Extraordinary-log Universality of Critical Phenomena in Plane Defects

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(Received 28 January 2023; revised 24 August 2023; accepted 13 October 2023; published 15 November 2023)

The recent discovery of the extraordinary-log (E-Log) criticality is a celebrated achievement in modern critical theory and calls for generalization. Using large-scale Monte Carlo simulations, we study the critical phenomena of plane defects in three- and four-dimensional O(n) critical systems. In three dimensions, we provide the first numerical proof for the E-Log criticality of plane defects. In particular, for $n = 2$, the critical exponent $\hat{q}$ of two-point correlation and the renormalization-group parameter α of helicity modulus conform to the scaling relation $\hat{q} = (n-1)/(2\pi\alpha)$, whereas the results for $n \geq 3$ violate this scaling relation. In four dimensions, it is strikingly found that the E-Log criticality also emerges in the plane defect. These findings have numerous potential realizations and would boost the ongoing advancement of conformal field theory.

DOI: 10.1103/PhysRevLett.131.207101

Introduction.—In the standard scenario of critical phenomena, the two-point correlation asymptotically decays as $g(r) \sim r^{-(d-2+\eta)}$ with spatial distance r, where d and η are spatial and anomalous dimensions, respectively [1].

Recently, a very unusual type of critical phenomena was unveiled in the context of surface critical behavior (SCB) [2]. Consider the O(n) model of pairwise-interacting unit-vector spins. The cases $n = 1$, 2, and 3, respectively, correspond to the Ising, XY, and Heisenberg models. In two dimensions, the Mermin-Wagner theorem prohibits spontaneous symmetry breaking for any finite temperature $T > 0$ with $n \geq 2$. Specifically, as T decreases, the XY model enters a quasi-long-range ordered phase via the Berezinskii-Kosterlitz-Thouless (BKT) transition [3–6], while the system with $n > 2$ remains disordered for all $T > 0$. However, the open surfaces of the critical three-dimensional (3D) O(n) models, with $n = 2$, 3, and 4, were observed to undergo a so-called special phase transition and enter the extraordinary phase, as the surface coupling strength is enhanced [7,8]. The nature of the extraordinary phase remained a long-standing puzzle until a recent renormalization-group study [2], which revealed the extraordinary-log (E-Log) critical phase for $2 \leq n < n_c$, with n_c an upper bound.

In the E-Log critical phase, the correlation function decays as a power law of distance logarithm, $g(r) \sim (\ln r)^{-(\hat{q}+1)}$, with $\hat{q}+1$ a critical exponent [2], which is extremely slowly in comparison with $r^{-(d-2+\eta)}$ for the standard scenario. Moreover, for a finite 3D lattice of side length L, $g(r, L)$ was numerically observed to exhibit a two-distance scaling behavior as $g(r, L) \sim c_1(\ln r)^{-(\hat{q}+1)} + c_2(\ln L)^{-\hat{q}}$, with c_1 and c_2 being constants [9]. In other words, the correlation function decays algebraically with the distance logarithm and then enters into a L-dependent plateau, of which the height decreases algebraically with the side-length logarithm (with exponent $\hat{q}$). On the other hand, the helicity modulus Υ, characterizing the response against a twist in boundary conditions [10], scales as $\Upsilon L \sim 2\alpha(\ln L)$, with α a renormalization-group parameter. A scaling relation reads [2,9]

$$\hat{q} = \frac{n-1}{2\pi\alpha}, \tag{1}$$

while the original formula means $\hat{q} + 1 = [(n-1)/2\pi\alpha]$ [2]. The E-Log criticality and scaling relation (1) were first verified at $n = 3$ [11]. For the XY model, the universality of $\hat{q}$ and α was confirmed in the E-Log critical regime [9]. Shortly afterwards, consistent estimates of $\hat{q}$ and α were obtained for $n = 2$ from different realizations of O(2) criticality [12–17] (Table I).

