

Boundary operator product expansion coefficients of the three-dimensional Ising universality class

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Recent advances in conformal field theory and critical phenomena have focused on the characterization of boundary or defects in a conformally invariant system. In this Letter, we study the critical behavior of the three-dimensional Ising universality class in the presence of a surface, realizing the ordinary, the special, and the normal universality classes. By combining high-precision Monte Carlo simulations of an improved model, where leading scaling corrections are suppressed, with a finite-size scaling analysis informed by conformal field theory, we determine unbiased, accurate estimates of universal boundary operator product expansion coefficients of experimental relevance. Furthermore, we improve the value of the scaling dimension of the surface field at the special transition by the estimate $\hat{\Delta}_\sigma = 0.3531(3)$.

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Introduction. The modern theory of critical phenomena is a cornerstone of contemporary physics, bridging key concepts from fundamental physics, statistical mechanics, and condensed matter physics. A central focus is the characterization of universal quantities—properties that assume specific values within a given universality class (UC), regardless of the underlying microscopic details of a system. Well-known examples include critical exponents, amplitude ratios, and coefficients in operator product expansions (OPEs). The latter in fact encode the renormalization group (RG) flow near fixed points, and are fundamental ingredients in the characterization of conformal invariance at a critical point [1]. In many realistic scenarios, it is necessary to extend beyond the standard field-theoretical and RG approaches to bulk criticality and consider the effects of boundaries, such as those encountered in surface critical phenomena [2]. Recent years have seen significant advances in our understanding of critical many-body systems with boundaries, such as classical [3–9] and quantum magnets [10–22], and gapless quantum systems with topologically protected boundary states [23–35]. While the overall phase diagrams of many such systems have been well characterized through field-theoretical and computational analyses, new and unexpected RG fixed points, such as the extraordinary log surface transition, have recently been predicted [36] and explored both within the RG and numerically [3–6,8,18,37]. Simultaneously, conformal field theory (CFT) has provided insights into various universal properties, such as boundary OPE (BOPE) coefficients, for critical three-dimensional systems

with surfaces. Using advanced approximate techniques, such as the truncated conformal bootstrap (TCB) [38] and the fuzzy sphere (FZ) construction [39], some of these OPE coefficients have been estimated recently [40,41]. However, unbiased estimates for these universal numbers often still remain unknown, even for the fundamental UC of the three-dimensional Ising model, which corresponds to scalar ϕ^4 theory. In this case, different characteristic surface UCs emerge, depending on the surface enhancement of interactions. For surface interactions preserving the $\mathbb{Z}_2$ symmetry, the ordinary UC and the extraordinary UC arise for weak and strong surface enhancement, respectively, with the special UC separating them. A finite surface-ordering field explicitly breaking the $\mathbb{Z}_2$ symmetry realizes the normal UC, equivalent to the extraordinary UC [42]. The presence of a surface restricts the conformal symmetry to the subgroup of transformations that leave the boundary invariant [43]. Accordingly, one distinguishes between *bulk* and *surface* operators, the latter admitting a usual OPE. Close to the surface, bulk operators admit a BOPE [44,45], whose form is fixed by CFT. Here, we bridge the gap between such a general structure and the actual universal coefficients of such OPEs for the three-dimensional Ising surface UCs by combining accurate and unbiased Monte Carlo (MC) simulations of an improved model and a CFT-motivated scaling analysis. The bulk Ising UC features two relevant operators: the $\mathbb{Z}_2$ -even energy operator ϵ and the $\mathbb{Z}_2$ -odd magnetization operator ϕ . Introducing coordinates $(\mathbf{x}, z)$, where $\mathbf{x}(z)$ is parallel (perpendicular) to the surface, the BOPE for the ordinary and special UC reads [45]

$$\phi(\mathbf{x}, z) \underset{z \rightarrow 0}{=} \frac{b_{\phi\sigma}}{(2z)^{\Delta_\phi - \hat{\Delta}_\sigma}} \sigma(\mathbf{x}) + \dots, \quad (1)$$

$$\epsilon(\mathbf{x}, z) \underset{z \rightarrow 0}{=} \frac{a_\epsilon}{(2z)^{\Delta_\epsilon}} + \frac{b_{\epsilon O}}{(2z)^{\Delta_\epsilon - \hat{\Delta}_O}} O(\mathbf{x}) + \dots. \quad (2)$$

Here, σ is the lowest-lying $\mathbb{Z}_2$ -odd surface operator, associated with the surface magnetization, with dimension $\hat{\Delta}_\sigma$, while O is the lowest-lying $\mathbb{Z}_2$ -even surface operator with

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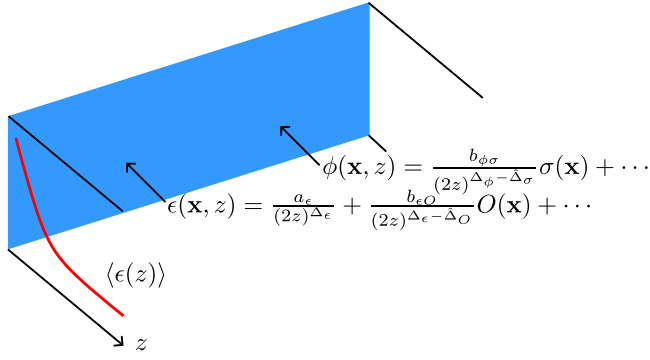


FIG. 1. Illustration of the BOPE.

