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M. P. Nightingale
University of Rhode Island, nightingale@uri.edu

H. W.J. Blöte

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Universality of surface correlation functions in three-dimensional models

M. P. Nightingale
Department of Physics, University of Rhode Island, Kingston, Rhode Island 02881

H. W. J. Blöte
Laboratorium voor Technische Natuurkunde, Technische Universiteit Delft, Postbus 5046, 2600 GA, Delft, The Netherlands
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Universality of surface critical behavior with respect to surface enhancement is studied for $O(n)$ models with $n = 1$ (Ising), $n = 2$ (planar rotor), and $n = 3$ (Heisenberg) on simple-cubic lattices. Finite-size methods are employed to estimate surface critical exponents for ordinary surface criticality. In addition, it is shown that universal scaling functions, independent of surface enhancement, can be constructed with all nonuniversal features of the finite-size scaling function of the spin-spin surface correlation functions incorporated in (1) a metric factor and (2) an irrelevant scaling field associated with the surface coupling strength.

I. INTRODUCTION

In real systems, the bulk critical behavior is modified by the presence of surfaces. For instance, in magnetic systems the correlation function between two spins separated by a distance r on the surface is known to decay with an exponent that differs from the bulk exponent. A further modification of the surface critical behavior may occur when the surface couplings are enhanced sufficiently to produce a surface-bulk tricritical point, which marks the onset of surface ordering even in the absence of bulk ordering. For a review of these phenomena, see Ref. 1.

Here we focus on the ordinary surface critical behavior in the absence of strong surface couplings. We investigate three universality classes containing the three-dimensional $O(1)$ (Ising), $O(2)$ (planar rotor), and $O(3)$ (Heisenberg) models. In particular, we are interested in the magnetic exponents describing the surface critical behavior, and in universal scaling functions describing the correlations in and near surfaces. The main issue addressed in this paper is the universality of these scaling functions with respect to surface enhancement.

Thus far, surface exponents have been determined by means of ϵ expansions,[2] by series expansions,[3] and by Monte Carlo simulations.[4] In the latter analysis of the $O(2)$ model by Landau *et al.*, systems were considered that do not map onto each other under scaling transformations and this may be one of the reasons why the data collapse of the surface layer magnetization was not completely satisfactory. In the present work, we avoid this problem by restricting ourselves to congruent systems. In addition, we perform a study of the corrections to scaling.

For our computations we employ a standard Monte Carlo method. The computations were done at the estimated critical points taken from the literature, a brief summary of which follows. For the Ising model, most Monte Carlo–based analyses[5–12] yield values near $K_c = 0.221653$ with quoted uncertainties of about 1 to a few times 10^{-6}. This value is somewhat larger than the preferred values given by Liu and Fisher[13] on the basis of series expansions, but it is in agreement with a series analysis given by Adler.[14] The critical point of the planar model is known less accurately. Series expansions yield $K_c = 0.4539$ (6)[3] and $K_c = 0.45386$,[15] in good agreement with results based on Monte Carlo simulations.[16–18] A more recent determination by means of the Monte Carlo transfer-matrix technique yielded $K_c = 0.45410$ (2) and $K_c = 0.45414$ (4), depending on the minimum system size used in the analysis.[19] For the Heisenberg model, series expansions by Ohno *et al.*[15] yield an estimated critical point at $K_c = 0.69196$ (we apologize for misquoting this value in our Ref. 20), which is close to $K_c = 0.6929$ (1) as obtained by standard Monte Carlo[21] and to $K_c = 0.69291$ (4) and $K_c = 0.69294$ (8) as obtained by a transfer-matrix Monte Carlo analysis,[19] again using different sets of system sizes.

In Sec. II we define our models, and we present a scaling analysis for the surface-surface and surface-bulk correlation functions. In Sec. III we analyze our numerical results and present data collapses for each of the three $O(n)$ models. Each data collapse includes three different values of the surface enhancement, thus demonstrating universality. This paper ends with a short conclusion and discussion in Sec. IV.