Since the E-Log criticality has been found merely for the SCB of 3D systems, a generalization is essential. Using large-scale Monte Carlo simulations, we provide smoking-gun evidence of the E-Log criticality in the plane defects sitting inside critical 3D Villain, XY, Heisenberg, and O(6) vector models. The emergence of the E-Log criticality is consistent with a very recent field-theoretic result [18]. Furthermore, we find that, while the values of $\hat{q}$ and α for $n = 2$ are compatible with scaling relation (1), violations of this well-established scaling relation are found for $n \geq 3$. Another important generalization is to the 4D XY model. Despite the trivial mean-field critical behavior in the bulk, we find that the plane defect can enter the E-Log critical phase via an exotic transition. Note that the O(n) spin model is perhaps the most important class of models in statistical mechanics and has broad application in

TABLE I. E-Log critical phases of O(n) systems. "BU" denotes bulk universality, and △ (▲) represents the conformity (inconformity) with scaling relation (1).

Surface critical phenomena					
BU	Model	$\hat{q}$	α	△/▲	year
3D O(3)	O(3) ϕ^4 [11]	2.1(2)	0.15(2)	△	2020
	O(3) ϕ^4 [12]		0.190(4)		2021
3D O(2)	XY [9]	0.59(2)	0.27(2)	△	2021
	O(2) ϕ^4 [12]		0.300(5)		2021
	Potts [13]	0.60(2)			2022
	clock [14]	0.59(1)	0.26(2)	△	2022
	Villain [16]	0.58(2)	0.28(1)	△	2022
	Potts [17]	0.59(3)			2023

Plane-defect critical phenomena					
BU	Model	$\hat{q}$	α	△/▲	year
3D O(2)	field theory [18]		0.600(10)		2023
	Villain, XY	0.29(2)	0.56(3)	△	present
3D O(3)	field theory [18]		0.540(8)		2023
	Heisenberg	0.63(3)	0.33(2)	▲	present
4D O(2)	XY	0.09(2)	0.97(7)		present

condensed-matter physics. In particular, we expect that the E-Log universality in the plane defects would find numerous realizations in the line defects of 2D and 3D quantum models for superfluidity, superconductivity, magnetism, etc.

E-Log universality in 3D plane-defect Villain model.—We consider a plane-defect Villain model on the simple-cubic lattice with Hamiltonian $\mathcal{H} = \frac{1}{2}\sum_{\langle \mathbf{rr}'\rangle}(\mathcal{J}^2_{\mathbf{rr}'}/C_{\mathbf{rr}'})$, where $\mathcal{J}_{\mathbf{rr}'} \in \{0, \pm1, \pm2, \ldots\}$ represents directed flows along the bonds between the nearest neighbors $\mathbf{r}$ and $\mathbf{r}'$, and $C_{\mathbf{rr}'}$ controls their relative weights. As in the standard Villain model [19–24], the flows are nondivergent and constitute closed directed loops. Periodic boundary conditions are imposed in each of the [100] (x), [010] (y), and [001] (z) directions. To involve a plane defect, we specify a plane that is perpendicular to the z direction [Fig. 1(a)]. If $\mathbf{r}$ and $\mathbf{r}'$ are both in the plane defect, we set $C_{\mathbf{rr}'} = W$; otherwise, we let $C_{\mathbf{rr}'} = K$. The bulk critical point K_c was located at $K = 0.333\,067\,04(7)$ with $W = K$ [25] and falls into 3D O(2) universality class.

We formulate a variant of Prokof'ev-Svistunov worm Monte Carlo algorithm that has two update schemes, respectively, for entire lattice and plane defect, and is very convenient for the measurements of correlation function and susceptibility in the plane defect; see the Supplemental Material [26] (which includes [27] and [25,28,29]).