dimension $\hat{\Delta}_O$. The BOPE is illustrated in Fig. 1. In addition, by fusing $\sigma(\mathbf{0})$ with $\phi(\mathbf{0}, z)$ one obtains [5]

$$\sigma(\mathbf{0})\phi(\mathbf{0}, z) \underset{z \rightarrow 0}{=} b_{\phi\sigma} \frac{2^{\hat{\Delta}_\sigma - \Delta_\phi}}{z^{\hat{\Delta}_\sigma + \Delta_\phi}} [1 + \beta_{\phi\sigma O} z^{\hat{\Delta}_O} O(\mathbf{0}) + \dots]. \quad (3)$$

In Eqs. (1)–(3), a_ϵ , $b_{\epsilon O}$, $b_{\phi\sigma}$, and $\beta_{\phi\sigma O}$ are universal BOPE coefficients. Dots indicate subleading contributions arising from descendants of σ and O , as well as surface operators of higher dimension. In the ordinary UC, there are no relevant $\mathbb{Z}_2$ -even operators, and the leading operator O in Eq. (2) is the displacement operator D , with dimension $\hat{\Delta}_D = 3$ [48,49]. In the special UC, the leading operator O is instead the relevant surface $\mathbb{Z}_2$ -even operator ϵ , associated with the deviation of the enhancement of surface interactions from its critical value.

In the normal UC, there are no relevant operators and the lowest surface operator is the displacement D . The $\mathbb{Z}_2$ symmetry is broken on the boundary, so that a classification of surface operators in terms of $\mathbb{Z}_2$ symmetry does not apply. Accordingly, Eq. (1) is modified as follows:

$$\phi(\mathbf{x}, z) \underset{z \rightarrow 0}{=} \frac{a_\phi}{(2z)^{\Delta_\phi}} + \frac{b_{\phi D}}{(2z)^{\Delta_\phi - 3}} D(\mathbf{x}) + \dots, \quad (4)$$

with a_ϕ and $b_{\phi D}$ universal BOPE coefficients. The BOPE of the energy operator holds as in Eq. (2), with $O = D$.

The various BOPE coefficients—the main target of this work—are summarized in Table I. They are extracted from the one- and two-point correlations that follow from Eqs. (1)–(4). In particular, in the ordinary and special UCs, we use the surface-bulk two-point correlator with leading scaling:

$$\langle \sigma(\mathbf{0})\phi(\mathbf{0}, z) \rangle = b_{\phi\sigma} \frac{2^{\hat{\Delta}_\sigma - \Delta_\phi}}{z^{\hat{\Delta}_\sigma + \Delta_\phi}} [1 + \beta_{\phi\sigma O} z^{\hat{\Delta}_O} \langle O(\mathbf{0}) \rangle], \quad (5)$$

while in the normal UC we exploit the one-point function with

$$\langle \phi(\mathbf{x}, z) \rangle = \frac{a_\phi}{(2z)^{\Delta_\phi}} + \frac{b_{\phi D}}{(2z)^{\Delta_\phi - 3}} \langle D(\mathbf{x}) \rangle. \quad (6)$$

Further, for all surface UCs considered, the one-point function of the energy operator obeys

$$\langle \epsilon(\mathbf{x}, z) \rangle = \frac{a_\epsilon}{(2z)^{\Delta_\epsilon}} + \frac{b_{\epsilon O}}{(2z)^{\Delta_\epsilon - \hat{\Delta}_O}} \langle O(\mathbf{x}) \rangle. \quad (7)$$

Model. We simulate the Blume-Capel model [50,51] on a three-dimensional lattice. Its reduced Hamiltonian is

$$\mathcal{H} = -\beta \sum_{\langle xx' \rangle} S_x S_{x'} + \delta \sum_x S_x^2, \quad S_x = -1, 0, 1, \quad (8)$$

such that the Gibbs weight is $\exp(-\mathcal{H})$. In Eq. (8), the first sum extends over nearest-neighbor sites and the second sum over all lattice sites. In the limit $\delta \rightarrow -\infty$, the Hamiltonian (8) reduces to the Ising model. In the (β, δ) plane, the model exhibits a line of continuous phase transitions in the Ising universality class for $\delta < \delta_{\text{tri}}$, terminating at a tricritical point at $\delta_{\text{tri}} = 2.006(8)$ [52,53]; see also Refs. [54,55] for previous determinations of δ_{tri} . For $\delta > \delta_{\text{tri}}$, the model undergoes a first-order phase transition. At $\delta = 0.656(20)$ [56], the Hamiltonian is “improved” [57], i.e., the leading scaling corrections, $\propto L^{-\omega}$, with $\omega = 0.832(6)$ [56], are suppressed. As in previous MC studies [47,58–64], here we fix $\delta = 0.655$ and $\beta = \beta_c = 0.387\,721\,735(25)$ [56], realizing an improved critical model in the Ising UC.

Results. In order to determine the normalization of bulk fields, we have first simulated the model on an $L \times L \times L$

TABLE I. Universal BOPE coefficients. The quoted uncertainties for TCB [46] and FZ results are only estimates of their systematic errors.

Ordinary UC						Method and references
$b_{\phi\sigma}$	a_ϵ	$b_{\epsilon D}$	$\beta_{\phi\sigma D}$	$\lambda_{\sigma\sigma D}$	C_D	
0.870(3)	−0.753(3)	−0.84(1)	1.05(3)	1.44(7)	0.0101(3)	MC, this work
0.869(7)	−0.750(3)					TCB [40]
0.87(2)	−0.74(4)	−0.92(4)			0.0089(2)	FZ [41]
Special UC						Method and references
$b_{\phi\sigma}$	a_ϵ	$b_{\epsilon\epsilon}$	$\beta_{\phi\sigma\epsilon}$	$\lambda_{\sigma\sigma\epsilon}$	$\lambda_{\epsilon\epsilon\epsilon}$	
1.435(3)	1.160(4)	3.09(5)	0.79(1)	0.86(1)	1.02(2)	MC, this work
Normal UC						Method and references
a_ϕ	$b_{\phi D}$	a_ϵ	$b_{\epsilon D}$	C_D		
2.6143(5)	0.242(2)	6.679(6)	1.69(1)	0.198(3)		MC, this work
2.60(5)	0.244(8)			0.193(5)		MC [5,47]
2.599(1)	0.25064(6)	6.607(7)	1.742(6)	0.182(1)		TCB [40]
2.58(16)	0.254(17)	6.4(9)	1.74(22)	0.176(2)		FZ [41]

TABLE II. Estimates of the scaling amplitudes as obtained from fits of MC data [67]. For every set of amplitudes, we indicate the corresponding UC and the scaling form.

