Boundary Critical Behavior of the Three-Dimensional Heisenberg Universality Class

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We study the boundary critical behavior of the three-dimensional Heisenberg universality class, in the presence of a bidimensional surface. By means of high-precision Monte Carlo simulations of an improved lattice model, where leading bulk scaling corrections are suppressed, we prove the existence of a special phase transition, with unusual exponents, and of an extraordinary phase with logarithmically decaying correlations. These findings contrast with naïve arguments on the bulk-surface phase diagram, and allow us to explain some recent puzzling results on the boundary critical behavior of quantum spin models.

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Introduction.—Critical phenomena in the presence of boundaries is a fertile source of interesting phenomena, and has attracted numerous experimental [1] and theoretical [2–4] investigations. In the simplest setting, one considers a d-dimensional system bounded $(d-1)$-dimensional surface, breaking the translation symmetry. For a critical system, the behavior at the surface is remarkably different than the bulk one. In fact, standard renormalization-group (RG) arguments predict that a given bulk universality class (UC) potentially splits into different surface UCs [3,5], resulting in a rich bulk-surface phase diagram. Surface UCs also determine the critical Casimir force [6–11]. For classical models, one generically distinguishes between the surface ordinary UC, where the surface exhibits critical behavior as a consequence of a critical bulk, the surface critical behavior in the presence of a disordered bulk (when such a transition exists), and the surface extraordinary UC, found for a critical bulk and strong enough surface enhancement. Finally, in the bulk-surface phase diagram these three transition lines meet at a multicritical point, the so-called special UC [2,3]. In this framework, one of the most important cases is the three-dimensional O(N) UC [12]. In the presence of a 2D surface, the scenario above is realized for $N=1$ (Ising) and $N=2$ (XY) cases. Surface critical behavior for the Heisenberg UC is instead not yet fully understood. Experiments have proven the realization of the ordinary surface UC for Gd samples at its bulk critical point, in the O(3) UC [13]. Since the Mermin-Wagner-Hohenberg theorem [14–16] forbids a surface transition, one could conclude that only the ordinary UC is realized. While early Monte Carlo (MC) simulations supported this picture [17], a later MC study claimed a possible Berezinskii-Kosterlitz-Thouless- (BKT) like surface transition [18]. This problem has recently attracted renewed attention in the context of quantum critical behavior, where several investigations reported puzzling results. MC simulations of dimerized spin-$1/2$ systems, exhibiting a classical Heisenberg bulk UC, have found nonordinary surface exponents for some geometrical settings [19–22]. Such a novel behavior has been attributed to a relevant topological θ term at the boundary, which is irrelevant for the bulk critical behavior [22]. A theory for a direct transition between a Néel and a valence-bond solid (VBS) in nonlocal 1D quantum systems has been put forward to explain the observed behavior [23]. Nevertheless, quite remarkably a MC study of a dimerized $S=1$ system reported a surface critical exponent close (although not identical) to that of the $S=1/2$ case [24], whereas VBS correlations decay faster than for the $S=1/2$ case [25]. Similar exponents have been found at the boundary of coupled Haldane chains [26]. For a $S=1$ system a topological θ term is absent, and so via a standard quantum-to-classical mapping [27] it should correspond to a classical 3D O(3) model with a surface. It is therefore unclear whether a boundary θ term is responsible for the observed nonordinary exponents for $S=1/2$ systems. In this context, a recent field-theoretical study has put forward different possible scenarios for the surface transition in the Heisenberg UC [28], the realization of which depends on the values of some amplitudes at the so-called normal surface UC [2–4,29,30]. Motivated by these developments, and by the need to understand the classical surface O(3) UC in 3D, we investigate here an improved lattice model by means of MC simulations. By tuning a surface coupling we unveil the existence of a boundary phase transition, separating the ordinary and extraordinary phases. Our findings provide an explanation for abovementioned results.