In Fig. 1(b), we map out a phase diagram. When the bulk is critical ($K = K_c$), a plane-defect transition occurs at $W = K_c$ as W is varied and has the effective thermodynamic renormalization exponent $y_t = 1/\nu_{3xy} - 1 \approx 0.4885$, with $\nu_{3xy} = 0.671\,83(18)$ [25] the correlation length exponent of 3D O(2) bulk criticality. This transition differs from the special transition for open surfaces in O(2) systems, which has $y_t = 0.58(1)$ [7,16]. Additionally, we confirm the field-theoretic prediction [30] of ordinary critical phase for $W < K_c$ at $K = K_c$ and the BKT-like transition with $K < K_c$. The BKT-like transition arises from the essential 2D critical behavior of plane defect in a disordered bulk [30]. For these plane-defect critical phenomena, Monte Carlo results are presented in the Supplemental Material [26].

We then explore the strong-W regime with $K = K_c$. Extensive worm-algorithm simulations are performed at $W = 0.5$, 1, 3 and 7, with L ranging from 4 to 128. At $L = 128$, the total number of generated closed loops for a specified W reaches 2.9×10^{10}. If the E-Log criticality happens, a fitting *Ansatz* of the large-distance correlation G

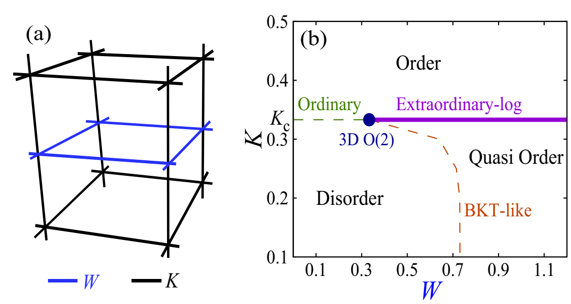

FIG. 1. A 3D lattice with a plane defect (a) and the phase diagram for the plane defect in 3D Villain model (b). W and K represent the interactions inside and outside the plane defect, respectively. There are quasi-long-range ordered, ordered, and disordered phases. The plane-defect critical phenomena include the ordinary, 3D O(2) and E-Log criticality at the bulk critical point K_c as well as the BKT-like transition for $K < K_c$.

in the plane defect is $G = a_0[\ln(L/l_0)]^{-\hat{q}}$, with a_0 a nonuniversal constant and l_0 a reference length. Generally speaking, numerical analyses of finite-size scaling (FSS) involving $\ln L$ are challenging. Such a difficulty can be alleviated at the cost of systematic fits. Throughout this Letter, we test the scaling *Ansatz* against data by least-squares fits. We monitor the evolution of χ^2 by changing the minimum size $L_{\min}$ involved. In principle, one searches for the smallest $L_{\min}$ relating to the χ^2 per degree of freedom (DOF) $\chi^2/\mathrm{DOF} = \mathcal{O}(1)$, which does not decrease drastically upon further increasing $L_{\min}$. Practically one prefers the fits with $\chi^2/\mathrm{DOF} \approx 1$. We should not trust any single fit and conclusions will be made by comparing preferred fits. For each W, we find that the estimate of $\hat{q}$ extrapolates to $\hat{q} \approx 0.29$. More precisely, for $W = 0.5$, 1, 3, and 7, we obtain $\hat{q} = 0.308(2)$, 0.301(2), 0.289(5), and 0.28(1) as well as $\chi^2/\mathrm{DOF} \approx 2.8$, 0.1, 2.8, and 1.5, respectively, with $L_{\min} = 16$. Based on these observations, by fixing $\hat{q} = 0.29$, we obtain $l_0 = 3.15(2)$, 0.684(2), 0.0153(2), and 0.0000100(3) as well as $\chi^2/\mathrm{DOF} \approx 2.4$, 1.4, 0.8, and 0.7, with $L_{\min} = 48$, 32, 64, and 48, for $W = 0.5$, 1, 3, and 7, respectively. Details of fits are given in the Supplemental Material [26]. The consistent estimates of $\hat{q}$ from various W indicate the uniqueness of logarithmic scaling and critical exponent.

