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 to explain some recent puzzling results on the boundary critical behavior of quantum spin models.

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 consider 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. For classical models, one generally 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, the most important case is the three-dimensional $O(N)$ UC [6]. 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 [7]. Since the Mermin-Wagner-Hohenberg theorem [8–10] forbids a surface transition, one could conclude that only the ordinary UC is realized. While early Monte Carlo (MC) simulations supported this picture [11], a later MC study claimed a possible Kosterlitz-Thouless-like surface transition [12]. This problem has recently attracted a 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 [13–16]. Such a novel behavior has been attributed to a relevant topological $\theta$–term at the boundary, which is irrelevant for the bulk critical behavior [16]. 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 [17]. 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 [18], whereas VBS correlations decay faster than for the $S = 1/2$ case [19]. Similar exponents have been found at the boundary of coupled Haldane chains [20]. For a $S = 1$ system a topological $\theta$–term is absent, and so via a standard quantum-to-classical mapping [21] it should correspond to a classical 3D $O(3)$ model with a surface. It is therefore unclear, whether a boundary $\theta$–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 [22], the realization of which depends on the values of some amplitudes at the so-called normal surface UC [2–4, 23, 24]. 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. The determination of critical exponents at the transition, and in the extraordinary phase provides an explanation for above-mentioned results.

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

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

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 $(\beta, \lambda)$ plane, the model exhibits a
second-order transition line in the Heisenberg UC [6, 25]. At \( \lambda = 5.17(11) \) the model is improved [26], i.e., leading bulk scaling corrections are suppressed. Negligible sub-leading bulk corrections decay fast as \( L^{-\omega_2}, \omega_2 \approx 2 \) [27]. For \( \lambda = 5.2 \), the model is critical at \( \beta = 0.68798521(8) \) [26]. The couplings \( \beta_{s,\perp}, \beta_{s,\tau} \) control the surface enhancement of the order parameter. Here we fix \( L_0 = L, \lambda = 5.2, \beta = 0.68798521, \beta_{s,\perp} = \beta_{s,\tau} = \beta_s \) and study the surface critical behavior on varying \( \beta_s \). 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 [28, 29].

The 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 [30]. To investigate the surface critical behavior we proceed in two steps. We first analyze RG-invariant quantities, with the aim of locating the on-set of a phase transition, and determine the fixed-point values. Then, we employ these results in a Finite-Size Scaling (FSS) [31] 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

\[
R = f((\beta_s - \beta_{s,c})L^{y_{sp}}),
\]

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

\[
U_4 \equiv \frac{\langle \bar{M}_s^2 \rangle^2}{\langle \bar{M}_s^2 \rangle^2}, \quad \bar{M}_s \equiv \sum_{i \in \text{surface}} \langle \phi_i \rangle.
\]

In Fig. 1 we show \( U_4 \) as function of \( \beta_s \) for lattice sizes \( L = 16, 32, 48, 64, 96, 128 \). We observe a crossing indicating a surface phase transition. Its existence is more evident when data are plotted on a larger scale [29]. 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 \( \lesssim 0.1\% \) 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 [32], including possible scaling corrections, as:

\[
R = R^* + \sum_{n=1}^{m} a_n (\beta_s - \beta_{s,c})^n L^{y_{sp} n} + \sum_{n=0}^{k} b_n (\beta_s - \beta_{s,c})^n L^{y_{sp} n},
\]