Model.—We simulate the ϕ^4 model, defined on a 3D $L_\parallel \times L_\parallel \times L$ lattice, with periodic boundary conditions (BCs) on directions corresponding to $L_\parallel$, and open BCs on the remaining direction. The reduced Hamiltonian, such that the Gibbs weight is $\exp(-\mathcal{H})$, is

$$\mathcal{H} = -\beta\sum_{\langle ij\rangle}\vec{\phi}_i\cdot\vec{\phi}_j - \beta_{s,\downarrow}\sum_{\langle ij\rangle_{s\downarrow}}\vec{\phi}_i\cdot\vec{\phi}_j \\ -\beta_{s,\uparrow}\sum_{\langle ij\rangle_{s\uparrow}}\vec{\phi}_i\cdot\vec{\phi}_j + \sum_i[\vec{\phi}_i^2 + \lambda(\vec{\phi}_i^2-1)^2], \tag{1}$$

where $\vec{\phi}_x$ is a three-components real field on the lattice site x, the first sum extends over the nearest-neighbor pairs where at least one field belongs to the inner bulk, the second and third sums pertain to the lower and upper surface, and the last term is summed over all lattice sites.

For $\lambda \to \infty$, the Hamiltonian (1) reduces to the classical O(3) model. In the (β, λ) plane, the bulk exhibits a second-order transition line in the Heisenberg UC [12,31]. At $\lambda = 5.17(11)$ the model is *improved* [32]; i.e., leading bulk scaling corrections $\propto L^{-\omega_1}$, $\omega_1 = 0.759(2)$, are suppressed and those due to the next-to-leading irrelevant bulk operator decay fast as $L^{-\omega_2}$, $\omega_2 \approx 2$ [33]. Additional corrections to scaling originate from the presence of surfaces. Improved lattice models are instrumental in high-precision MC simulations [12], and in particular in boundary critical phenomena [34–43]. For $\lambda = 5.2$, the model is critical at $\beta = 0.687\,98521(8)$ [32]. The couplings $\beta_{s,\downarrow}$, $\beta_{s,\uparrow}$ control the surface enhancement of the order parameter. Here we fix $L_\parallel = L$, $\lambda = 5.2$, $\beta = 0.687\,985\,21$, $\beta_{s,\downarrow} = \beta_{s,\uparrow} = \beta_s$ and study the surface critical behavior on varying β_s. We compute improved estimators of surface observables by averaging them over the two surfaces. MC simulations are performed by combining Metropolis, overrelaxation, and Wolff single-cluster updates [44,45].

Special transition.—For $\beta_s = \beta$ there is no surface enhancement and at the bulk critical point the model realizes the ordinary UC. Its critical behavior will be studied elsewhere [46]. To investigate the surface critical behavior we proceed in two steps. We first analyze RG-invariant quantities, with the aim of locating the onset of a phase transition, and determine the fixed-point values. Then, we employ these results in a finite-size scaling (FSS) [47] analysis to compute universal critical exponents. In the vicinity of a surface transition at $\beta_s = \beta_{s,c}$, and neglecting for the moment scaling corrections, a RG-invariant observable R satisfies

$$R = f((\beta_s - \beta_{s,c})L^{y_{\rm sp}}), \tag{2}$$

where $y_{\rm sp}$ is the scaling dimension of the relevant scaling field associated with the transition. We consider the surface Binder ratio U_4:

$$U_4 \equiv \frac{\langle (\vec{M}_s^2)^2 \rangle}{\langle \vec{M}_s^2 \rangle^2}, \qquad \vec{M}_s \equiv \sum_{i \in \text{surface}} \vec{\phi}_i. \tag{3}$$

In Fig. 1 we show U_4 as function of β_s for lattice sizes $L = 16,\ 32,\ 48,\ 64,\ 96,\ 128$. We observe a crossing indicating a surface phase transition. Its existence is visually more evident when data are plotted on a larger scale [45]. The slope of U_4 appears to increase rather slowly with L, such that a rather high precision in the MC data ($\approx 10^{-5}$) is needed in order to show the crossing. Within such a high accuracy, scaling corrections are visible, although for instance the data for $L = 16$ deviate by a mere