II. SURFACE CRITICAL BEHAVIOR OF THREE-DIMENSIONAL $O(n)$ MODELS

We investigate $O(n)$ ($n = 1$, 2, and 3) models defined on simple cubic lattices of $L \times L \times L$ sites. The systems have periodic boundary conditions in two of the principal, say, x and y, directions, and free surfaces perpendicular to the third, the z direction. For each site $\mathbf{r} = (x, y, z)$

with $1 \leq x, y, z \leq L$ we introduce n-component unit vectors $\mathbf{S}_\mathbf{r} = (S_{\mathbf{r}1}, \ldots, S_{\mathbf{r}n})$. The general reduced Hamiltonian (in units of $-1/k_\mathrm{B}T$) of the models under consideration can be written as

$$\mathcal{H} = \sum_{(\mathbf{r},\mathbf{r}')} \mathbf{s}_\mathbf{r} \cdot \mathbf{s}_{\mathbf{r}'} \ , \tag{1}$$

where $\mathbf{s}_\mathbf{r} = \sqrt{K}\mathbf{S}_\mathbf{r}$ if $\mathbf{r}$ is a bulk site, i.e., $\mathbf{r} = (x, y, z)$, with $1 \neq z \neq L$, and $\mathbf{s}_\mathbf{r} = \sqrt{\epsilon K}\mathbf{S}_\mathbf{r}$ for surface sites i.e., $\mathbf{r} = (x, y, z)$ with $z = 1$ or $z = L$, while the summation is over all nearest-neighbor pairs of sites implied by the boundary conditions mentioned above. We consider only systems with surface interactions no stronger than in the bulk, i.e., $\epsilon \leq 1$.

To analyze the surface critical behavior, finite-size scaling was applied to the following correlation functions and generalized susceptibilities, which were computed with standard Monte Carlo techniques at the bulk critical point as a function of the enhancement ϵ. Two surface susceptibilities were computed, viz., the standard reduced surface susceptibility

$$\chi_{11} = \left\langle \sum_{i,j=1}^{L} \mathbf{S}_{1,1,1} \cdot \mathbf{S}_{i,j,1} \right\rangle \tag{2}$$

and the analogous cross susceptibility associated with correlations of spins on one surface with spins on the other surface,

$$\chi_{12} = \left\langle \sum_{i,j=1}^{L} \mathbf{S}_{1,1,1} \cdot \mathbf{S}_{i,j,L} \right\rangle. \tag{3}$$

In addition, we considered two correlation functions. The surface-surface spin-spin correlation function g_{ss} is defined as

$$g_{\mathrm{ss}}(r, \epsilon) = \langle \mathbf{S}_{1,1,1} \cdot \mathbf{S}_{r+1,1,1} \rangle, \tag{4}$$

where $\langle \cdot \rangle$ denotes the thermal average. The surface-bulk correlation function g_{sb} is defined as

$$g_{\mathrm{sb}}(r, \epsilon) = \langle \mathbf{S}_{1,1,1} \cdot \mathbf{S}_{1,1,r+1} \rangle. \tag{5}$$

For the analysis of the numerical results, we apply finite-size scaling. First we review the scaling behavior of the surface-bulk correlation function. Unfortunately, surface critical behavior is subject to strong corrections to scaling due to the irrelevant field $u(\epsilon)$ associated with the surface enhancement. Fortunately, however, the associated exponent is known; it has the value -1 in three dimensions.[22] The correlation function $g_{\mathrm{ss}}(r, L, \epsilon)$ of two spins at distance r on the surface of a system of linear dimension L with surface coupling ϵK_c is expected to be of the scaling form

$$g_{\mathrm{ss}}(r, L, \epsilon) = L^{-2x_{h_1}} m'(\epsilon)^2 G_{\mathrm{ss}}\left(\frac{r}{L}, \frac{u(\epsilon)}{L}\right). \tag{6}$$

Here x_{h_1} is the critical dimension of the surface magnetization. The corresponding renormalization exponent y_{h_1} is given by $x_{h_1} + y_{h_1} = 2$. Equation (6) is a straightforward generalization of the bulk scaling form proposed by Privman and Fisher,[23] with $m'(\epsilon)$ playing the role of the metric factor conjugate to the surface spins. Similarly, the correlation function $g_{\mathrm{sb}}(r, L, \epsilon)$ of a spin on the surface and a spin at a distance r into the bulk is expected to be of the following scaling form

$$g_{\mathrm{sb}}(r, L, \epsilon) = L^{-x_h - x_{h_1}} m\, m'(\epsilon) G_{\mathrm{sb}}\left(\frac{r}{L}, \frac{u(\epsilon)}{L}\right), \tag{7}$$

where x_h is the critical dimension of the bulk magnetization, which is related to the exponent y_h by $x_h + y_h = 3$; m is the metric factor conjugate to the bulk spin variables, i.e., the bulk analog of m'. Note that m is independent of enhancement ϵ.

