Boundary Criticality of the 3D O(N) Model: From Normal to Extraordinary

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(Received 13 December 2021; revised 5 March 2022; accepted 22 April 2022; published 27 May 2022)

It was recently realized that the three-dimensional O(N) model possesses an extraordinary boundary universality class for a finite range of $N \geq 2$. For a given N, the existence and universal properties of this class are predicted to be controlled by certain amplitudes of the normal universality class, where one applies an explicit symmetry breaking field to the boundary. In this Letter, we study the normal universality class for $N = 2$, 3 using Monte Carlo simulations on an improved lattice model and extract these universal amplitudes. Our results are in good agreement with direct Monte Carlo studies of the extraordinary universality class serving as a nontrivial quantitative check of the connection between the normal and extraordinary classes.

DOI: 10.1103/PhysRevLett.128.215701

Introduction.—When a physical systems is in the vicinity of a continuous phase transition, various observables develop power-law singularities which have a character of universality: they are determined by the gross features of the system, such as dimensionality and symmetry, and not by the details of local interactions. Renormalization-group (RG) theory allows us to understand the emergence of universality as the result of the existence of fixed points in a suitably defined flow of Hamiltonians. Accordingly, systems exhibiting identical critical behavior define a given universality class (UC) [1]. The presence of a boundary gives rise to rich phenomena, which have attracted a large amount of experimental [2] and theoretical [3–5] studies. General RG arguments show that a given bulk UC class, describing the critical behavior far away from the boundary, potentially admits different surface UCs [1]. Further, surface critical exponents and other universal data generally differ from those of the bulk [3,4]. Surface UCs also determine the critical Casimir force [6–12]. While boundary criticality is a mature subject, it has recently received renewed attention driven in part by advances in conformal field theory [13–23] and developments in topological phases of quantum matter. Many topological phases including quantum Hall states, topological insulators, and certain quantum spin liquids possess protected boundary states. While it was initially thought that this protection relies on the presence of a bulk energy gap, examples where the boundary state survives in some form even as the bulk gap closes were later discovered [24–32]. The study of such "gapless topological states" and their boundaries lies in the domain of boundary critical phenomena. As gapless topological states were investigated in the context of quantum magnets [33–41], it was realized that even for the simplest model of *classical* magnets—the O(N) model—basic questions about the boundary phase diagram remain open [42–44].

The much investigated classical O(N) model [45] provides a prototypical example of boundary criticality. In three dimensions, for $N = 1$, 2, the bulk-surface phase diagram hosts a surface transition line, where the bulk is disordered and the surface critical behavior belongs to that of 2D O(N) UC. This line terminates at the bulk transition line dividing it into ordinary and extraordinary surface UCs; the termination point is the so-called special UC [3,4]. Surprisingly, the surface phase diagram for $N > 2$ is still not fully settled. For $d = 3$ and $N > 2$ there is no surface transition for a disordered bulk [45], thus the topology of the phase diagram does not necessarily dictate the existence of the extraordinary UC or the special multicritical point [46,47]. Yet, a recent field-theoretical analysis in Ref. [42] has pointed out that if one treats N as a continuous parameter, the extraordinary UC survives for a range $2 < N < N_c$, where N_c is a currently unknown constant. Further, the extraordinary UC in the region $2 \leq N < N_c$ exhibits a surface order parameter correlation function that falls off as

$$\langle \vec{\phi}(\mathbf{x}) \cdot \vec{\phi}(0) \rangle \sim \frac{1}{(\log \mathbf{x})^q}, \tag{1}$$

thus, it was labeled the "extraordinary-log" UC in Ref. [42]; this should be contrasted to the extraordinary transition for $N = 1$ or in $d > 3$ where the above correlation function approaches a constant at large separation. In fact, for $N = 3$ a recent numerical simulation [43] finds firm evidence of a special transition with exponents differing from those of the ordinary UC and a phase consistent with the extraordinary-log UC, implying $N_c > 3$ [48]. For $N = 2$, the "logarithmic" character of the extraordinary phase was also verified numerically [44].

Reference [42] showed that for a given N the existence of the extraordinary-log phase and its properties [such as the exponent q in Eq. (1)] are determined by certain universal amplitudes of the normal boundary UC. The latter is realized when an explicit symmetry breaking field is applied to the boundary [3,4,49,50].