Borrowing the insights into FSS from the E-Log criticality of SCB, we obtain the FSS $\chi_s = a_1 L^2[\ln(L/l_0)]^{-\hat{q}}$ of the plane-defect susceptibility χ_s, with a_1 a nonuniversal constant. For $W = 0.5$, the fit with $L_{\min} = 16$ yields $\hat{q} = 0.322(1)$ and has a huge χ^2/DOF ($\chi^2/\mathrm{DOF} \approx 7.0$), which reduces to $\chi^2/\mathrm{DOF} \approx 2.7$ at $L_{\min} = 32$ with $\hat{q} = 0.309(3)$. For $W = 1$, 3, and 7, we obtain $\hat{q} = 0.310(1)$, 0.295(3), and 0.29(1) as well as $\chi^2/\mathrm{DOF} \approx 1.7$, 3.2, and 3.0, respectively. When $\hat{q} = 0.29$ is fixed, we obtain $l_0 = 4.08(3)$ ($W = 0.5$), 0.866(3) ($W = 1$), 0.01909(9) ($W = 3$), and 0.0000119(3) ($W = 7$) with $0.3 \lessapprox \chi^2/\mathrm{DOF} \lessapprox 1.4$. Hence, the estimates of $\hat{q}$ are close to those from G.

From the FSS analyses of G and χ_s, we estimate $\hat{q} = 0.29(2)$. In Figs. 2(a) and 2(b), by plotting G and $\chi_s L^{-2}$ versus $\ln(L/l_0)$, where the values of l_0 are from fits, the mutually consistent scaling formulae and critical exponent are illustrated.

We analyze the helicity modulus Υ, which is defined through the fluctuations of winding number $\mathcal{W}_x$ of directed flows along a periodic direction (say x direction), namely, $\Upsilon = \langle \mathcal{W}_x^2 \rangle / L$. For the E-Log criticality in a 3D system, Υ scales as $\Upsilon L \sim \ln L$. This behavior is roughly illustrated by the data in Fig. 2(c). We perform least-squares fits to $\Upsilon L = \alpha(\ln L) + b + cL^{-\omega}$, where α can be universal, ω denotes the exponent of leading finite-size corrections, whereas b and c are nonuniversal. Unlike the scaling form $\Upsilon L = 2\alpha(\ln L) + b + cL^{-\omega}$ that applies to SCB involving two open surfaces, the prefactor is α due to the uniqueness of plane defect. We look into the fits using $\omega = 0.789$ [31,32] or $\omega = 1$, and find that the inclusion of a correction term stabilizes fits. For $W = 0.5$, 1, 3, and 7, we obtain $\alpha = 0.555(3)$, 0.562(4), 0.580(6), and 0.57(1) as well as $\chi^2/\mathrm{DOF} \approx 0.2$, 0.7, 2.0, and 2.2, respectively, with $L_{\min} = 16$. Comparing all preferred fits (Supplemental Material [26]), we estimate $\alpha = 0.56(3)$.

The universal results of $\hat{q}$ and α from different W prove the universality of the E-Log criticality. Furthermore, the values of $\hat{q}$ and α cannot be related to any known E-Log criticality, indicating a new universality class. In the Supplemental Material [26], it is demonstrated that $\hat{q}$ and α from direct fits are consistent with those from the conversions according to Eq. (1), and such consistency is even more obvious at $\chi^2/\mathrm{DOF} \approx 1$. Thus, scaling relation (1) is validated for the present E-Log universality.