UC	Fit results		Equation
Bulk	$E_0 = 1.204\,234(8)$	$U_E = 3.496(6)$	(10)
	$\mathcal{N}_S^2 = 0.185\,66(7)$	$B_{\phi\phi} = 3.386(7)$	(11)
	$\mathcal{N}_E^2 = 1.1790(8)$	$B_{\epsilon\epsilon} = 5.00(8)$	(12)
	$B'_{\epsilon\epsilon} = -9(1)$		
Ordinary	$\mathcal{N}_\sigma^2 = 0.383(1)$	$B_{\sigma\sigma} = 4.3(2)$	(15)
	$A_\epsilon = -0.545(2)$	$B_\epsilon = -26.8(8)$	(16)
	$z_0 = 1.01(3)$		
	$M_{\phi\sigma} = 0.392(1)$	$B_{\phi\sigma} = 3.15(9)$	(17)
Special	$\mathcal{N}_\sigma^2 = 0.3544(6)$	$B_{\sigma\sigma} = 1.49(1)$	(15)
	$A_\epsilon = 0.840(3)$	$B_\epsilon = 5.92(7)$	(16)
	$z_0 = 0.53(2)$		
	$M_{\phi\sigma} = 0.3282(6)$	$B_{\phi\sigma} = 1.38(1)$	(17)
Normal (+, o)	$z_0 = 0.50(2)$		
	$\mathcal{E}_0 = 1.322\,91(1)$	$U_\mathcal{E} = 2.12(2)$	(19)
	$\mathcal{N}_\epsilon^2 = 1.48(2)$	$B_{\epsilon\epsilon} = 1.77(3)$	(20)
	$A_\epsilon = 4.835(4)$	$B_\epsilon = -2.68(8)$	(16)
	$z_0 = 1.43(1)$		
	$A_\phi = 1.126\,44(6)$	$B_\phi = -1.000(15)$	(21)
	$z_0 = 1.437(3)$		

lattice, with periodic boundary conditions (BCs). We sample the local order parameter S_x and the local energy E_x , defined as

$$E_x \equiv S_x \sum_{\substack{x' \text{ n. n.} \\ \text{of } x}} S_{x'} = S_x \sum_{n=1}^3 (S_{x+e_n} + S_{x-e_n}), \quad (9)$$

where e_n is the unit vector in direction n , so that the sum extends over all nearest-neighbor sites of x . The expectation value of E_x and its finite-size amplitude is obtained by fitting [65] $E_{\text{bulk}} \equiv (1/L^3) \sum_x \langle E_x \rangle$ to

$$E_{\text{bulk}} = E_0 + U_E L^{-\Delta_\epsilon}, \quad (10)$$

where $\Delta_\epsilon = 1.412\,625(10)$ [66] is the scaling dimension of the relevant even operator, related to the standard exponent ν by $\Delta_\epsilon = 3 - 1/\nu$ [1]. See Appendix A for a discussion of the scaling forms used in this work. Fits of MC data [67] allow us to infer estimates of the coefficients E_0 and U_E . In Table II, we report them, together with other amplitudes discussed below. We fit the two-point function of S_x and E_x to [5]

$$\langle S_x S_0 \rangle = \frac{\mathcal{N}_S^2}{x^{2\Delta_\phi}} \left[1 + B_{\phi\phi} \left(\frac{x}{L} \right)^{\Delta_\epsilon} + Cx^{-2} \right], \quad (11)$$

$$\langle E_x E_0 \rangle_c = \frac{\mathcal{N}_E^2}{x^{2\Delta_\epsilon}} \left[1 + B_{\epsilon\epsilon} \left(\frac{x}{L} \right)^{\Delta_\phi} + B'_{\epsilon\epsilon} \left(\frac{x}{L} \right)^{2\Delta_\epsilon} + Cx^{-2} \right], \quad (12)$$

where $\Delta_\phi = 0.518\,1489(10)$ [66] is the scaling dimension of the relevant odd operator, related to the standard exponent

η by $\Delta_\phi = (1 + \eta)/2$ [1] and the subscript c indicates the connected part of the correlations. Equations (11) and (12) are valid for $(x/L) \ll 1$ and $x \gtrsim x_0$, with x_0 a nonuniversal length, associated with short-distance behavior. Incidentally, from the results in Table II we can compute the universal finite-size amplitude of the energy operator $u_\epsilon = U_E/\mathcal{N}_E = 3.220(6)$ and the bulk OPE coefficients $\lambda_{\phi\phi\epsilon} = B_{\phi\phi}/u_\epsilon = 1.052(3)$, $\lambda_{\epsilon\epsilon\epsilon} = B_{\epsilon\epsilon}/u_\epsilon = 1.55(2)$, in line with MC $\lambda_{\phi\phi\epsilon} = 1.051(1)$, $\lambda_{\epsilon\epsilon\epsilon} = 1.533(5)$ [68], and conformal bootstrap $\lambda_{\phi\phi\epsilon} = 1.051\,8537(41)$, $\lambda_{\epsilon\epsilon\epsilon} = 1.532\,435(19)$ [66] estimates. To realize the various boundary UCs, we generalize the Hamiltonian (8), imposing open BCs on one direction and periodic BC in the remaining two, thus realizing an $L \times L \times L$ lattice with two surfaces $\mathcal{S}_\downarrow$ and $\mathcal{S}_\uparrow$, each of size L^2 . The reduced Hamiltonian thus reads