where \( \omega \) 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 \( L_{\text{min}} \) taken into account. Results are overall stable, exhibiting however a small detectable drift on increasing \( L_{\text{min}} \), which is larger than the statistical accuracy of the fit. Furthermore a good \( \chi^2/\text{DOF} \) (DOF denotes the degrees of freedom) is found only for \( L_{\text{min}} \geq 48 \). In line with the above observation on the slope of \( U_4 \), the fitted value of \( y_{sp} \) is unusually small. Increasing \( m \) to 2 does not change significantly \( \chi^2/\text{DOF} \), indicating that the approximation \( m = 1 \) is adequate [29]. The small value of \( y_{sp} \) can potentially result in slowly-decaying analytical scaling corrections \( \propto L^{-y_{sp}} \), originating from nonlinearities in the scaling field [33]. To check their relevance, we have repeated the fits including a quadratic correction to the relevant scaling field \( (\beta_s - \beta_{s,c}) \rightarrow (\beta_s - \beta_{s,c}) + B(\beta_s - \beta_{s,c})^2 \). 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 [29]. Including scaling corrections in the analysis, fits leaving \( \omega \) as a free parameter give a value compatible with 1 [29]. Indeed, scaling corrections \( \propto L^{-1} \) are expected for non-periodic BC [34, 35]. 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 \( \chi^2/\text{DOF} \). By judging conservatively the variation of estimates we obtain the critical-point value of \( U_4^* = 1.0652(4) \). We employ this result to evaluate critical exponents using the method of FSS at fixed phenomenological coupling [36, 37]. This technique consists in an analysis of MC data done by fixing the value of an RG-invariant observables \( R \) (here, \( R = U_4 \)), thereby trading the fluctuations of \( R \) with fluctuations of a parameter driving the transition (here, \( \beta_s \)). This method has been used in several high-precision MC studies of critical phenomena [26, 38–40], and can lead to significant gains in the error bars [37, 38]. A discussion of the method can be found in Ref. [37]. For this analysis we have complemented MC data shown in Fig. 1 with an additional simulation at \( L = 192 \).
Table I. To compute the surface magnetic exponent $\eta$

This result also agrees with the less precise fits shown in the results in Table II we estimate in Ref. [42]. In Table II we report the various results of $O$ computed using the boundary-flip algorithm [41], with a direction parallel to the surfaces. The ratio $Z$ of an RG-invariant observable $R$ belonging to the right-hand side of Eq. (4), with $m = 1$, neglecting scaling corrections, fits below 4.

$$\frac{dR}{d\beta_s} = AL^{y_p} (1 + BL^{-1})$$

We consider $R = U_4$ and the ratio $R = Z_a/Z_p$ of the partition function with antiperiodic and periodic BC on a direction parallel to the surfaces. The ratio $Z_a/Z_p$ is computed using the boundary-flip algorithm [41], with the generalization to $O(N)$-symmetric models discussed in Ref. [42]. In Table II we report the various results of fits to Eq. (5). By looking conservatively at the variation of the results in Table II we estimate

$$y_p = 0.36(1), \quad \nu_p \equiv 1/y_p = 2.78(8).$$

This result also agrees with the less precise fits shown in Table I. To compute the surface magnetic exponent $\eta$

TABLE III. Fits of $\chi_s$ 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).

we measure the surface susceptibility

$$\chi_s = 1 \int \sum_{i,j \in \text{surf}} \vec{\phi}_i \cdot \vec{\phi}_j.$$  

In agreement with standard surface FSS [2], we fit MC data for $\chi_s$ at fixed $U_4$ to

$$\chi_s = AL^{1 - \eta} (1 + BL^{-1}),$$

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

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

We checked that varying the fixed value $U_4^* = 1.0652(4)$ within one error bar gives negligible variations in the resulting critical exponents [29]. Finally, FSS at fixed $U_4^*$ allows to estimate $\beta_{s,c}$ as [29]:

$$\beta_{s,c} = 1.1678(2).$$

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 $8 \leq L \leq 384$. In Figs. 2(a) and 2(b) we plot the ratio $\xi/L$ of the surface correlation length $\xi$ [43] over the lattice size $L$, and the product $\Upsilon L$, where $\Upsilon$ is the helicity modulus [44, 45]. Both quantities exhibit a logarithmic growth with $L$, indicating
in the presence of a 2D surface. We have proven the boundary critical behavior of the classical 3D $O(3)$ UC, in the presence of a 2D surface. We have proven the existence of a special phase transition, with unusual exponents, and of an extraordinary phase with slowly-decaying correlations, supporting the “extra-ordinary-log” scenario of Ref. [22]. These findings provide an explanation to recent MC results on the boundary critical behavior of quantum spin models [13–16, 18–20]. The exponent $\eta_{\parallel}$ reported for such models 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 $\varepsilon$–expansion series [3, 48–50] by setting $\varepsilon = 1$ and $N = 3$ [15]. However, the $\varepsilon$–expansion result for $y_{sp}$ differs significantly from Eq. (6) [29]. 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, $(\beta_s - \beta_{s,c})L^{y_{sp}} = O(1)$, 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 Ref. [18, 20], where a topological $\theta$–term is absent. Also, we observe that the exponent $\eta_{\parallel}$ reported in Refs. [18, 20] 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. [22]. 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. [17], nonperturbative corrections to $\eta_{\parallel}$ due to the topological $\theta$–term are expected to be small [22]. This would explain the similarity of the $\eta_{\parallel}$ exponent in dimerized $S = 1/2$ models [14–16] with that of the special transition (Eq. (9)). Finally, to close the loop, it would highly desirable to investigate the boundary critical behavior of quantum spin models with a tunable surface coupling, such as those considered in Refs. [16, 18], so as to detect a surface phase transition and compare with the present findings.