E-Log criticality in 3D plane-defect O(n) *vector models.*—We consider the plane-defect O(n) vector models with Hamiltonian $\mathcal{H} = -\sum_{\langle \mathbf{r}\mathbf{r}' \rangle} C_{\mathbf{r}\mathbf{r}'} \vec{S}_{\mathbf{r}} \cdot \vec{S}_{\mathbf{r}'}$, where $\vec{S}_{\mathbf{r}}$ represents n-component unit-vector spins. Using the Wolff cluster Monte Carlo algorithm [33], we sample the helicity modulus $\Upsilon = (1/L^d)\{(2/n)\langle E \rangle - [2/n(n-1)] \sum_{a<b} \langle (T_{\mathbf{e}_x}^{(a,b)})^2 \rangle \}$ with $E = \sum_{\mathbf{r}} C_{\mathbf{r}(\mathbf{r}+\mathbf{e}_x)} \vec{S}_{\mathbf{r}} \cdot \vec{S}_{\mathbf{r}+\mathbf{e}_x}$ and $T_{\mathbf{e}_x}^{(a,b)} = \sum_{\mathbf{r}} C_{\mathbf{r}(\mathbf{r}+\mathbf{e}_x)} (S_{\mathbf{r}}^a S_{\mathbf{r}+\mathbf{e}_x}^b - S_{\mathbf{r}}^b S_{\mathbf{r}+\mathbf{e}_x}^a)$, where $(S_{\mathbf{r}}^a,\ S_{\mathbf{r}}^b)$ represents pairs of components of $\vec{S}_{\mathbf{r}}$, as well as the

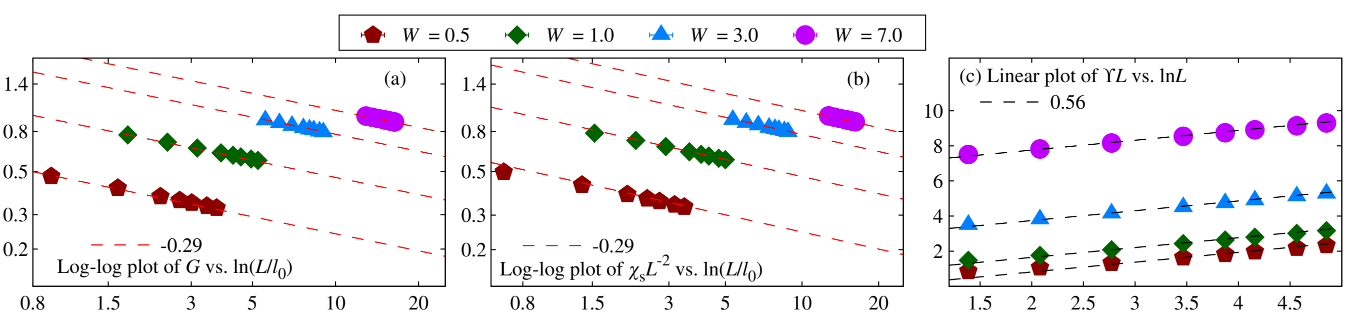

FIG. 2. The two-point correlation G (a), the scaled susceptibility $\chi_s L^{-2}$ (b) and the scaled helicity modulus ΥL (c) for the E-Log critical phase of the 3D plane-defect Villain model. In panels (a) and (b), the horizontal coordinates are set as $\ln(L/l_0)$, where the values of l_0 are from least-squares fits, and the plots are further made on log-log scales. The slopes -0.29 and 0.56 of dashed lines stand for $-\hat{q}$ and α, respectively.