Motivated by these recent developments, in this Letter we study the normal surface UC of the three dimensional O(N) model, for $N = 2$ and $N = 3$, by means of Monte Carlo (MC) simulations of an *improved* lattice model [45], where the leading bulk irrelevant scaling field is suppressed. Through a finite-size scaling analysis of MC data we determine certain universal amplitudes of the normal UC. Such amplitudes are *per se* of interest, as they provide a quantitative description of the normal UC; for $N = 1$ they have been studied in Ref. [51]. Furthermore, exploiting the analysis of Ref. [42], our results confirm the existence of the extraordinary-log UC for $N = 3$, and allow us to compute the universal exponent q in Eq. (1) for $N = 2$ and $N = 3$. Our results are in good agreement with the value of q found in direct studies of the extraordinary phase in Refs. [43,44].

Model.—We study the classical lattice ϕ^4 model by means of MC simulations. It is defined on a three-dimensional $L_\parallel \times L_\parallel \times L$ lattice, with periodic boundary conditions (BCs) along the lateral directions with size $L_\parallel$, and open BCs along the remaining direction. The reduced Hamiltonian $\mathcal{H}$, such that the Gibbs weight is $\exp(-\mathcal{H})$, is

$$\mathcal{H} = -\beta \sum_{\langle ij \rangle} \vec{\phi}_i \cdot \vec{\phi}_j - \beta_s \sum_{\langle ij \rangle_s} \vec{\phi}_i \cdot \vec{\phi}_j - \vec{h}_s \cdot \sum_{i \in s} \vec{\phi}_i + \sum_i [\vec{\phi}_i^2 + \lambda(\vec{\phi}_i^2 - 1)^2], \tag{2}$$

where $\vec{\phi}_x$ is an N-components real field on the lattice site x and the first sum extends over the nearest-neighbor pairs where at least one site belongs to the inner bulk. The second and third sums extend over the lattice sites on the surface. The last term in Eq. (2) is summed over all lattice sites. In Eq. (2) the coupling constant β determines the critical behavior of the bulk, while β_s controls the surface coupling. Finally, we have introduced a symmetry-breaking boundary field $\vec{h}_s = h_s \vec{e}_N$ along the Nth direction.

For $\lambda \to \infty$, the Hamiltonian (2) reduces to the hard spin O(N) model. In the (β, λ) plane, the bulk exhibits a second-order transition line in the O(N) UC [45,52,53]. For $N = 2$ the model is *improved* for $\lambda = 2.15(5)$ [53], i.e., the leading bulk irrelevant scaling field with dimension $y_i = -0.789(4)$ [54] is suppressed. At $\lambda = 2.15$ the model is critical for $\beta = 0.508\,749\,88(6)$ [55]. For $N = 3$ the model is improved for $\lambda = 5.17(11)$ and the suppressed leading irrelevant scaling field has dimension $y_i = -0.759(2)$ [56]. At $\lambda = 5.2$, the model is critical at $\beta = 0.687\,985\,21(8)$ [56]. Improved models are instrumental to obtain accurate results in critical phenomena [45], in particular in boundary critical phenomena [43,51,57–65], because the broken translational invariance generically gives rise to additional scaling corrections, which cumulate to those arising from bulk irrelevant operators. The latter are suppressed for improved lattice models, hence enabling a more accurate analysis.

In the MC simulations presented here we set β and λ to the central value of the bulk critical point in the improved models, and $\beta_s = \beta$. Note that the boundary parameters β_s, h_s are chosen to be identical on the two surfaces: this realizes the normal UC on both surfaces, and allows us to compute improved estimators of surface observables by averaging them over the two surfaces. The geometry is fixed by $L = L_\parallel$. MC simulations are performed by combining Metropolis, overrelaxation, and Wolff single-cluster updates [66]; details of the algorithm are reported in Ref. [43], and the implementation of the Wolff algorithm in the presence of a symmetry-breaking surface field is discussed in Ref. [51]. The inclusion of a boundary field breaks the O(N) symmetry to O(N-1). Accordingly, we distinguish the components of $\vec{\phi}$ defining $\vec{\phi} \equiv (\vec{\varphi}, \sigma)$, where σ is the component parallel to the surface field, and $\vec{\varphi}$ is a $(N-1)$-component vector orthogonal to it. As discussed below, we measure the magnetization profile $\langle \sigma \rangle$ and various surface-surface and surface-bulk two-point functions.

Besides the model realizing the normal UC, we also perform some MC simulations of the ϕ^4 model with periodic BCs, with the aim of determining the bulk field normalization. In this case, the Hamiltonian is as in Eq. (2), without the surface terms.