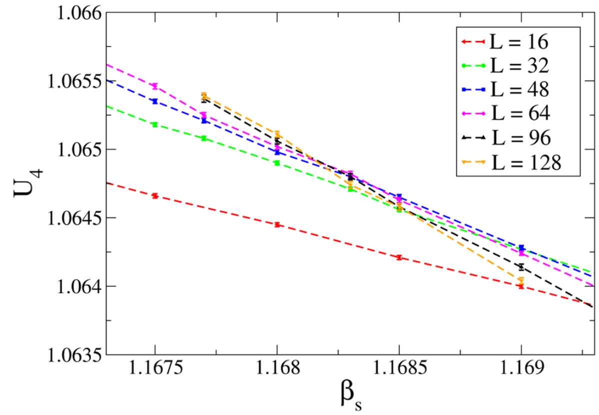

FIG. 1. Plot of the RG-invariant quantity U_4 defined in Eq. (3) as a function of β_s. MC error bars [59–62] are $\approx 10^{-5}$.

$\lesssim 0.1\%$ from the data at $L = 64$. For a quantitative determination of critical parameters, we expand the right-hand side of Eq. (2) in Taylor series [48], including possible scaling corrections, as

$$R = R^* + \sum_{n=1}^{m} a_n (\beta_s - \beta_{s,c})^n L^{n y_{\rm sp}} + L^{-\omega} \sum_{n=0}^{k} b_n (\beta_s - \beta_{s,c})^n L^{n y_{\rm sp}}, \tag{4}$$

where ω is the leading correction-to-scaling exponent. We first consider fits of $R = U_4$ neglecting scaling corrections and for $m = 1$. Corresponding results are reported in Table I, as a function of the minimum lattice size $L_{\rm min}$ taken into account. Results are overall stable, exhibiting however a small detectable drift on increasing $L_{\rm min}$, which is larger than the statistical accuracy of the fit. Furthermore, a good χ^2/d.o.f. (d.o.f. denotes the degrees of freedom) is found only for $L_{\rm min} \geq 48$. In line with the above observation on the slope of U_4, the fitted value of $y_{\rm sp}$ is unusually small. Increasing m to 2 does not change significantly χ^2/d.o.f., indicating that the approximation $m = 1$ is adequate [45]. The small value of $y_{\rm sp}$ can potentially result in slowly decaying analytical scaling corrections $\propto L^{-y_{\rm sp}}$,

TABLE I. Fits of $R = U_4$ to the right-hand side of Eq. (4), with $m = 1$, neglecting scaling corrections $\propto L^{-\omega}$ (above), and including corrections to scaling with $\omega = 1$ and $k = 0$ (below).

$L_{\rm min}$	U_4^*	$\beta_{s,c}$	$y_{\rm sp}$	χ^2/d.o.f.
16	1.063 85(5)	1.169 41(6)	0.27(2)	50.2
32	1.064 63(2)	1.168 47(3)	0.40(2)	3.9
48	1.064 81(3)	1.168 27(3)	0.40(3)	1.0
64	1.064 87(4)	1.168 21(5)	0.39(4)	1.0
96	1.0649(2)	1.1681(2)	0.36(11)	0.9
16	1.065 57(5)	1.167 64(5)	0.40(2)	1.0
32	1.0654(1)	1.167 79(9)	0.39(2)	0.8