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Supercomputer JUWELS at Jülich Supercomputing Centre (JSC) [51].

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### Supplemental Material

**MONTE CARLO SIMULATIONS**

We report here some technical details on the MC simulations. To update the model we combine a Metropolis sweep over the entire lattice, followed by an overrelaxation sweep, and $L$ single-cluster updates. For the Metropolis step, we update each lattice site in a lexicographic order, and for each site we consider a proposal to update the $\alpha$–component $\phi_i^{(\alpha)}$ of the field $\vec{\phi}_i$ as

$$
\phi_i^{(\alpha)} \rightarrow \phi_i^{(\alpha)} + r \Delta,
$$

(S.1)

where $r \in [-1/2, 1/2]$ is a uniformly distributed random number and $\Delta$ is chosen to have a good acceptance. We fix $\Delta = 2$, for which we have an acceptance of about $48\%$. On a given lattice site, we loop over all components of $\vec{\phi}_i$. A Metropolis sweep is followed by an overrelaxation sweep over the entire lattice, where each $\vec{\phi}_i$ is updated as

$$
\vec{\phi}_i \rightarrow 2 \frac{\vec{\phi}_i \cdot \vec{\phi}_{nn}}{\vec{\phi}_{nn} \cdot \vec{\phi}_{nn}} \vec{\phi}_{nn} - \vec{\phi}_i,
$$

(S.2)

where $\vec{\phi}_{nn}$ is the sum of $\{\vec{\phi}_j\}$ which are nearest neighbors of $i$. The update of Eq. (S.2) is a reflection of $\vec{\phi}_i$ and it is in principle always accepted, since $\vec{\phi}_i \cdot \vec{\phi}_j$ remains unchanged. However, for a small denominator on the right-hand side of Eq. (S.2), such an update is potentially numerically unstable. To fix this, we accept the move only if the variation of $\vec{\phi}_i \cdot \vec{\phi}_j$ does not exceed a threshold, set to $10^{-12}$. For each Wolff single-cluster update [28], we flip the $\alpha$ component of the fields in a cluster built around a randomly chosen root site, iterating over all components of $\vec{\phi}$.

The second-moment surface correlation length on a finite size $L$ is defined as

$$
\xi = \frac{1}{2 \sin(\pi/L)} \sqrt{\frac{C(0)}{C(2\pi/L)}} - 1,
$$

(S.3)

where $C(p)$ is the Fourier transform of the surface correlations. In Eq. (S.3) we average $C(2\pi/L)$ over the two possible minimum momenta $\vec{p} = (2\pi/L, 0)$ and $\vec{p} = (0, 2\pi/L)$. We refer to Appendix A of Ref. [52] for a discussion of the definition of $\xi$ in a finite size.

The helicity modulus $\Upsilon$ describes the response of the system to a twist in the h.c. [44]. To fix the notation, we recall that in the model (1) we impose periodic BC on the directions 1 and 2, parallel to the surfaces, and open BC on the remaining direction 3. To include a torsion over the components $\alpha$ and $\beta$ of $\vec{\phi}$, we replace

$$
\vec{\phi}_x \cdot \vec{\phi}_{x+\hat{e}_1} \rightarrow \vec{\phi}_x R_{\alpha,\beta}(\theta) \vec{\phi}_{x+\hat{e}_1}, \quad \vec{x} = (x_1, x_{1,f}, x_2, x_3),
$$