Next, we address the question how the scaling functions depend on the irrelevant surface scaling field. Under a transformation rescaling by a factor b, the surface magnetic field h_1 scales as $h_1 \to b^{y_{h_1}} h_1$. We assume that the effect of the irrelevant field is to modify this scaling transformation to $h_1 \to b^{y_{h_1}}[1 + u(\epsilon)/L]h_1$. To obtain a scaling relation that reflects this, one replaces the metric factor m' by $[1 + u(\epsilon)/L]m'$. In other words, the irrelevant enhancement field yields a modified metric factor, which is in effect a rescaling of the ordinate of a scaling plot. A further generalization allows for a rescaling of the abscissa as well, and the final form we chose reads

$$g_{\mathrm{ss}}(r, L, \epsilon) = L^{-2x_{h_1}} m'(\epsilon)^2 \left(1 + \frac{u_{\mathrm{ss}}(\epsilon)}{L}\right) \Gamma_{\mathrm{ss}}(\rho_{\mathrm{ss}}), \tag{8}$$

where

$$\rho_{\mathrm{ss}} = \frac{1}{2} - \left(\frac{1}{2} - \frac{r}{L}\right)\left(1 + c_{\mathrm{ss}}\frac{u_{\mathrm{ss}}(\epsilon)}{L}\right), \tag{9}$$

with c_{ss} an unknown constant. Because of the periodic boundary conditions, Γ_{ss} is symmetric about $\rho_{\mathrm{ss}} = 1/2$. This symmetry is absent in the surface-bulk correlation function, yet we chose the analogous form

$$g_{\mathrm{sb}}(r, L, \epsilon) = L^{-x_h - x_{h_1}} m\, m'(\epsilon) \left(1 + \frac{u_{\mathrm{sb}}(\epsilon)}{L}\right) \Gamma_{\mathrm{sb}}(\rho_{\mathrm{sb}}), \tag{10}$$

with

$$\rho_{\mathrm{sb}} = \frac{1}{2} - \left(\frac{1}{2} - \frac{r}{L}\right)\left(1 + c_{\mathrm{sb}}\frac{u_{\mathrm{sb}}(\epsilon)}{L}\right). \tag{11}$$

We note that, in principle, Eq. (8) should have an additional factor of $1 + u_{\mathrm{ss}}/L$, and that it should not be necessary to distinguish between u_{ss} and u_{sb}. However, it may be expected that the bulk irrelevant fields will contribute corrections to scaling similar to those in Eqs. (8) and (10), thus obscuring this relation between the two scaling forms.

The scaling behavior of the surface susceptibility χ_{11} can be obtained by integration of Eq. (8):

$$\chi_{11}(L, \epsilon) = L^{2-2x_{h_1}}[a(\epsilon) + b(\epsilon)/L] + c(\epsilon). \tag{12}$$

The scaling relation for the cross susceptibility χ_{12} between the two surfaces must be similar. However, we argue that the constant $c(\epsilon)$ is zero in this case, since the correlation between surface spins (at a distance $\sim L$) decays as $L^{-2x_{h_1}}$: Substitution in Eq. (3), and replacing the sums by integrals, yields a vanishing contribution for $L \to \infty$ when $x_{h_1} > 1$, a condition that is satisfied for the present $O(n)$ models.