Normal universality class.—In this section, we discuss the normal surface UC of the O(N) model in $d = 3$. Unless otherwise stated, all operators in this section [e.g., $\vec{\phi} = (\vec{\varphi}, \sigma)$] denote continuum fields; when referring to fields of the lattice model (2), we use the subscript "lat." To leading order, the bulk field $\vec{\phi}_{\rm lat} \propto \vec{\phi}$. The boundary operator spectrum contains two "protected" operators whose existence is mandated by bulk conservation laws and whose scaling dimensions are known exactly [49,50,67]: (i) The "tilt" operator t^i of dimension $\hat{\Delta}_t = d - 1 = 2$, which is an O($N$-1) vector ($i = 1 \ldots N-1$). This operator is induced on the boundary when the symmetry breaking field $\vec{h}_s$ is tilted—thus the nomenclature [68]. (ii) The displacement operator D of dimension $\hat{\Delta}_D = d = 3$, which is an O(N-1) scalar. Perturbing the boundary with this operator is equivalent to moving the location of the boundary, justifying the name "displacement." These are believed to be the two lightest boundary operators.

In particular, on the lattice the boundary field $\varphi^i_{\mathrm{lat}} \propto t^i$. The boundary operator product expansion (OPE) holds for $z \to 0$:

$$\sigma(\mathbf{x}, z) = \frac{a_\sigma}{(2z)^{\Delta_\phi}} + b_D (2z)^{3-\Delta_\phi} D(\mathbf{x}) + \ldots,$$
$$\varphi^i(\mathbf{x}, z) = b_t (2z)^{2-\Delta_\phi} t^i(\mathbf{x}) + \ldots, \qquad (3)$$

where Δ_ϕ is the bulk scaling dimension of $\vec{\phi}$. The coefficients a_σ, b_t, b_D are universal, assuming that the bulk and boundary operators are normalized. a_σ and b_t will be the main target of this Letter—as was shown in Ref. [42], their ratio controls the existence and universal properties of the extraordinary-log phase (in the absence of a boundary magnetic field). Defining

$$\alpha \equiv \frac{\pi}{2}\left(\frac{a_\sigma}{4\pi b_t}\right)^2 - \frac{N-2}{2\pi}, \qquad (4)$$

the extraordinary-log phase exists when $\alpha > 0$. Further, the exponent q in Eq. (1) is given by

$$q = \frac{N-1}{2\pi\alpha}. \qquad (5)$$

We extract a_σ and b_t from the following correlators, which in a semi-infinite geometry take the form

$$\langle \sigma(z) \rangle = \frac{a_\sigma}{(2z)^{\Delta_\phi}}, \qquad \langle t^i(0) \varphi^j(\mathbf{x}, z) \rangle = \delta_{ij} b_t \frac{(2z)^{2-\Delta_\phi}}{(\mathbf{x}^2 + z^2)^2}. \qquad (6)$$

The bulk field ϕ^a, $a = 1\ldots N$, is normalized so that in an infinite geometry $\langle \phi^a(x)\phi^b(0)\rangle = \delta^{ab} x^{-2\Delta_\phi}$, while t^i is normalized so that in a semi-infinite geometry $\langle t^i(\mathbf{x}) t^j(0) \rangle = \delta^{ij} \mathbf{x}^{-4}$. Thus, in a lattice model, to fix the normalizations above and to find a_σ, b_t we will need to measure four different correlators. On the lattice, we expect both finite size scaling corrections and corrections to scaling [69].

Results.—We study first the XY UC. In order to determine the normalization of the bulk field, we have simulated the ϕ^4 model for $N = 2$, with periodic BCs and at the critical point, for lattice sizes $L = 32$–192. In Fig. 1(a) we show the two-point function $\langle \vec{\phi}(x) \cdot \vec{\phi}(0) \rangle$, rescaled to the expected decay $x^{-2\Delta_\phi}$. Here and below we use $\Delta_\phi = 0.519\,088(22)$, $\Delta_\epsilon = 1.511\,36(22)$ [70]. We fit the MC data to

$$\langle \vec{\phi}(x) \cdot \vec{\phi}(0) \rangle = \mathcal{N}_{\mathrm{bulk}} x^{-2\Delta_\phi} \left[1 + B_\epsilon \left(\frac{x}{L}\right)^{\Delta_\epsilon} + C x^{-2} \right], \qquad (7)$$

where the leading finite-size correction $\propto L^{-\Delta_\epsilon}$ is due to the energy operator in the OPE of $\phi^a \times \phi^a$, while the correction