(S.4)

where $R_{\alpha,\beta}(\theta)$ is a rotation matrix that rotates the $\alpha$ and $\beta$ components of $\vec{\phi}$ by an angle $\theta$. In Eq. (S.4) we have slightly generalized the notation, such that $\vec{x} = (x_1, x_2, x_3)$ indicates the lattice site as a three-dimensional vector, and $\hat{e}_1$ is the unit vector in the 1–direction. The torsion of Eq. (S.4) results in a 2–dimensional “defect” plane at $x_1 = x_{1,f}$ with size $S = L_3 L = L^2$. The helicity modulus $\Upsilon$ is defined as [44]

$$
\Upsilon \equiv \frac{L}{S} \frac{\partial^2 F(\theta)}{\partial \theta^2} \bigg|_{\theta = 0}.
$$

(S.5)

To obtain an easy expression for $\Upsilon$, it is useful, instead of having a plane-defect at $x_1 = x_{1,f}$, to smear out the torsion over all length $L$ orthogonal to the plane. Specifically, by a change of variables in the partition sum (a series of rotations), one can write an equivalent Hamiltonian where now the replacement (S.4) is

$$
\vec{\phi}_x \cdot \vec{\phi}_{x+\hat{e}_1} \rightarrow \vec{\phi}_x R_{\alpha,\beta}(\theta/L) \vec{\phi}_{x+\hat{e}_1}, \quad \forall \vec{x}.
$$

(S.6)

Using Eq. (S.6) the helicity modulus $\Upsilon$ is written as [45]

$$
\begin{align*}
\Upsilon^{(\alpha,\beta)} &= \beta \sum_{\vec{x} \in \text{bulk}} \vec{\phi}_x \cdot \vec{\phi}_{x+\hat{e}_1} + \beta_{\downarrow} \sum_{\vec{x} \in \text{surface}\downarrow} \vec{\phi}_x \cdot \vec{\phi}_{x+\hat{e}_1} \\
&\quad + \beta_{\uparrow} \sum_{\vec{x} \in \text{surface}\uparrow} \vec{\phi}_x \cdot \vec{\phi}_{x+\hat{e}_1},
\end{align*}
$$

where $R_{\alpha,\beta}(\theta)$ is a rotation matrix that rotates the $\alpha$ and $\beta$ components of $\vec{\phi}$ by an angle $\theta$. In Eq. (S.4) we have slightly generalized the notation, such that $\vec{x} = (x_1, x_2, x_3)$ indicates the lattice site as a three-dimensional vector, and $\hat{e}_1$ is the unit vector in the 1–direction. The torsion of Eq. (S.4) results in a 2–dimensional “defect” plane at $x_1 = x_{1,f}$ with size $S = L_3 L = L^2$. The helicity modulus $\Upsilon$ is defined as [44]

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\end{align*}
$$

(S.6)

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&\quad + \beta_{\uparrow} \sum_{\vec{x} \in \text{surface}\uparrow} \vec{\phi}_x \cdot \vec{\phi}_{x+\hat{e}_1},
\end{align*}
$$

where, to obtain an improved estimator, we have averaged over the $N(N-1)/2 = 3$ pairs of components $(\alpha, \beta)$ where the torsion is applied. A further improved estimator of $\Upsilon$ is obtained by averaging over the directions 1
and 2 for the torsion:

\[
\begin{align*}
\Upsilon &= \frac{1}{2L^2} \left[ \frac{2}{3} (E) - \sum_{\tilde{e}=\tilde{e}_1,\tilde{e}_2} \frac{1}{3} \sum_{\alpha<\beta} \left( T^{(\alpha,\beta)}_{\tilde{e}} \right)^2 \right], \\
E &\equiv \beta \sum_{\tilde{e}=\tilde{e}_1,\tilde{e}_2} \tilde{\phi}^z \cdot \tilde{\phi}_{\tilde{X}+\tilde{e}} + \beta s_{\uparrow} \sum_{\tilde{x} \in \text{surface} \uparrow} \tilde{\phi}^z \cdot \tilde{\phi}_{\tilde{X}+\tilde{e}} \\
&\quad + \beta_{s\uparrow} \sum_{\tilde{x} \in \text{surface} \uparrow} \tilde{\phi}^z \cdot \tilde{\phi}_{\tilde{X}+\tilde{e}}, \\
T^{(\alpha,\beta)}_{\tilde{e}} &\equiv \beta \sum_{\tilde{x} \in \text{bulk}} \left( \phi^{(\alpha)}_{\tilde{x}} \phi^{(\beta)}_{\tilde{X}+\tilde{e}} - \phi^{(\beta)}_{\tilde{x}} \phi^{(\alpha)}_{\tilde{X}+\tilde{e}} \right) \\
&\quad + \beta s_{\downarrow} \sum_{\tilde{x} \in \text{surface} \downarrow} \left( \phi^{(\alpha)}_{\tilde{x}} \phi^{(\beta)}_{\tilde{X}+\tilde{e}} - \phi^{(\beta)}_{\tilde{x}} \phi^{(\alpha)}_{\tilde{X}+\tilde{e}} \right) \\
&\quad + \beta_{s\uparrow} \sum_{\tilde{x} \in \text{surface} \uparrow} \left( \phi^{(\alpha)}_{\tilde{x}} \phi^{(\beta)}_{\tilde{X}+\tilde{e}} - \phi^{(\beta)}_{\tilde{x}} \phi^{(\alpha)}_{\tilde{X}+\tilde{e}} \right).
\end{align*}
\]  
\(\text{(S.8)}\)