III. NUMERICAL RESULTS

The Monte Carlo data for the models described by Eq. (1) with $n = 1$, 2, and 3, and for system sizes $L = 4, 6, \ldots, 20$ were obtained by means of conventional Metropolis methods. For each n, the models were studied at three different values of the surface enhancement ϵ, namely, $\epsilon_1 = 1.0$ for $n = 1$, 2, and 3; $\epsilon_2 = (19/20)^2$ for $n = 1$ and 0.8 for $n = 2$ and 3; and $\epsilon_3 = (9/10)^2$ for $n = 1$ and 0.6 for $n = 2$ and 3. Squares of simple fractions were chosen for $n = 1$ for reasons of computational efficiency. The simulations were performed at the numerically determined critical points: $K = 0.221653$ for $n = 1$, $K = 0.45410$ for $n = 2$, and $K = 0.69285$ for $n = 3$ (see Sec. I). Data for χ_{11} and χ_{12}, used for the determination of y_{h_1}, are shown in Table I.

For χ_{11} we have applied least-squares fits according to

$$\chi_{11}(L, \epsilon_i) \approx a_i L^{2y_{h_1}-2} + c_i, \tag{13}$$

for $i = 1, 2$, and 3 and $L = L_0, L_0 + 2, \ldots, 20$. It was not found necessary to include a correction proportional to $b(\epsilon_i)$ as given by Eq. (12) in this case, since such fits did not produce significantly different results. The value of L_0 can be varied to eliminate successive small system sizes which may be subject to finite-size corrections not included in the fitted expression. Increasing L_0 reduces the influence of such corrections, but it increases the error margins of the fit. Results of these fits are shown in Table II. The fits to χ_{12} were of the form

$$\chi_{12}(L, \epsilon_i) \approx (d_i + b_i/L) L^{2y_{h_1}-2}. \tag{14}$$

The correlation functions $g_{\rm ss}$ and $g_{\rm sb}$ at a distance equal to half the system size were fitted by the expressions

$$g_{\rm ss}\left(\frac{L}{2}, L, \epsilon_i\right) \approx p_i L^{2y_{h_1}-4}(r_i + s_i/L) \tag{15}$$

and

$$g_{\rm sb}\left(\frac{L}{2}, L, \epsilon_i\right) \approx t_i L^{y_{h_1}+y_h-5}(v_i + w_i/L), \tag{16}$$

TABLE I. Monte Carlo results for the $O(n)$ surface susceptibilities. The first column shows the spin dimensionality n, the second column the system size L, and the third column the length of the simulations in 10^6 of sweeps. The surface susceptibilities χ_{11} and χ_{12} are listed for three surface enhancements: $\epsilon_1 = 1.0$; $\epsilon_2 = 0.95^2$ for $n = 1$ and 0.8 for $n = 2$ and 3; $\epsilon_3 = 0.9^2$ for $n = 1$ and 0.6 for $n = 2$ and 3. Statistical inaccuracies are shown in parentheses.