$$\mathcal{H} = -\beta \sum_{\langle x, x' \rangle} S_x S_{x'} + \delta \sum_x S_x^2 - \beta_s \sum_{\langle x, x' \rangle \in \mathcal{S}_\downarrow \cup \mathcal{S}_\uparrow} S_x S_{x'} + h_\downarrow \sum_{x \in \mathcal{S}_\downarrow} S_x + h_\uparrow \sum_{x \in \mathcal{S}_\uparrow} S_x, \quad (13)$$

where the first sum extends over the nearest-neighbor sites for which at least one site belongs to the bulk, the second over all sites, the third sum over all nearest-neighbor pairs on the boundaries, and the fourth and fifth sums each extend over a single surface. In Eq. (13), we have imposed the same coupling β_s on both surfaces, while we allow for different boundary fields $h_\downarrow$ and $h_\uparrow$ on the two surfaces. The various surface UCs studied here are realized by setting the bulk couplings β , δ to the improved critical point $\delta = 0.655$, $\beta = \beta_c = 0.387\,721\,735(25)$ [56], and then tuning the boundary parameters β_s , $h_\downarrow$, $h_\uparrow$. Due to the reduced translation symmetry, we adopt a slightly different definition for the local energy observable $E_{x,z}$, summing over nearest-neighbor sites along the directions parallel to the surfaces only:

$$E_{x,z} \equiv S_{x,z} \sum_{n=1}^2 (S_{x+e_n,z} + S_{x-e_n,z}). \quad (14)$$

We first consider the ordinary UC, which is realized by setting $\beta_s = \beta$ and $h_\downarrow = h_\uparrow = 0$. To extract the normalization of the boundary field, we fit the surface two-point function to

$$\langle S_{x,0} S_{0,0} \rangle = \frac{\mathcal{N}_\sigma^2}{x^{2\hat{\Delta}_\sigma}} \left[1 + B_{\sigma\sigma} \left(\frac{x}{L} \right)^{\hat{\Delta}} + Cx^{-2} \right], \quad (15)$$

where $\hat{\Delta}_\sigma = 2 - 0.7249(6)$ [59] is the scaling dimension of the lowest odd surface operator σ and $\hat{\Delta}$ is the dimension of the leading even surface operator appearing in the BOPE $\sigma \times \sigma$, which is the displacement D , with $\hat{\Delta}_D = 3$ [48,49]. We fit the energy profile to

$$\langle E_{x,z} \rangle = \frac{2}{3} E_0 + \frac{A_\epsilon}{(2\bar{z})^{\Delta_\epsilon}} \left[1 + B_\epsilon \left(\frac{\bar{z}}{L} \right)^{\hat{\Delta}} + \frac{C}{\bar{z}^2} \right], \quad (16)$$

where $\bar{z} \equiv z + z_0$, with z_0 a model-dependent correction-to-scaling amplitude [5], $\hat{\Delta} = 3$, and we fix E_0 to the estimate given in Table II; the factor $2/3$ in front of E_0 accounts for the different definitions used in the bulk [Eq. (9)] and with open BCs [Eq. (14)]. The BOPE coefficient $b_{\phi\sigma}$ is extracted from

the surface-bulk two-point function, which we fit to

$$\langle S_{\mathbf{x},0} S_{\mathbf{x},z} \rangle = \frac{M_{\phi\sigma}}{\bar{z}^{\hat{\Delta}_\sigma + \Delta_\phi}} \left[1 + B_{\phi\sigma} \left(\frac{\bar{z}}{L} \right)^{\hat{\Delta}} + \frac{C}{\bar{z}^2} \right], \quad (17)$$

where $\bar{z} \equiv z + z_0$, $\hat{\Delta}_\sigma = 2 - 0.7249(6)$ [59] is the dimension of the lowest-lying odd surface operator, and as in Eq. (16) $\hat{\Delta} = 3$.

The special UC is realized in the model (13) by setting $\beta_s = 0.549\,14(2)$ [69]. The analysis of the MC data is analogous to the ordinary UC, with the important difference in the presence of a *relevant* surface $\mathbb{Z}_2$ -even operator ε , so that in Eqs. (15)–(17) we have $\hat{\Delta} = \hat{\Delta}_\varepsilon = 2 - 0.718(2)$ [69]. In this work, we have determined a new estimate of the scaling dimension of the lowest odd operator [67]:

$$\hat{\Delta}_\sigma = 0.3531(3), \quad (18)$$

improving an available estimate $\hat{\Delta}_\sigma = 0.3535(6)$ [69]. In fitting the surface-surface and surface-bulk correlations, we use in Eqs. (15) and (17) the value given in Eq. (18). For the special UC, we also study the scaling behavior of the surface energy. We fit $E_{\text{surf}} \equiv (1/L^2) \sum_{\mathbf{x}} \langle E_{\mathbf{x},0} \rangle$ to

$$E_{\text{surf}} = \mathcal{E}_0 + U_\varepsilon L^{-\hat{\Delta}_\varepsilon}. \quad (19)$$