originating from nonlinearities in the scaling field [49]. To check their relevance, we have repeated the fits including a quadratic correction to the relevant scaling field $(\beta_s - \beta_{s,c}) \to (\beta_s - \beta_{s,c}) + B(\beta_s - \beta_{s,c})^2$. We obtain identical results, and the fitted values of B vanish within error bars; therefore analytical scaling corrections are negligible for the range of data in exam [45]. Fits including the term $\propto L^{-\omega}$, with a free ω parameter, are consistent with $\omega \gtrsim 1$ [45]. Since a correction term $\propto L^{-1}$ is in any case expected for nonperiodic BCs [50,51], we can safely assume that leading scaling corrections are $\propto L^{-1}$. To obtain more accurate results, we have repeated the fits to Eq. (4) setting $\omega = 1$ and $k = 0$. Corresponding results reported in Table I are stable, with a good χ^2/d.o.f. By judging conservatively the variation of estimates, we obtain the critical-point value of $U_4^* = 1.0652(4)$. We use this result to evaluate critical exponents with the method of FSS at fixed phenomenological coupling [52,53]. This technique consists in an analysis of MC data done by fixing the value of a RG-invariant observable R (here, $R = U_4$), thereby trading the fluctuations of R with fluctuations of a parameter driving the transition (here, β_s). This method has been used in several high-precision MC studies of critical phenomena [32,54–56], and can lead to significant gains in the error bars [53,54]. A discussion of the method can be found in Ref. [53]. For this analysis we have complemented MC data shown in Fig. 1 with an additional simulation at $L = 192$. To compute the exponent $y_{\rm sp}$, we consider derivatives of a RG-invariant observable R with respect to β_s, at fixed $U_4 = 1.0652$. According to FSS, and including leading L^{-1} scaling corrections,

$$\frac{dR}{d\beta_s} = AL^{y_{\rm sp}}(1 + BL^{-1}). \tag{5}$$

We consider $R = U_4$ and the ratio $R = Z_a/Z_p$ of the partition function with antiperiodic and periodic BCs on a direction parallel to the surfaces, sampled with the boundary-flip algorithm [57,58]. In Table II we report the various results of fits to Eq. (5). By looking conservatively at the variation of the results, we estimate

$$y_{\rm sp} = 0.36(1), \qquad \nu_{\rm sp} \equiv 1/y_{\rm sp} = 2.78(8). \tag{6}$$

This result also agrees with the less precise fits shown in Table I. To compute the surface magnetic exponent $\eta_\parallel$ we measure the surface susceptibility:

$$\chi_s = \frac{1}{L^2} \sum_{i,j \in \text{surface}} \vec{\phi}_i \cdot \vec{\phi}_j. \tag{7}$$

In agreement with standard surface FSS [2], we fit MC data for χ_s at fixed U_4^* to

$$\chi_s = AL^{1-\eta_\parallel}(1 + BL^{-1}), \tag{8}$$

TABLE II. Fits of $dR/d\beta_s$ to Eq. (5) for $R = U_4$ and $R = Z_a/Z_p$ at fixed $U_4^* = 1.0652$. Fits above are obtained setting $B = 0$ in Eq. (5), i.e., neglecting scaling corrections, fits below include the term BL^{-1}.

Observable	$L_{\rm min}$	$y_{\rm sp}$	χ^2/d.o.f.
$dU_4/d\beta_s$	16	0.3952(7)	37.9
	32	0.381(2)	4.7
	48	0.374(2)	0.2
	64	0.372(4)	0.2
	96	0.369(6)	0.03
$d(Z_a/Z_p)/d\beta_s$	16	0.364(3)	0.8
	32	0.362(5)	1.0
	48	0.364(9)	1.3
	64	0.35(2)	0.01
	96	0.34(3)	0.03
$dU_4/d\beta_s$	16	0.361(3)	0.4
	32	0.357(6)	0.3
	48	0.366(11)	0.07
$d(Z_a/Z_p)/d\beta_s$	16	0.36(1)	1.0
	32	0.35(2)	1.3
	48	0.29(4)	0.4

where as above we allow for a correction-to-scaling term $\propto L^{-1}$. Fit results are reported in Table III. We estimate

$$\eta_\parallel = -0.473(2). \tag{9}$$

We checked that varying the fixed value $U_4^* = 1.0652(4)$ within one error bar gives negligible variations in the resulting critical exponents [45]. Finally, FSS at fixed U_4^* allows us to estimate $\beta_{s,c} = 1.1678(2)$ [45].