In this work we have used the improved expression of Eq. (S.8) and checked that it is consistent with Eq. (S.7).

Finally, to validate the program, we have performed a series of tests, the most crucial of which are as follows. By setting periodic BC, we have checked the MC results for a small value of \(\beta\) with the high-temperature series of Ref. [25]. Also, for periodic BC we have reproduced the universal values of the RR-invariants reported in Ref. [26]. Furthermore, we have set \(\beta = 0\) in the Hamiltonian (1) and computed the surface observables which correspond to 2 independent bidimensional surfaces. The results have been successfully compared with MC simulations of the same model in two dimensions, and periodic BC.

**ADDITIONAL ANALYSIS AT FIXED \(U_4\) AT THE SPECIAL TRANSITION**

We consider here the impact on the fitted critical exponents of varying the fixed value of \(U_4 = 1.0652(4)\) between one error bar. In Tables VI and VII we report fits for \(y_{sp}\) and \(\eta\), where we fix \(U_4 = 1.0648\) and \(U_4 = 1.0656\).

**FIT OF \(\beta_{s,c}\)**

FSS at fixed RG-invariant \(R = R_f\) allows to determine the value of the critical surface coupling \(\beta_{s,c}\) at the special transition. For each lattice size \(L\), the FSS analysis results in a pseudocritical coupling \(\beta_{s,c}^{(f)}(L)\) that converges to \(\beta_{s,c}\) for \(L \to \infty\) as

\[
\beta_{s,c}^{(f)}(L) = \beta_{s,c} + AL^{-c},
\]

where \(e = y_{sp}\) for a generic fixed value \(R_f\), and \(e = y_{sp} + \omega\) if \(R_f\) corresponds to the critical one [36, 37]. In Table VIII we report the results of fit to Eq. (S.9). We consider a variation of \(U_4 = 1.0652(4)\) between one error bar. Fits of \(\beta_{s,c}^{(f)}(L)\) at the lower bound of \(U_4\), i.e., at fixed \(U_4 = 1.0648\), deliver a large \(\chi^2/\text{DOF}\). Furthermore, for \(L_{\text{min}} = 32\) the fit is unstable. For the central value \(U_4 = 1.0652\), as well as for the upper bound \(U_4 = 1.0656\) fits are overall stable, and with a good \(\chi^2/\text{DOF}\). Nevertheless, there is a small deviation between the fitted values of \(\beta_{s,c}\) at \(U_4 = 1.0652\) and at \(U_4 = 1.0656\). Therefore, the quoted estimate of Eq. (10) is chosen to be compatible with both these fits.

**FIT IN THE EXTRAORDINARY PHASE**

In Table IX we report fit results of the surface susceptibility \(\chi_s\) to \(AL^2 \ln(L/l_0)^{-q}\), and of the correlations
TABLE IV. Fits of $U_4$ to Eq. (4) at the special transition, with $m = 2$, neglecting scaling corrections (above), and with $m = 1$ including analytical scaling corrections (below).