Further, to extract the normalization of the surface energy, we fit its two-point function to

$$\langle E_{\mathbf{x},0} E_{0,0} \rangle = \frac{\mathcal{N}_\varepsilon^2}{x^{2\hat{\Delta}_\varepsilon}} \left[1 + B_{\varepsilon\varepsilon} \left(\frac{x}{L} \right)^{\hat{\Delta}_\varepsilon} + Cx^{-2} \right]. \quad (20)$$

To realize the normal UC, we set $\beta_s = \beta$ and $h_\downarrow = \infty$ in Eq. (13), thereby polarizing a surface with fixed spins $S = 1$. For the opposite surface, we have considered two cases: a surface with $h_\uparrow = 0$, realizing the ordinary UC, and a surface identical to the lower one, with $h_\uparrow = \infty$. We refer to these BCs as $(+, o)$, and $(+, +)$, respectively. The determination of the BOPE coefficients in the $(+, +)$ BCs delivers results somewhat less precise, though in full agreement with those obtained with $(+, o)$ BCs. Here, we discuss the analysis of the $(+, o)$ case [67]. In the normal UC, there are no relevant surface operators, and the lowest-lying operator entering in Eq. (16) is the displacement D , with $\hat{\Delta} = 3$. Furthermore, due to the broken $\mathbb{Z}_2$ symmetry, a nonvanishing order-parameter profile emerges in this case, which we fit to

$$\langle S_{\mathbf{x},z} \rangle = \frac{A_\phi}{(2\bar{z})^{\Delta_\phi}} \left[1 + B_\phi \left(\frac{\bar{z}}{L} \right)^3 + \frac{C}{\bar{z}^2} \right], \quad \bar{z} \equiv z + z_0. \quad (21)$$

Discussion. As we discuss in Appendix A, using the fitted amplitudes of Table II, one can determine the BOPE coefficients introduced above. In particular, $b_{\phi\sigma} = M_{\phi\sigma} 2^{\Delta_\phi - \hat{\Delta}_\sigma} / (\mathcal{N}_S \mathcal{N}_\sigma)$ [Eq. (16)], $a_\varepsilon = (3/2) A_\varepsilon / \mathcal{N}_E$ [Eq. (17)], and, for the normal UC, $a_\phi = A_\phi / \mathcal{N}_\phi$ [Eq. (21)]. In the ordinary and normal UCs, the finite-size corrections are proportional to the amplitude u_D of the displacement operator D . This enters also in the boundary expansion of the energy-momentum tensor $T_{zz} = -\sqrt{C_D} D$, where C_D is the universal norm coefficient [70]. On a finite geometry, $\langle T_{zz} \rangle = \Theta / L^3$, where Θ is the universal amplitude of the critical Casimir force [71–78]. The universal norm C_D can be related to the

finite-size correction of the one-point function of the energy and, for the normal UC, of the order parameter [5,70,79]

$$C_D = -\frac{2^d \Delta_\varepsilon \Theta}{S_d B_\varepsilon} = -\frac{2 \Delta_\varepsilon \Theta}{\pi B_\varepsilon}, \quad (22)$$

$$C_D = -\frac{2^d \Delta_\phi \Theta}{S_d B_\phi} = -\frac{2 \Delta_\phi \Theta}{\pi B_\phi}, \quad (23)$$

where $S_d = 2\pi^{d/2} / \Gamma(d/2)$ and $d = 3$. Employing the value of Θ reported in Appendix B, one can determine C_D , as well as the amplitude $u_D = \Theta / \sqrt{C_D}$; for the ordinary UC, we obtain $u_D = 3.00(5)$. In the case of the normal UC, Eqs. (22) and (23) provide two different estimators for C_D . In Table I, we quote C_D as obtained from Eq. (23), which is more precise and in full agreement with that obtained from Eq. (22): $C_D = 0.202(6)$. The finite-size amplitude u_D is found to be $u_D = 1.34(2)$ [using Eq. (22)] and $u_D = 1.35(1)$ [using Eq. (23)]. The BOPE coefficients $b_{\varepsilon D}$ and $b_{\phi D}$ are extracted from a_ε and a_ϕ with the identities [70]

$$\frac{b_{\varepsilon D}}{\Delta_\varepsilon a_\varepsilon} = \frac{1}{S_d \sqrt{C_D}}, \quad (24)$$

$$\frac{b_{\phi D}}{\Delta_\phi a_\phi} = \frac{1}{S_d \sqrt{C_D}}. \quad (25)$$

Again, in the case of the normal UC, employing on the right-hand side of Eqs. (24) and (25) C_D as extracted from the energy operator [Eq. (22)] gives results in full agreement with, though slightly less precise than, those quoted in Table I. Other BOPE coefficients can be extracted as $\beta_{\phi\sigma D} = B_{\phi\sigma} / u_D$ and $\lambda_{\sigma\sigma D} = B_{\sigma\sigma} / u_D$. In the special UC, finite-size corrections are unrelated to the displacement operator and are due to the lowest-lying $\mathbb{Z}_2$ -even operator ε . Its finite-size amplitude u_ε can be conveniently obtained from results in Table II as $u_\varepsilon = U_\varepsilon / \mathcal{N}_\varepsilon = 1.74(2)$. Then, BOPE coefficients are obtained as $b_{\varepsilon\varepsilon} = 2^{-\hat{\Delta}_\varepsilon} B_\varepsilon a_\varepsilon / u_\varepsilon$, $\beta_{\phi\sigma\varepsilon} = B_{\phi\sigma} / u_\varepsilon$, and $\lambda_{\sigma\sigma\varepsilon} = B_{\sigma\sigma} / u_\varepsilon$. The finite-size scaling (FSS) analysis of the surface energy correlations [Eq. (20)] allows us to extract a further OPE coefficient $\lambda_{\varepsilon\varepsilon\varepsilon} = B_{\varepsilon\varepsilon} / u_\varepsilon$. The remaining BOPE coefficients a_ε and $b_{\phi\sigma}$ are obtained as for the ordinary UC. In Table I, we summarize our results and compare them with available results in the literature. For several quantities, we are not aware of previous calculations. Whenever a comparison with previous works is available, we generally observe a reasonable agreement, with a small but significant deviation especially in the estimates of C_D . In the case of the normal UC, our results significantly improve the precision of the universal coefficients obtained in Ref. [5] by reanalyzing some MC results of Ref. [47]. We stress that, different from the TCB and FZ techniques, our method, based on a combination of MC simulations and a FSS analysis, is numerically exact. As outlined above, and in the Supplemental Material [67], for some BOPE independent estimates deliver perfectly consistent values, thus underscoring their robustness and the reliability of the quoted uncertainties: We expect our results to provide a benchmark for future studies. Future improvements might be obtained by searching for an improved model where also the leading boundary irrelevant operator, the displacement D , is suppressed. Such a realization, if at all possible, requires, however, a fine-tuning of surface interactions. Some of the coefficients of Table I are experimentally accessible, in particular those of the normal UC, obtained in critical