Extraordinary phase.—The existence of a surface phase transition implies an extraordinary phase for $\beta_s > \beta_{s,c}$. To investigate it, we have simulated the model at $\beta_s = 1.5$, for lattice sizes $8 \le L \le 384$. In Figs. 2(a) and 2(b) we plot the ratio ξ/L of the surface correlation length ξ [63] over the lattice size L, and the product ΥL, where Υ is the helicity modulus [65,66]. Both quantities exhibit a logarithmic growth with L, indicating a violation of standard FSS.

TABLE III. Fits of χ_s at fixed $U_4 = 1.0652$ to the right-hand side of Eq. (8) neglecting the scaling corrections $\propto L^{-1}$ (above), and including them (below).

$L_{\rm min}$	$\eta_\parallel$	χ^2/d.o.f.
16	−0.477 60(7)	146.9
32	−0.4753(1)	12.3
48	−0.4746(2)	3.1
64	−0.4742(2)	1.4
96	−0.4736(4)	0.2
16	−0.4721(2)	0.4
32	−0.4725(4)	0.2
48	−0.4723(8)	0.3

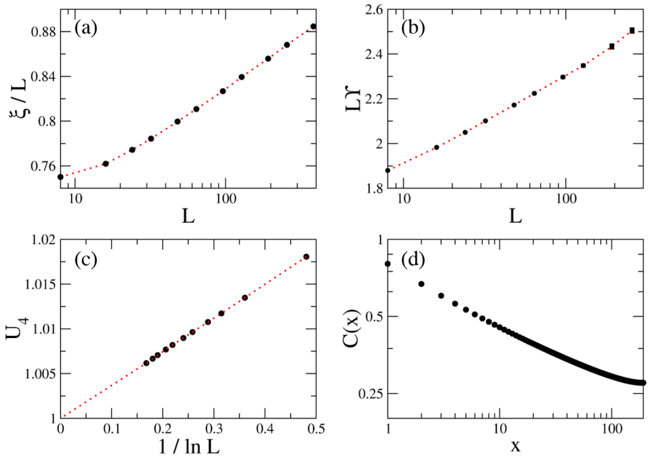

FIG. 2. Observables for $\beta_s = 1.5$, in the extraordinary phase. The ratio ξ/L (a) and ΥL (b) in semilogarithmic scale. (c) The surface Binder ratio U_4 as a function of $1/\ln L$. Dotted lines are a guide to the eye. (d) The surface correlations of the order parameter for $L = 348$. When not visible, statistical error bars are of the order of or smaller than the point size.

The surface Binder ratio U_4 shown in Fig. 2(c) is rather close to 1, and exhibits a logarithmic approach to 1. Nevertheless, the surface is not ordered: its two-point function $C(x) \equiv \langle \vec{\phi}_0 \cdot \vec{\phi}_x \rangle$ for the largest lattice size $L = 384$ shown in Fig. 2(d) exhibits a slow, visible decay. Furthermore, for an ordered surface, $\xi/L \sim L$ and $\Upsilon \sim \mathrm{const}$, in contrast with Figs. 2(a) and 2(b). These findings support the scenario of a so-called "extra-ordinary-log" phase, recently put forward in Ref. [28]. In such a phase, $C(x \to \infty) \propto \ln(x)^{-q}$, where q is a universal exponent determined by some amplitudes in the normal UC. Fits of $C(L/2)$, $C(L/4)$ to $\ln(L/l_0)^{-q}$, and of χ to $L^2 \ln(L/l_0)^{-q}$ [67], provide an estimate of $q \simeq 2.1(2)$ [45]. Moreover, in the "extra-ordinary-log" phase $U_4 - 1 \propto (\ln L)^{-2}$, $(\xi/L)^2 \simeq (\alpha/2)\ln(L)$ and $\Upsilon L \simeq 2\alpha \ln(L)$, for $L \to \infty$, with $\alpha = 1/(\pi q)$ a universal RG parameter [67]. Indeed, fits of $(\xi/L)^2$ to $(\alpha/2)\ln L + B$ give $\alpha \approx 0.14$, showing however some drift in the estimate as a function of the minimum lattice size taken into account. Such a value is nevertheless consistent with the estimate of q reported above, which corresponds to $\alpha \simeq 0.15(2)$. Corresponding fits of $L\Upsilon$ give less stable results. Judging from the trends in the fit results, one can conclude $\alpha \gtrsim 0.11$, again roughly consistent with previous estimates. We stress that error bars reported above should be taken with some grain of salt, since they stem from fits that neglect subleading corrections; these are likely to be important, as illustrated, e.g., by other critical models with marginal perturbations [68]. A more quantitative precise assessment of the extraordinary phase is outside the scope of the present work.