n	L	10^6 sweeps	$\chi_{11}(\epsilon_1)$	$\chi_{12}(\epsilon_1)$	$\chi_{11}(\epsilon_2)$	$\chi_{12}(\epsilon_2)$	$\chi_{11}(\epsilon_3)$	$\chi_{12}(\epsilon_3)$
1	4	5	4.235 (2)	1.272 (3)	3.535 (2)	0.859 (2)	2.992 (2)	0.590 (2)
1	6	5	5.153 (4)	1.207 (5)	4.084 (2)	0.759 (3)	3.337 (2)	0.494 (3)
1	8	5	5.696 (5)	1.117 (6)	4.390 (3)	0.679 (4)	3.519 (3)	0.429 (3)
1	10	5	6.076 (6)	1.038 (8)	4.597 (4)	0.615 (5)	3.646 (3)	0.384 (4)
1	12	5	6.345 (7)	0.975 (8)	4.749 (4)	0.556 (5)	3.733 (3)	0.351 (4)
1	14	5	6.561 (8)	0.924 (10)	4.851 (5)	0.524 (6)	3.804 (4)	0.322 (4)
1	16	5	6.727 (9)	0.883 (11)	4.955 (4)	0.487 (4)	3.860 (3)	0.303 (4)
1	18	5	6.879 (9)	0.820 (12)	5.030 (5)	0.464 (5)	3.909 (4)	0.285 (4)
1	20	5	6.978 (9)	0.798 (12)	5.092 (4)	0.448 (5)	3.940 (4)	0.270 (4)
2	4	2.4	4.226 (2)	1.246 (3)	2.996 (1)	0.591 (2)	2.162 (1)	0.266 (1)
2	6	2.4	5.223 (3)	1.224 (4)	3.359 (2)	0.506 (2)	2.302 (1)	0.214 (1)
2	8	2.8	5.821 (4)	1.153 (5)	3.564 (2)	0.448 (2)	2.380 (1)	0.185 (1)
2	10	8.4	6.240 (3)	1.088 (4)	3.703 (1)	0.406 (2)	2.432 (1)	0.164 (1)
2	12	3.4	6.563 (5)	1.036 (6)	3.807 (2)	0.374 (3)	2.469 (1)	0.149 (1)
2	14	2.3	6.806 (7)	0.981 (9)	3.887 (3)	0.352 (3)	2.502 (1)	0.138 (2)
2	16	2.8	7.016 (7)	0.946 (9)	3.951 (3)	0.335 (3)	2.529 (1)	0.130 (1)
2	18	5	7.168 (6)	0.897 (8)	4.007 (2)	0.316 (3)	2.547 (1)	0.124 (1)
2	20	4	7.324 (7)	0.894 (9)	4.051 (3)	0.297 (3)	2.563 (1)	0.119 (1)
3	4	0.6	4.232 (3)	1.238 (4)	3.033 (2)	0.608 (3)	2.192 (2)	0.280 (2)
3	6	0.4	5.271 (5)	1.256 (8)	3.429 (3)	0.528 (4)	2.347 (2)	0.227 (2)
3	8	0.4	5.925 (8)	1.171 (11)	3.662 (4)	0.482 (5)	2.438 (3)	0.198 (3)
3	10	0.4	6.405 (10)	1.152 (14)	3.820 (5)	0.428 (6)	2.497 (3)	0.179 (3)
3	12	0.4	6.755 (13)	1.101 (17)	3.943 (6)	0.421 (7)	2.537 (3)	0.158 (3)
3	14	0.4	6.987 (15)	1.036 (20)	4.023 (7)	0.393 (8)	2.571 (3)	0.154 (4)
3	16	0.4	7.271 (17)	1.016 (22)	4.096 (7)	0.372 (8)	2.604 (4)	0.149 (4)
3	18	0.4	7.408 (18)	0.948 (25)	4.170 (8)	0.335 (10)	2.623 (4)	0.134 (4)
3	20	0.4	7.587 (21)	0.927 (26)	4.225 (9)	0.352 (10)	2.641 (4)	0.130 (4)

TABLE II. Results for the $O(n)$ surface magnetic exponent y_{h_1} as determined from the surface susceptibilities χ_{11} and χ_{12}, and the correlation functions g_{ss} and g_{sb}. The first column shows the spin dimensionality n, and the second column the quantity from which y_{h_1} was determined. Error margins in the third decimal place are shown between parentheses. Unsatisfactory fits (as apparent from excessive χ^2 residues) are indicated by asterisks.

n	Q	$y_{h_1}(L_0=4)$		$y_{h_1}(L_0=6)$		$y_{h_1}(L_0=8)$		$y_{h_1}(L_0=10)$	
1	χ_{11}	0.712	(*)	0.728	(6)	0.715	(13)	0.732	(29)
1	χ_{12}	0.736	(5)	0.746	(9)	0.764	(17)	0.791	(43)
1	g_{ss}	0.606	(*)	0.702	(*)	0.710	(15)	0.724	(33)
1	g_{sb}	0.738	(*)	0.793	(12)	0.792	(26)	0.817	(48)
2	χ_{11}	0.759	(*)	0.778	(6)	0.771	(11)	0.751	(22)
2	χ_{12}	0.780	(5)	0.795	(8)	0.807	(18)	0.820	(44)
2	g_{ss}	0.723	(*)	0.760	(*)	0.781	(18)	0.782	(24)
2	g_{sb}	0.814	(*)	0.839	(7)	0.813	(12)	0.799	(23)
3	χ_{11}	0.784	(*)	0.773	(13)	0.767	(28)	0.828	(62)
3	χ_{12}	0.789	(11)	0.818	(28)	0.769	(51)	0.722	(86)
3	g_{ss}	0.754	(*)	0.779	(18)	0.757	(28)	0.758	(46)
3	g_{sb}	0.828	(*)	0.872	(21)	0.821	(40)	0.865	(94)

where $y_h = 2.486$ for $n = 1$,[13,24,11,4] $y_h = 2.483$ for $n = 2$,[25,17] as well as for $n = 3$.[25]