adsorption experiments [80–84]. We are not aware of experimental determinations for other UCs, though in principle coefficients could be accessed by spatially resolved probes, e.g., x-ray scattering under grazing incidence [85]. The technique used here can be clearly employed for other boundary UCs. In particular, it would be interesting to extend the study to the $O(N)$ model, $N > 1$. While a surface ordinary UC is always present, the special transition exists only for $N \leq N_c$ [36], with $N_c \approx 5$ [37]. For the $O(N)$ UC, precise estimates of the critical exponents at the ordinary UC are available [7] and the exponents at the special transition have been numerically determined in Refs. [3,86,87], whereas a numerically reliable determination of BOPE coefficients is presently not available.

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Data availability. The data that support the findings of this article are openly available [89].

Appendix A: Scaling forms. A crucial ingredient for a numerically reliable determination of universal quantities is the formulation of precise scaling ansatzes, where one identifies the leading corrections to the scaling behavior of critical observables. Here, this is accomplished by a scaling analysis motivated by the CFT describing the UCs studied and its connection to the simulated lattice model. Most of the scaling forms used in this work in order to fit the MC data are generalizations of those derived in the Supplemental Material of Ref. [5]. Here, we briefly recall the essential steps in this derivation. Lattice observables are generally expanded in terms of CFT fields belonging to the same symmetry sector. In particular, for bulk observables,

$$\begin{aligned} S_x &= \mathcal{N}_S(1 + c_S \vec{\nabla}^2)\phi, \\ S_x^2 - \langle S_x^2 \rangle &= \mathcal{N}_{S^2}(1 + c_{S^2} \vec{\nabla}^2)\epsilon, \\ E_x - \langle E_x \rangle &= \mathcal{N}_E(1 + c_E \vec{\nabla}^2)\epsilon, \end{aligned} \quad (\text{A1})$$

where the constants $\mathcal{N}_S$, $\mathcal{N}_{S^2}$, $\mathcal{N}_E$, c_S , c_{S^2} , and c_E are model-dependent. With this expansion, Eq. (10) follows immediately by taking the expectation value on a finite volume. Moreover, the finite-size amplitude U_E is given by $U_E = \mathcal{N}_E u_\epsilon$, where u_ϵ is the universal finite-size amplitude of the energy operator,

$$\langle \epsilon \rangle = \frac{u_\epsilon}{L^{\Delta_\epsilon}}. \quad (\text{A2})$$

We notice that, using Eq. (A1), one can in principle expect an additional correction $\propto L^{-2-\Delta_\epsilon}$ to the right-hand side of

Eq. (10): Our fit analysis shows that such a term is negligible within the precision of MC data. Given that also S^2 couples to the energy operator, a FSS form for $S_{\text{bulk}}^2 \equiv (1/V) \sum_x S_x^2$ analogous to Eq. (10) holds

$$S_{\text{bulk}}^2 = S_0^2 + U_{S^2} L^{-\Delta_\epsilon}, \quad (\text{A3})$$

where $U_{S^2} = \mathcal{N}_{S^2} u_\epsilon$.

Using the bulk OPEs $\phi \times \phi = \lambda_{\phi\phi\epsilon} \epsilon$ and $\epsilon \times \epsilon = \lambda_{\epsilon\epsilon\epsilon} \epsilon$, one obtains Eqs. (11) and (12) [5], as well as an analogous formula for the correlations of S^2 :

$$\langle S_x^2 S_0^2 \rangle_c = \frac{\mathcal{N}_{S^2}^2}{x^{2\Delta_\epsilon}} \left[1 + B_{\epsilon\epsilon} \left(\frac{x}{L} \right)^{\Delta_\epsilon} + Cx^{-2} \right]. \quad (\text{A4})$$

We notice that the subleading correction $\propto (x/L)^{2\Delta_\epsilon}$ in Eq. (12) is due to the fact that we consider the connected part of the correlations: Such a term is absent in Eq. (11). In principle, a subleading term $\propto (x/L)^{2\Delta_\epsilon}$ is also present in Eq. (A4): Due to a reduced precision of the S^2 correlations, our analysis shows that such a correction is not relevant [67]. In Eqs. (11), (12), and (A4), the finite-size coefficients are related to the OPE constants by

$$\begin{aligned} B_{\phi\phi} &= \lambda_{\phi\phi\epsilon} u_\epsilon, \\ B_{\epsilon\epsilon} &= \lambda_{\epsilon\epsilon\epsilon} u_\epsilon. \end{aligned} \quad (\text{A5})$$