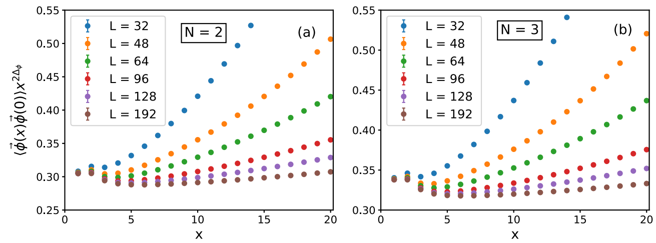

FIG. 1. Bulk two-point function for (a) $N = 2$ and (b) $N = 3$, rescaled to the large-distance decay exponent $2\Delta_\phi$. Error bars are smaller than symbol size.

$\propto x^{-2}$ comes from the next-to-leading irrelevant operator in the action and from descendant operators in the expansion of the lattice field $\vec{\phi}_i$ in terms of continuum fields [69]. Equation (7) holds for $(x/L) \ll 1$ and $x \gtrsim x_0$, with x_0 a nonuniversal length governing the two-point function at short distance. The analysis of various fits [71–73] to Eq. (7) allows us to infer [69]

$$\mathcal{N}_{\mathrm{bulk}} = 0.281\,52(15), \qquad B_\epsilon = 2.758(10). \qquad (8)$$

Next, we study the surface critical behavior. As discussed above, in order to implement the normal UC, we simulated the ϕ^4 model at the critical point with open BCs and a symmetry-breaking surface field. Preliminary MC data suggested a reduction of corrections to scaling for a surface field $h_s = 1.5\beta_s$. Our MC simulations reported below have thus been done at this value of h_s, for lattice sizes $L = 32$–192. To extract the normalization of the surface field component φ, we have computed its two-point function along the surface. We show it in Fig. 2(a), rescaled to its expected large-distance decay exponent 4. In this case finite-size corrections are rather small, such that we fit the data to [74]

$$\langle \vec{\varphi}(\mathbf{x}) \cdot \vec{\varphi}(0) \rangle = \mathcal{N}_\varphi \mathbf{x}^{-4}(1 + C\mathbf{x}^{-2}), \qquad (9)$$

where, analogous to Eq. (7), the leading correction to scaling $\propto \mathbf{x}^{-2}$ originates from the expansion of the lattice operator in terms of continuum ones. Fits to Eq. (9) deliver [69]

$$\mathcal{N}_\varphi = 0.328(3). \qquad (10)$$

In Fig. 2(c), we show the magnetization profile $\langle \sigma(z) \rangle$ as a function of the distance from the surface z, and rescaled to its asymptotic decay exponent Δ_ϕ. For this quantity, scaling and finite-size corrections are relevant and we fit MC data to

$$\langle \sigma(z) \rangle = M_\sigma (z + z_0)^{-\Delta_\phi} \left[1 + B_\sigma \left(\frac{z + z_0}{L}\right)^3 \right], \qquad (11)$$

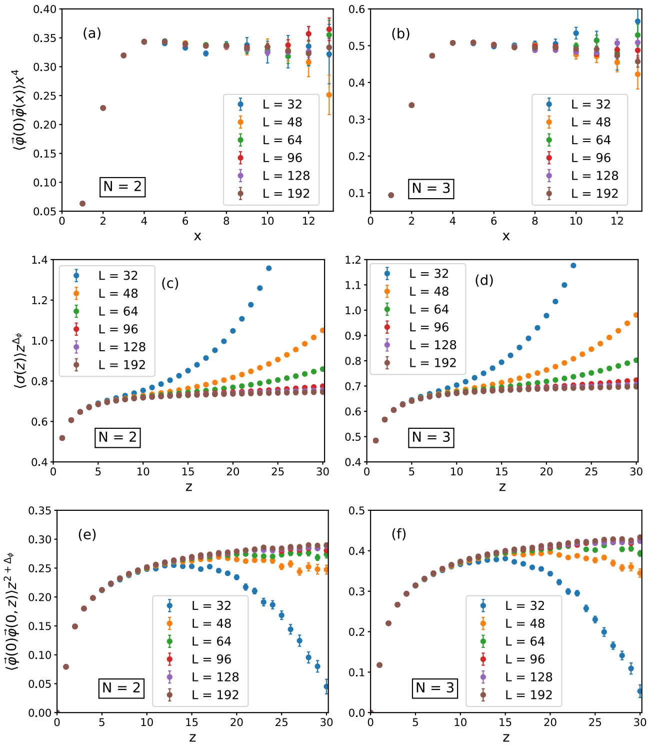

FIG. 2. Plots of surface observables. (a) and (b) Two-point functions of the surface field component φ, for $N = 2$ and $N = 3$, rescaled to the large-distance decay exponent 4. (c) and (d) Order-parameter profile as a function of the distance from the surface, rescaled to the large-distance decay exponent Δ_ϕ. (e) and (f) Surface-bulk correlation functions of the field component φ, rescaled to the large-distance decay exponent $2 + \Delta_\phi$.