The results are included in Table II for $L_0 = 4$–10. The best convergence (as evident from the finite-size dependence of the residue of the fits) is found on the basis of the susceptibility data, in particular the χ_{12} data. In some cases the results from the correlation functions deviate somewhat more than expected for purely statistical errors. Perhaps we are observing the influence of the bulk correction-to-scaling exponent which may interfere with the irrelevant surface exponent. From the data in Table II we finally estimate $y_{h_1} = 0.740$ (15) for $n = 1$, $y_{h_1} = 0.790$ (15) for $n = 2$, and $y_{h_1} = 0.79$ (2) for $n = 3$.

Using these results for y_{h_1}, we attempt to produce a data collapse for each of $n = 1$, 2, and 3 on the basis of Eq. (8). A least-squares fit was applied according to

$$g_{ss}(r,L,\epsilon_i) \approx A_i L^{2y_{h_1}-4}\left(1+\frac{u_i}{L}\right)\left\{1+\sum_{k=2}^{8}{}' \Gamma_k^{ss}\left[\left(\frac{1}{2}-\frac{r}{L}\right)\left(1+\frac{cu_i}{L}\right)\right]^k\right\}, \tag{17}$$

where the primed sum indicates that k is restricted to be even, since Γ_{ss} is an even function. For $L > 6$, $r > 3$ and $r \geq L/5$, we obtain the set of parameters shown in Table III.

According to Eqs. (8) and (17) the quantity

$$\Gamma_{ss}(\rho) = A_i^{-1}\left(1+\frac{u_i}{L}\right)^{-1} L^{4-2y_{h_1}} g_{ss}(r,L,\epsilon_i) \tag{18}$$

depends only on the surface enhancement only via

$$\rho = \frac{1}{2} - \left(\frac{1}{2}-\frac{r}{L}\right)\left(1+c\frac{u_i}{L}\right), \tag{19}$$

which approaches r/L for small u_i/L.

Figure 1 shows $\ln\Gamma_{ss}$ as a function of ρ for the case of the Ising model. The plot contains data points for all

TABLE III. Parameters as determined for the data collapses shown in Figs. 1–6.

Parameter	Surface-surface			Surface-bulk		
	$O(1)$	$O(2)$	$O(3)$	$O(1)$	$O(2)$	$O(3)$
A_0	10.162	8.246	9.053	2.752	2.486	2.593
A_1	5.013	2.245	2.614	2.041	1.428	1.513
A_2	2.801	0.808	0.934	1.574	0.883	0.946
u_0	-1.092	-0.809	-1.241	-1.452	-1.335	-1.518
u_1	0.685	2.249	1.396	-0.953	-0.438	-0.639
u_2	1.710	2.670	1.971	-0.551	0.111	-0.120
c	0.4399	0.401	0.433	1.145	1.122	1.112
Γ_1	0	0	0	3.798	3.601	3.807
Γ_2	16.342	15.14	15.948	-13.118	-8.580	-12.675
Γ_3	0	0	0	233.447	186.95	225.245
Γ_4	170.763	178.1	139.776	-955.645	-774.16	-907.279
Γ_5	0	0	0	2006.53	1709.72	1882.656
Γ_6	-248.45	-717.7	-43.377	0	0	0
Γ_8	18996.16	19498	16389.066	0	0	0