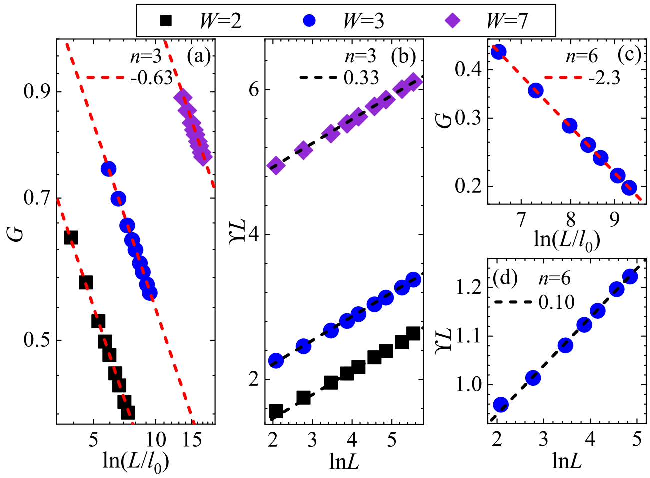

FIG. 3. Same as Figs. 2(a) and 2(c) but for the E-Log critical phases of the 3D plane-defect Heisenberg and O(6) vector models.

two-point correlation $G = \langle \vec{S}_{\mathbf{r}} \cdot \vec{S}_{\mathbf{r}'} \rangle$ with $\mathbf{r}' - \mathbf{r} = (L/2, 0)$ in the plane defect.

We consider the $n = 2$ (XY) case on the simple-cubic lattice with $K = K_c = 1/2.201\,844\,1$, where K_c is the bulk critical point [25], and simulate at $W = 1$, 3, and 7. For G and Υ, we perform FSS analyses using the scaling *Ansatz* for the E-Log criticality. In the Supplemental Material [26], using a specially designed χ^2 test, we confirm that $\hat{q}$ and α agree with those from the plane-defect Villain model. Thus far, all uncovered E-Log critical phenomena conform to scaling relation (1).

We now study the E-Log universality for the $n = 3$ (Heisenberg) case on the simple-cubic lattice. We start by simulating the $W = K$ case up to $L = 384$ and obtain $K_c \approx 0.693\,002\,88$, which surpasses the most accurate result $K_c = 0.693\,003(2)$ in literature [7]. We then simulate at $W = 2$, 3, and 7 with $K = 0.693\,002\,88$, and confirm the existence of E-Log criticality (Supplemental Material [26]). Furthermore, we find the universality of $\hat{q}$ and α with $\hat{q} = 0.63(3)$ and $\alpha = 0.33(2)$, which violate scaling relation (1). With the estimated $\hat{q}$ and α, the FSS of G and Υ are displayed in Figs. 3(a) and 3(b), respectively.

Because of the upper bound $n_c \approx 5$, the E-Log criticality does not exist for $n > 5$ in the open surfaces of 3D systems [34]. By contrast, for the plane-defect O(6) vector model, we find the E-Log criticality with $\hat{q} = 2.3(1)$ and $\alpha = 0.10(1)$ at $K = K_c = 1.428\,653$ [35] and $W = 3$ [Figs. 3(c) and 3(d)], which again violates scaling relation (1).

Exotic plane-defect transition and E-Log universality in 4D XY model.—The E-Log criticality has merely been found in the plane defects and open surfaces of 3D systems. Is there an E-Log universality class for any other spatial dimension? We consider the plane-defect XY model on 4D hypercubic lattices [Fig. 4(a)] with $K = K_c$, for which one has $K_c = 1/3.314\,437$ [36].

At $W = K_c$, the effective plane-defect thermodynamic renormalization exponent y_t vanishes, since $y_t = 1/\nu_{4xy} - 2$ and $\nu_{4xy} = 1/2$ apply, and the interaction enhancement can be exactly marginal, marginally relevant or marginally irrelevant. The scaled second-moment correlation length ξ/L indicates a transition at $W_c \approx 0.41$ by the deviation from scale invariance for $W > W_c$ [Fig. 4(b)]. In the Supplemental Material [26], we perform systematic FSS analyses using various scaling *Ansätze*: a standard scaling with L^{y_t} (with or without logarithmic corrections) and a scaling with $y_t = 0$ but involving $\ln L$. The estimates of W_c from preferred least-squares fits are compatible with $W_c = 0.41(2)$. Hence, our results reveal a transition at W_c, which is compatible with the marginally irrelevant scenario, since W_c is significantly larger than K_c. Similar to the FSS at $W = K_c$, G scales as $G \sim L^{-2}$ at $W = 0.1$, indicating a critical behavior for $W < W_c$ governed by the Gaussian fixed point.