where the perturbation of the surface action with the displacement operator D produces the replacement $z \to z + z_0$, with z_0 a nonuniversal constant, and the leading finite-size correction originates from the OPE (3) [69]; the latter is also known as distant wall correction [6,75,76]. Fits to Eq. (11) allow us to estimate [69]

$$M_\sigma = 0.7540(3), \qquad B_\sigma = 1.21(6), \qquad z_0 = 1.018(6). \tag{12}$$

In Fig. 2(e) we show the surface-bulk correlation function $\langle \varphi(0)\varphi(0,z)\rangle$ of the field component φ, where one point is on the surface and the other a distance z away from the surface, so that the vector separating the two points is orthogonal to the surface; the correlations are rescaled to the large-distance decay exponent $2 + \Delta_\phi$. These correlations are affected by significant scaling corrections, while finite-size corrections, though not negligible, are smaller than in the case of $\langle \sigma(z)\rangle$. Together with the relatively fast large-distance decay, $\sim z^{-2-\Delta_\phi}$, this makes the analysis of the surface-bulk correlations more involved. A good ansatz for the MC data is

$$\langle \vec{\varphi}(0)\cdot\vec{\varphi}(0,z)\rangle = M_\varphi (z+z_0)^{-2-\Delta_\phi}\left[1 + B_\varphi \left(\frac{z+z_0}{L}\right)^3 + C(z+z_0)^{-2}\right], \tag{13}$$

where we have included the corrections considered in Eqs. (9) and (11) [69]. To avoid overfitting, in fits to Eq. (13) we plug in the result for z_0 of Eq. (12), varying its value within one error bar quoted there. From the various fits we estimate

$$M_\varphi = 0.3146(8), \qquad B_\varphi = -0.7(2). \tag{14}$$

In the analysis of the MC data for the Heisenberg normal UC, we proceed analogous to the case $N = 2$, using the critical exponents $\Delta_\phi = 0.518\,920(25)$ and $\Delta_\epsilon = 1.5948(2)$ [56]. To extract the normalization of the bulk field ϕ, we simulated the ϕ^4 model for $N = 3$, periodic BCs, and at the critical point, for lattice sizes $L = 32$–192. In Fig. 1(b) we show the two-point function of ϕ, rescaled to the expected decay $x^{-2\Delta_\phi}$. From fits of the correlations to Eq. (7) we obtain [69]

$$\mathcal{N}_{\text{bulk}} = 0.312\,30(15), \qquad B_\epsilon = 2.432(7). \tag{15}$$

Concerning the surface critical behavior, preliminary MC simulations of the model (2) with $N = 3$ suggested a reduction of subleading corrections for a surface field $h_s = 1.4\beta_s$. Here, we present results for this choice of h_s, and lattice sizes $L = 32$–192. In Fig. 2(b) we show the surface correlations. Fits of $\langle \vec{\varphi}(\mathbf{x})\cdot\vec{\varphi}(0)\rangle$ to Eq. (9) allow us to estimate [69]

$$\mathcal{N}_\varphi = 0.481(3). \tag{16}$$

Fits of the order-parameter profile $\langle \sigma(z)\rangle$, shown in Fig. 2(d), deliver the following results:

$$M_\sigma = 0.7062(2), \qquad B_\sigma = 1.07(5), \qquad z_0 = 1.031(4). \tag{17}$$

In Fig. 2(f) we show the surface-bulk correlation function $\langle \vec{\varphi}(0)\cdot\vec{\varphi}(0,z)\rangle$. We fit it to Eq. (13), employing the estimate of z_0 given in Eq. (17). From the various fits we obtain [69]

$$M_\varphi = 0.4674(8), \qquad B_\varphi = -0.7(1). \tag{18}$$

Discussion.—According to the discussion above of the normal UC and of the scaling forms in Ref. [69], the results of our scaling analysis of MC data allow us to extract universal amplitudes a_σ, b_t of the normal UC via

TABLE I. Final results: universal amplitudes a_σ, b_t, and b_D in Eq. (3) together with the corresponding value of α, Eq. (4). We also tabulate $\alpha_{\rm eo}$ found in Refs. [43,44] by direct MC simulations of the extraordinary region. For $N = 1$ we present the values of a_σ, b_D extracted from MC results of Refs. [51,58].