Moreover, the subleading amplitude $B'_{\epsilon\epsilon}$ is related to the finite-size amplitude of the energy by $B'_{\epsilon\epsilon} = -u_\epsilon^2$, which holds within the available numerical precision. Combining the expansion (A1) with the BOPE (4), we derive in Ref. [5] Eq. (21) and show that $A_\phi = \mathcal{N}_S a_\phi$. The scaling form of the energy profile (16) follows analogously, and we have $A_\epsilon = (2/3)\mathcal{N}_E a_\epsilon$; here, as in Eq. (16), the factor 2/3 is due to the fact that in the definition of energy profile [Eq. (14)] we sum over two lattice directions, as opposed to the definition for the bulk observable [Eq. (9)], where the sum is over all three directions. Further, the finite-size correction is related to BOPEs as $B_\epsilon = 2^{\hat{\Delta}_O} b_{\epsilon O} u_O / a_\epsilon$, with u_O the universal finite-size amplitude of the leading boundary operator O in Eq. (2):

$$\langle O \rangle = \frac{u_O}{L^{\hat{\Delta}_O}}. \quad (\text{A6})$$

The profile of the S^2 observable, being coupled to the energy operator [Eq. (A1)], satisfies a scaling form identical to Eq. (16):

$$\begin{aligned} \langle S_{x,z}^2 \rangle &= S_0^2 + \frac{A_{S^2}}{(2(z+z_0))^{\Delta_\epsilon}} \left[1 + B_\epsilon \left(\frac{z+z_0}{L} \right)^{\hat{\Delta}} \right. \\ &\quad \left. + C(z+z_0)^{-2} \right], \end{aligned} \quad (\text{A7})$$

with S_0^2 extracted by Eq. (A3). Analogous to the above discussion, we have $A_{S^2} = \mathcal{N}_{S^2} a_\epsilon$. We notice that B_ϵ in Eqs. (16) and (A7) are the same universal amplitude. At the special transition, the observable S^2 on the surface couples to the $\mathbb{Z}_2$ -even operator ε ; hence, its surface average $S_{\text{surf}}^2 \equiv (1/L^2) \sum_{\vec{x}} \langle S_{\vec{x},0}^2 \rangle$ satisfies a finite-size behavior analogous to Eq. (19):

$$S_{\text{surf}}^2 = \Sigma_0 + U_{\varepsilon^2} L^{-\hat{\Delta}_\varepsilon}. \quad (\text{A8})$$

Correlations involving surface quantities follow from a similar expansion of the lattice observables in boundary CFT

fields:

$$\begin{aligned} S_{\mathbf{x},0} &= \mathcal{N}_\sigma (1 + c_\sigma \vec{\nabla}^2) \sigma, \\ S_{\mathbf{x},0}^2 - \langle S_{\mathbf{x},0}^2 \rangle &= \mathcal{N}_{\sigma^2} (1 + c_{\sigma^2} \vec{\nabla}^2) O, \\ E_{\mathbf{x},0} - \langle E_{\mathbf{x},0} \rangle &= \mathcal{N}_O (1 + c_O \vec{\nabla}^2) O, \end{aligned} \quad (\text{A9})$$

where O is the lowest-lying $\mathbb{Z}_2$ -even surface operator, $O = D$ the displacement operator in the ordinary and in the normal UC, and $O = \varepsilon$ the relevant boundary $\mathbb{Z}_2$ -even operator in the special UC. From this expansion and the OPE of $\sigma \times \sigma$, it follows that $B_{\sigma\sigma}$ in Eq. (15) is related to the OPE coefficient $\lambda_{\sigma\sigma O}$ by

$$B_{\sigma\sigma} = \lambda_{\sigma\sigma O} u_O. \quad (\text{A10})$$

Further, using Eq. (A9), one obtains Eq. (20) and an analogous scaling form for the two-point function of S^2 on the surface at the special UC:

$$\langle S_{\mathbf{x},0}^2 S_{\mathbf{0},0}^2 \rangle = \frac{\mathcal{N}_{\sigma^2}^2}{x^{2\hat{\Delta}_\varepsilon}} \left[1 + B_{\varepsilon\varepsilon} \left(\frac{x}{L} \right)^{\hat{\Delta}_\varepsilon} + C x^{-2} \right]. \quad (\text{A11})$$

We notice that the $B_{\varepsilon\varepsilon}$ in Eqs. (20) and (A11) are the same amplitude, related to the OPE coefficient $\lambda_{\varepsilon\varepsilon\varepsilon}$ by

$$B_{\varepsilon\varepsilon} = \lambda_{\varepsilon\varepsilon\varepsilon} u_\varepsilon, \quad (\text{A12})$$

where u_ε is the universal finite-size amplitude of ε [see Eq. (A6)]. Finally, the scaling behavior of the surface-bulk correlation (17) follows from Eqs. (A1) and (5), with $M_{\phi\sigma} = b_{\phi\sigma} 2^{\hat{\Delta}_\sigma - \hat{\Delta}_\phi} \mathcal{N}_S \mathcal{N}_\sigma$ and $B_{\phi\sigma} = \beta_{\phi\sigma} u_O$ [5].

