwen are exact in any finite order in one dimension. Both generate interactions of increasing complexity between the cells in higher orders. The magnetization profiles generated for the chain using Eq. (15) and the first-order cumulant transformation show a plateau structure with a decay which is much slower than exponential. In the limit of small K, m_i is exact to first order in K, since the first-order cumulant expansion is exact in this order. However, for i arbitrarily large one finds contributions to m_i of order K^2. To obtain the exact result $m_i \sim K^{i-1}$ as i increases, the cumulant expansion must be carried out to increasingly high orders. The lowest-order Niemeijer–van Leeuwen cumulant expansion and presumably the cluster expansion as well would appear to be a rather poor starting point for calculating a realistic magnetization profile. We note that second- and third-order calculations of bulk properties[26-28] reveal at best a slow convergence of the cumulant expansion.

B. $d=2$

In the two-dimensional semi-infinite Ising model with a free surface no surface transitions take place at finite temperatures, since such a transition would be essentially one dimensional. Our RG calculations are consistent with this exact result whereas mean-field theory is not. The only transition the system exhibits is the ordinary transition, for which the exact[29] result $y_{h_1}=\frac{1}{2}$ is known. In Table IV the results of the cluster calculation with weight function $M1=M2$ (the two weight functions are identical for a square cell of four site spins) are compared with the majority-rule results of Ref. 2. For weight function $M1=M2$ there is a slight improvement in the value of y_{h_1}, which, however, should not be regarded as very significant in view of the sizeable deviations of y_{h_1} and the bulk critical quantities from their exact values.

Note added in proof. In important recent work A. J. Bray and M. A. Moore [Phys. Rev. Lett. 38, 1046 (1977); University of Manchester preprint to be published] have calculated the surface critical exponents to first order in $\epsilon=4-d$ and have proposed scaling relations relating most of the surface critical exponents to bulk exponents. For comparison with our calculated values in Table III we include some of their results here: For the ordinary transition $y_{h_1}^{O}=\frac{1}{2}(d-y_t^{d=3})=0.72\pm0.02$. For the surface-bulk transition $y_{t_1}^{SB}=y_t^{d=3}-1=0.56\pm0.04$, $y_{h_1}^{SB}=2-\frac{1}{3}\epsilon+O(\epsilon^2)=1.667$.

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[11]The matrix in Table I is somewhat more complicated than the corresponding expression in Ref. 2 since we have not restricted our attention to the subspace $K_{\|} = K_{\perp} = K_b$ and have considered other weight functions besides MR for the surface spins.
[12]The cluster calculations with $M1$ and $M2$ show an extra fixed point E' with coordinates $(\infty, 0, K_b^*)$ not found in the cumulant results. There is no finite value of $K_{\|}$ which maps onto E'. All trajectories in the plane $K_b = K_b^*$ leaving E' go to E. Near E' $K_1' = \lambda_{\perp} K_{\perp}$, where $\lambda_{\perp} = 1.07$. We suspect that the existence of two fixed points E and E' is an unphysical artifact of the cluster approximation for weight functions $M1$ and $M2$ and that there should be a single fixed point $E = E'$ just as one finds with the cumulant expansion. (This is almost the case. If one looks for fixed points of Eqs. (7a) and (7b) as a function of K_b, one finds that E and E' merge for K_b only 3% less than K_b^*. For smaller values of K_b only a single attractive fixed point with coordinates $K_{\|} = \infty$, $K_{\perp} = 0$ remains). Both the cumulant and the cluster transformations with $M1$ and $M2$ also have a fixed point G at $(\infty, 0, \infty)$ unstable with respect to perturbations in $K_{\perp}$. With a fixed point E at $(\infty, 0, K_b^*)$ attractive with respect to perturbations in $K_{\perp}$ and an attractive fixed point at (∞, ∞, ∞) an additional fixed point such as G is necessary for topological reasons.
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[17]Where fixed points SF, E, and E' in Table II have coordinates $K_{\|}^* = \infty$ and $K_{\perp}^* = 0$, the eigenvectors of T_{ij}^* have the expected form $m_1^* = 1$; $m_i^* = 0$, $i \neq 1$. In the cluster calculation of fixed point E with weight functions $M1$ and $M2$, $K_{\perp}^* \neq 0$. Here m_i^* decreases monotonically with i from the value 1 for the surface layer and shows unphysical steps similar to those in Figs. 6(a)–6(b). For step n, $m_{2^n}^* \sim 2^{n(\beta_1^E - \beta)/\nu}$, which is consistent with a plausible ansatz, Eqs. (17a)–(17c), for the magnetization profile.
[18]In the cumulant expansion the maximum eigenvalue of the matrix T_{ij} exceeds 1 in certain regions of $\vec{K}$ space, and straightforward application of Eq. (15) may lead to an m_i greater than the maximum possible value 1. This problem does not occur in the cluster calculation.
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[21]For i well away from the surface and slowly varying, Eqs. (9a) and (9b) take for form $m_i(t) \approx b^{-\beta/\nu} m_{i/b}(b^{1/\nu} t)$, where $y_t = \nu^{-1}$, $\xi \sim t^{-\nu}$ and in our approximation $A + B + C = b^{y_h - d} = b^{-\beta/\nu}$. This scaling equation for m_i is compatible with any ansatz with the form of Eq. (17a).
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