| $L_{\text{min}}$ | $U_4^*$ | $\beta_{s,c}$ | $y_{\text{sp}}$ | $\chi^2$/DOF |
|-----------------|----------|----------------|-----------------|---------------|
| 16              | 1.06386(5) | 1.16939(6) | 0.28(2) | 52.1 |
| 32              | 1.06463(2) | 1.16847(3) | 0.40(2) | 4.1 |
| 48              | 1.06481(3) | 1.16827(3) | 0.41(3) | 1.0 |
| 64              | 1.06487(4) | 1.16821(5) | 0.40(4) | 1.1 |

TABLE V. Fits of $U_4$ to Eq. (4) at the special transition, with $m = 1$ and a free parameter $\omega$.

| $L_{\text{min}}$ | $U_4^*$ | $\beta_{s,c}$ | $y_{\text{sp}}$ | $\omega$ | $\chi^2$/DOF |
|-----------------|----------|----------------|-----------------|----------|---------------|
| 16              | 1.0651(2) | 1.1680(1) | 0.40(2) | 1.5(2) | 0.8 |
| 32              | 1.0650(5) | 1.1681(2) | 0.39(2) | 2.4(1.7) | 0.8 |

Using the well-known $\varepsilon$–expansion result of $1/\nu$ [49, 50]

\[
1/\nu = 2 - N + 2 \frac{N + 2}{N + 8} \varepsilon - \frac{(N + 2)(13N + 44)}{2(N + 8)^2} \varepsilon^2 + O(\varepsilon)^3,
\]

the $\varepsilon$–expansion series for $y_{\text{sp}}$ is

\[
y_{\text{sp}} = 1 - N + 2 \frac{N + 2}{N + 8} \varepsilon + \frac{(N + 2)(32 + 4N)\pi^2}{2(N + 8)^3} - 19N - 92 \varepsilon^2 + O(\varepsilon)^3.
\]

Setting $N = 3$ in Eq. (S.10) and Eq. (S.13), a simple summation to $\varepsilon = 1$ gives $\eta_{\parallel} = -0.445$, $y_{\text{sp}} = 1.081$. Employing a [1/1] Padé resummation, we find $\eta_{\parallel} = -0.445$, $y_{\text{sp}} = 0.791$. Alternatively, one can analyze the series of $\Phi$, and compute $y_{\text{sp}} = \Phi/\nu$ using $\nu = 0.7112$ [25]. In this case, we obtain $y_{\text{sp}} = 0.938$ for a direct summation, and $y_{\text{sp}} = 0.657$ for a [1/1] Padé approximation.
TABLE IX. Fits for $q$ in the extraordinary phase, as extracted from the surface susceptibility $\chi_s$ and the surface correlations $C(L/2)$ and $C(L/4)$. $L_{\text{min}}$ is the minimum lattice size taken into account.
| Obs. | $L_{\text{min}}$ | $\alpha$ | $\chi^2$/DOF |
|------|----------------|-----------|--------------|
|      |                |           |              |
| 8    | 0.0795(1)      | 4406.0    |              |
| 16   | 0.1103(2)      | 474.6     |              |
| 24   | 0.1228(3)      | 100.8     |              |
| 32   | 0.1291(5)      | 30.0      |              |
| 48   | 0.1355(7)      | 7.1       |              |
| 64   | 0.1384(9)      | 2.6       |              |
| 96   | 0.142(2)       | 0.4       |              |
| 128  | 0.142(2)       | 0.4       |              |
| 192  | 0.145(5)       | 0.2       |              |

$(\xi/L)^2$

| Obs. | $L_{\text{min}}$ | $\alpha$ | $\chi^2$/DOF |
|------|----------------|-----------|--------------|
|      |                |           |              |
| 8    | 0.0773(1)      | 110.7     |              |
| 16   | 0.0852(3)      | 9.9       |              |
| 24   | 0.0897(7)      | 1.8       |              |
| 32   | 0.091(1)       | 1.9       |              |
| 48   | 0.094(2)       | 1.4       |              |
| 64   | 0.096(3)       | 1.5       |              |
| 96   | 0.104(5)       | 0.8       |              |
| 128  | 0.111(9)       | 0.3       |              |

$\Upsilon L$

| Obs. | $L_{\text{min}}$ | $\alpha$ | $\chi^2$/DOF |
|------|----------------|-----------|--------------|
|      |                |           |              |

TABLE X. Fits of $\alpha$ as extracted from $(\xi/L)^2$ and $\Upsilon L$, as a function of the minimum lattice size taken into account.