Appendix B: Critical Casimir amplitude. Given a three-dimensional system $L_\parallel \times L_\parallel \times L$ with lateral size $L_\parallel$, the critical Casimir force F_C is defined by

$$F_C \equiv - \frac{\partial [L(\mathcal{F}^{(s)} - f_{\text{bulk}}^{(s)})]}{\partial L} \bigg|_{L_\parallel, T}, \quad (\text{B1})$$

where $\mathcal{F}^{(s)}$ is the singular part of the free energy per volume $L_\parallel^2 L$ and in units of $k_B T$, and $f_{\text{bulk}}^{(s)}$ is its thermodynamic limit $f_{\text{bulk}}^{(s)} = \lim_{L_\parallel, L \rightarrow \infty} \mathcal{F}^{(s)}$. At a critical point $T = T_c$ and for homogeneous BCs, or in the absence of a relevant length,

$$F_C = \frac{\Theta}{L^3}. \quad (\text{B2})$$

At the critical point, $\mathcal{F}^{(s)}(T = T_c) = A/L^3$. The critical Casimir amplitude Θ is related to the finite-size amplitude A of $\mathcal{F}^{(s)}$ by $\Theta = 2A$.

To compute the critical Casimir amplitude, we employ the so-called coupling-parameter approach [90]. In essence, this consists in a combination of MC sampling and a numerical integration, yielding the free energy difference between systems with thicknesses L and $L - 1$ and identical lateral sizes. We refer to Refs. [47,60] for a discussion on the implementation. For the numerical integration, we use the Gauss-Kronrod method with 41/20 nodes, allowing for an accurate convergence of the integral; by comparing the resulting quadrature with 41 and 20 nodes, we checked that the systematic error of the quadrature is negligible with respect to the statistical error bar. The free energy difference $I(L)$ at criticality is then

TABLE III. Fits of the critical Casimir amplitude [Eq. (B3)] as a function of the minimum lattice size $L_{\min}$ taken into account, for three BCs considered here; d.o.f. denotes the number of degrees of freedom of a fit.

BCs: (o, o)				
$L_{\min}$	$F_{\text{bulk}}(\beta_c)$	Θ	C	$\chi^2/\text{d.o.f.}$
8	0.075 736 842(44)	0.3005(14)	−0.184(11)	0.8
12	0.075 736 839(51)	0.3009(37)	−0.189(44)	1.1
16	0.075 736 895(57)	0.2907(66)	−0.01(11)	0.1
BCs: $(+, o)$				
$L_{\min}$	$F_{\text{bulk}}(\beta_c)$	Θ	C	$\chi^2/\text{d.o.f.}$
8	0.075 737 047(23)	0.5818(11)	−1.1665(89)	20.9
12	0.075 736 947(25)	0.5959(19)	−1.382(26)	1.9
16	0.075 736 923(29)	0.6013(34)	−1.496(64)	1.0
BCs: $(+, +)$				
$L_{\min}$	$F_{\text{bulk}}(\beta_c)$	Θ	C	$\chi^2/\text{d.o.f.}$
8	0.075 736 644(41)	−0.7794(16)	1.561(13)	2.7
12	0.075 736 715(47)	−0.7896(37)	1.695(45)	0.5
16	0.075 736 740(54)	−0.7945(65)	1.78(11)	0.3

fitted to

$$I(L) = F_{\text{bulk}}(\beta_c) + \frac{\Theta}{(L - 1/2)^3} + \frac{C}{(L - 1/2)^4}, \quad (\text{B3})$$

where $F_{\text{bulk}}(\beta_c)$ is the bulk free energy density at criticality, Θ is the desired Casimir amplitude, and the last term is due to $1/L$ scaling corrections. We note that for the BCs considered here, previous MC studies have considered the limit of infinite lateral size $L_\parallel$, whereas in this work we have chosen a geometry with equal sizes on all directions. Indeed, like any other FSS quantity, the Casimir amplitude depends on the aspect ratio $\rho = L/L_\parallel$ of the system. The dependence on ρ for three-dimensional models in the Ising universality class and periodic BCs has been studied in Ref. [91] with field-theoretical methods and in Ref. [92] with MC simulations. Furthermore, the aspect-ratio dependence has been investigated for nonhomogeneous BCs, in the presence of a chemical step and in the limit $\rho \rightarrow 0$ in Refs. [47,61]. In this situation, the chemical step forms a line defect and gives rise to a linear ρ dependence of the critical Casimir force on ρ , for $\rho \rightarrow 0$, allowing to extract its contribution to the Casimir force. In two dimensions, the aspect-ratio dependence of the Casimir force in Ising models with various BCs has been investigated in Refs. [93–96]. For three of the BCs studied here, we have computed $I(L)$ for lattice sizes $L = 8, 12, 16, 24, 32, 48$, and 64 . Corresponding fits to Eq. (B3) are reported in Table III. Inspecting the fit results, we infer the following estimates of the critical Casimir amplitude Θ :

$$\Theta = 0.301(4) \quad (o, o) \text{ BCs}, \quad (\text{B4})$$

$$\Theta = 0.601(4) \quad (+, o) \text{ BCs}, \quad (\text{B5})$$

$$\Theta = -0.790(4) \quad (+, +) \text{ BCs}. \quad (\text{B6})$$

As noted above, all these amplitudes pertain to a model with aspect ratio $\rho = 1$. Interestingly, for (o, o) BCs, we

obtain a positive, i.e., repulsive critical Casimir amplitude. This is in stark contrast with slab limit $\rho = 0$, where the amplitude is negative $\Theta = -0.030(5)$ [60]. For $(+, o)$ BCs, Θ is significantly larger than for $\rho = 0$, where $\Theta = 0.492(5)$ [60]. In the case of $(+, +)$ BCs, we find instead that the critical Casimir amplitude Θ is rather close to the $\rho = 0$

limit, where $\Theta = -0.820(15)$ [58]. The data in Table III allow us to estimate the critical bulk free energy density. Considering the spread in the fitted values for different BCs, we conservatively estimate $F_{\text{bulk}}(\beta_c) = 0.075\,7368(1)$, improving the estimate $F_{\text{bulk}}(\beta_c) = 0.075\,7368(4)$ of Ref. [58].

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