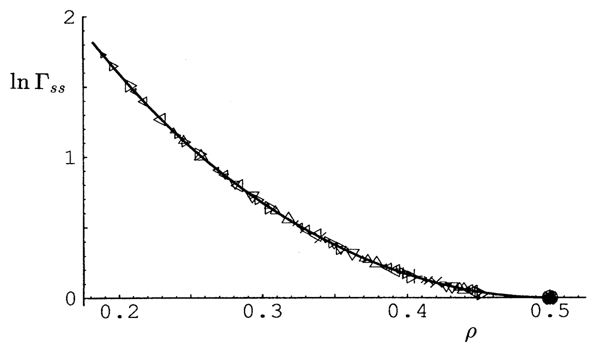

FIG. 1. Data collapse of the surface-surface correlation function of the $O(1)$ (Ising) model as defined in the text. The statistical errors in the data points do not exceed the size of the symbols. The shape of symbols indicates the finite size: $L = 8$: $\circ$; $L = 10$: $+$; $L = 12$: $\times$; $L = 14$: $\bigtriangledown$; $L = 16$: $\bigtriangleup$; $L = 18$: $\triangleleft$; $L = 20$: $\triangleright$. The three symbol sizes indicate the three surface enhancement parameters (see text). Larger symbols correspond to stronger surface couplings.

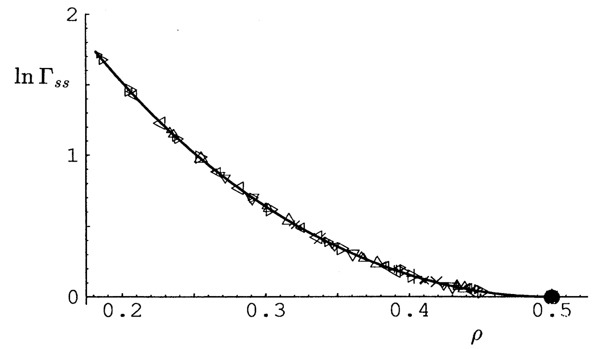

FIG. 2. Data collapse of the surface-surface correlation function of the $O(2)$ (planar) model as defined in the text. For more details, see the caption of Fig. 1.

three values of the surface coupling enhancement. The curve shows the fit according to Eq. (17). It is apparent from this figure that all data collapse on a single curve. This is an unambiguous manifestation of universality. Note that the factors rescaling the axes in Eq. (17) are determined by a least-squares fit, so that by counting fitting parameters we could have expected only two points in common between any two sets of data with different coupling enhancements.

For the planar rotor and Heisenberg models we performed the same analysis. The results, which are similar to those of the $O(1)$ case, are shown in Figs. 2 and 3.

Finally, the same procedure was applied to the surface-bulk correlation function. The fit in this case was made by assuming the form

$$g_{\rm sb}(r,L,\epsilon_i) \approx A_i L^{y_h+y_{h_1}-5}\left(1+\frac{u_i}{L}\right)\left\{1+\sum_{k=1}^{5}\Gamma_k^{\rm sb}\left[\left(\frac{1}{2}-\frac{r}{L}\right)\left(1+\frac{cu_i}{L}\right)\right]^k\right\} \tag{20}$$

using the same set of values L and r as for the surface-surface correlations.

The results are included in Table III. The data collapses according to Eq. (20) are shown in Figs. 4–6 in terms of the logarithm of Γ_{sb} vs ρ, where Γ_{sb} is defined in analogy with Eq. (18).

IV. DISCUSSION

We have estimated surface critical exponents and have determined the scaling functions of the surface-surface and surface-bulk correlation functions in three-dimensional $O(n)$ models. These scaling functions are universal but restricted to the boundary conditions chosen (periodic in two directions, open in the third one) and the aspect ratio (equal sizes in the three directions).

The data collapses are satisfactory, but the residues of the fits are larger than expected on the basis of statistics. Noticeable deviations of the data points from the universal curves in Figs. 1–6 occur for the smaller system sizes. These deviations can be attributed to the fact that our

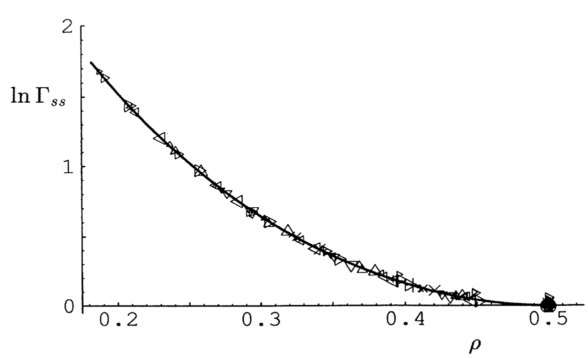

FIG. 3. Data collapse of the surface-surface correlation function of the $O(3)$ (Heisenberg) model as defined in the text. For more details, see the caption of Fig. 1.