N	a_σ	b_t	b_D	α	$\alpha_{\rm eo}$
1	2.60(5)		0.244(8)		
2	2.880(2)	0.525(4)		0.300(5)	0.27(2) [44]
3	3.136(2)	0.529(3)		0.190(4)	0.15(2) [43]

$$a_\sigma = \frac{2^{\Delta_\phi} M_\sigma}{\sqrt{\mathcal{N}_{\rm bulk}/N}}, \qquad b_t = \frac{2^{\Delta_\phi} M_\varphi}{4\sqrt{N-1}\sqrt{\mathcal{N}_{\rm bulk}/N}\sqrt{\mathcal{N}_\varphi}}. \tag{19}$$

a_σ is obtained from the amplitude of the order-parameter profile M_σ (11) and the normalization of the bulk field $\mathcal{N}_{\rm bulk}$ (7), while b_t is obtained in terms of the amplitude of the surface-bulk correlations M_φ (13), and the bulk and surface normalizations $\mathcal{N}_{\rm bulk}$, (7); $\mathcal{N}_\varphi$, (9). We collect our results for a_σ, b_t in Table I, including the value of α obtained from a_σ and b_t via Eq. (4). For both $N = 2$ and $N = 3$, $\alpha > 0$, which indicates that the extraordinary-log UC exists, in accord with MC results of Refs. [43,44]. Reference [42] predicts that α controls various universal properties of the extraordinary-log phase, including the exponent q in Eq. (1), which is related to α via Eq. (5). α found here agrees well with α extracted from direct MC simulations of the extraordinary region [43,44], listed in Table I as $\alpha_{\rm eo}$. This provides a highly nontrivial check of the theory in Ref. [42]. As pointed out in Ref. [43], the error bar on $\alpha_{\rm eo}$ should be taken with a grain of salt given the difficulty of fitting to the form in Eq. (1) and the presence of subleading logarithmic corrections. Thus, we expect the method for determining α presented here to be more reliable than directly simulating the extraordinary-log phase. We also present results for the coefficients a_σ, b_D in Eq. (3) for the normal UC of the Ising model ($N = 1$) [69,77–84], extracted from MC studies in Refs. [51,58]. A numerical conformal bootstrap study of the normal UC of the O(N) model with $N \geq 2$ was conducted in parallel to our work [68]. Our results for a_σ and b_t are within the bounds produced by positive bootstrap and agree reasonably well with the approximate truncated bootstrap results. For $N = 1$, both a_σ and b_D in Table I agree within error bars with the truncated bootstrap findings of Ref. [85].

We conclude by outlining some possible future directions. It will be interesting to extend the calculations presented here to the O(N) model with $N > 3$, with an eye to determining the critical value N_c where the extraordinary-log UC disappears. $N = 4$ is a natural first target since bootstrap calculations [68], as well as previous MC simulations [86], suggest that the extraordinary transition still exists in this case. Another extension is to study the free energy density for the normal UC in the geometry considered here, which combined with the coefficient B_σ in Eq. (11) and a_σ, allows one to determine the OPE coefficient b_D in Eq. (3), as well as the universal coefficient C_D, characterizing the boundary OPE of the energy-momentum tensor $T_{zz} \overset{z\to 0}{\to} -\sqrt{C_D} D$ [67]. (In fact, this is how for the Ising model b_D in Table I was obtained [87].) Further interesting avenues for future research would be to consider the $N \to 0$ limit [88–93], which describes the physics of dilute polymers [1,45,94], and O(N) loop models [95,96], which provide an extension of the standard O(N) model to noninteger values of N.

We are very grateful to Marco Meineri for discussions. M. M. thanks Ilya Gruzberg, Abijith Krishnan, Marco Meineri, and Jay Padaysi for a collaboration on a related project. We thank Jian-Ping Lv for useful communications. F. P. T. is funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation)–Project No. 414456783. We gratefully acknowledge the Gauss Centre for Supercomputing e.V. for funding this project by providing computing time through the John von Neumann Institute for Computing (NIC) on the GCS Supercomputer JUWELS at Jülich Supercomputing Centre (JSC) [97]. M. M. is supported by the National Science Foundation under Grant No. DMR-1847861.

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