Discussion.—In this work we have elucidated the boundary critical behavior of the classical 3D O(3) UC, in the presence of a 2D surface. A previous MC study, assuming the existence of the ordinary UC only, did not consider RG-invariant observables and reported just a crossover to the ordinary UC for a strong enough surface enhancement [17]. A later study observed a flattening in the curves of the RG-invariant $Q_{11} \equiv 1/U_4$ for large enough surface coupling, and interpreted this as the onset of a BKT-like transition, without further investigations [18]. Here, by means of large-statistics MC simulations of an improved model, where leading scaling corrections are suppressed, and a quantitative FSS analysis, we have proven the existence of a standard special phase transition, with an unusually small, but finite, leading relevant exponent. The extraordinary phase displays slowly decaying correlations and, remarkably, a logarithmic violation of FSS, supportive of the "extra-ordinary-log" scenario of Ref. [28]. A comprehensive theory of such a rather uncommon FSS violation is presently unavailable; hopefully, this work will stimulate research in this direction. These findings also provide an explanation to recent MC results on the boundary critical behavior of quantum spin models [19–22, 24–26]. The exponent $\eta_\parallel$ found for some geometrical settings is close to that of the special transition, Eq. (9), thus suggesting that those quantum spin models are "accidentally" close to the special transition. The observed $\eta_\parallel$ is also close to a simple evaluation of the two-loops ε-expansion series [3,69–71] by setting $\varepsilon = 1$ and $N = 3$ [21]. However, the ε-expansion result for y_{sp} differs significantly from Eq. (6) [45]. Generally, the realization of the special UC requires a fine-tuning of boundary couplings, because the corresponding fixed point is unstable. Nevertheless, the unusually small value of y_{sp} [Eq. (6)] implies a slow crossover from the special fixed point when the model is tuned away from the special transition. In other words, a small y_{sp} results in a (relatively) large region, $(\beta_s - \beta_{s,c})L^{y_{\mathrm{sp}}} = O(1)$, where FSS is controlled by the special fixed point and the observed exponents are close to those of the special UC, without the need of a fine-tuning. This plausibly explains at least the results for $S = 1$ quantum models of Refs. [24,26], where a topological θ term is absent. Also, we observe that the exponent $\eta_\parallel$ reported in Refs. [24,26] deviates for about 15% from $\eta_\parallel$ at the special point [Eq. (9)], suggesting that the models are not exactly at the special transition. Concerning the $S = 1/2$ case, we notice that the small value of y_{sp} implies that the special fixed point is located at a small, possibly perturbatively accessible, value of the coupling constant g^* of the field theory studied in Ref. [28]. Accordingly, if the special transition occurs in the presence of VBS order, $\eta_\parallel$ is expected to be identical to the $S = 1$ case, whereas for a direct magnetic-VBS transition, as advocated in Ref. [23], nonperturbative corrections to $\eta_\parallel$ due to the topological θ term are expected to be small [28]. This would explain the similarity of the $\eta_\parallel$ exponent in dimerized $S = 1/2$ models [20–22] with that of the special transition [Eq. (9)]. Finally, to close the loop, it would be highly desirable to investigate the boundary critical behavior of quantum spin models with a tunable surface coupling, such as those considered in Refs. [22,24], so as to detect a surface phase transition and compare with the present findings.

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