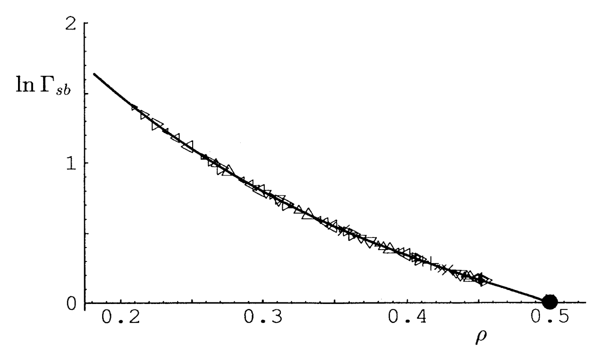

FIG. 4. Data collapse of the surface-bulk correlation function of the $O(1)$ (Ising) model as defined in the text. For more details, see the caption of Fig. 1

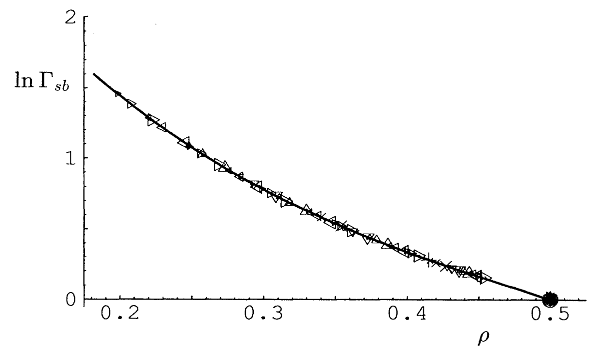

FIG. 5. Data collapse of the surface-bulk correlation function of the $O(2)$ (planar) model as defined in the text. For more details, see the caption of Fig. 1.

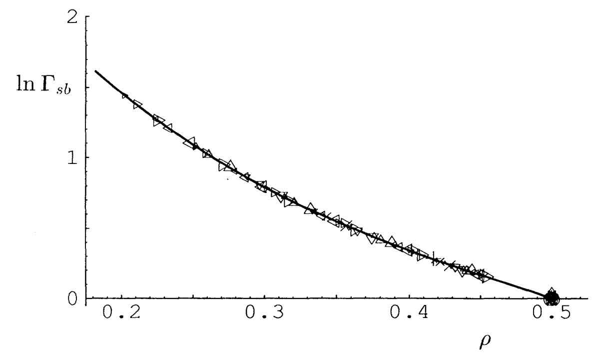

FIG. 6. Data collapse of the surface-bulk correlation function of the $O(3)$ (Heisenberg) model as defined in the text. For more details, see the caption of Fig. 1.

fits deal with the effects of many simultaneous sources of corrections to scaling: The irrelevant surface enhancement field, irrelevant bulk fields, and various higher-order corrections might all contribute. Furthermore, our choice of a specific scaling form to take the irrelevant surface enhancement field into account, although plausible, lacks solid theoretical justification. This becomes particularly clear if one compares the signs and magnitudes of the parameters u_i as estimated from the surface-surface and surface-bulk correlation functions in Table III. If the u_i could be attributed to one single source, both estimates should be consistent.

Finally, the singular parts of both susceptibilities χ_{11} and χ_{12} contain metric factors $m'(\epsilon)^2$. These factors cancel in the singular amplitude ratios a_i/d_i ; thus we expect these ratios to be universal. Indeed, the fits show that $a_i/d_i = 2.64$ (6) for $n = 1$, $a_i/d_i = 3.60$ (6) for $n = 2$, and $a_i/d_i = 4.22$ (5) for $n = 3$.

Remarkably, the data collapses produced for the three $O(n)$ models ($n = 1$, 2, and 3) are rather similar. Not only the magnetic critical exponents, but also the surface magnetic scaling functions appear to be almost the same for the three models.

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