For $W > W_c$, we find the E-Log criticality. Figure 4(c) shows, for $W = 1$, 3, and 6, that G scales as $G \sim [\ln(L/l_0)]^{-\hat{q}}$ with the universal exponent $\hat{q} = 0.09(2)$. Divergence of ΥL^2 upon increasing L is inferred from Fig. 4(d). Using least-squares fits, we find that Υ scales as

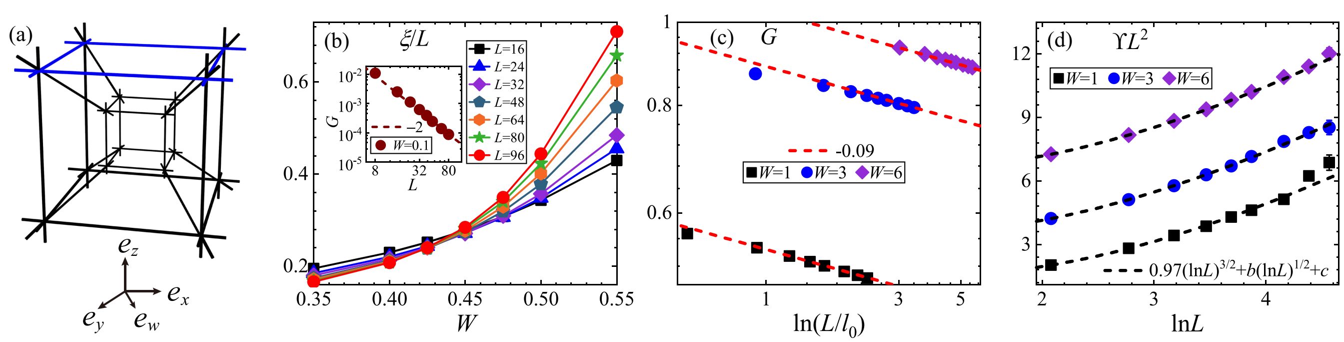

FIG. 4. Plane-defect criticality of 4D XY model at $K = K_c$. (a) A 4D hypercubic lattice with a plane defect. (b) The scaled second-moment correlation length ξ/L versus W. Inset: log-log plot of G versus L at $W = 0.1$. (c) Log-log plot of G versus $\ln(L/l_0)$ for $W = 1$, 3, and 6, where the values of l_0 are from least-squares fits. The slope -0.09 of dashed lines stands for $-\hat{q}$. (d) ΥL^2 versus $\ln L$. The dashed lines stand for $\Upsilon L^2 = 0.97(\ln L)^{3/2} + b(\ln L)^{1/2} + c$, where b and c are from least-squares fits.

$\Upsilon L^2[\ln(L/l_0)]^{-1/2} \sim \alpha \ln(L/l_0)$ with the universal parameter $\alpha = 0.97(7)$. In this FSS formula, the left-hand side relates to the FSS $\Upsilon_{4D} \sim L^{-4}(\xi_{4D})^2 \sim L^{-2}[\ln(L/l_0)]^{1/2}$ of 4D bulk criticality with the exponents -2 and $1/2$ for leading scaling and logarithmic correction respectively [36], whereas the E-Log universality accounts for $\alpha \ln(L/l_0)$ in the right-hand side.

Summary and discussions.—We study the plane-defect criticality of the O(n) model with $n = 2$, 3, and 6 in three dimensions and $n = 2$ in four dimensions, and obtain convincing evidence of the E-Log criticality for each situation. In three dimensions, the E-Log criticality for $n \geq 3$ violates scaling relation (1), which holds for $n = 2$. For a plane defect in the critical 4D *XY* system, the presence of E-Log universality and exotic transition is also evidenced. These findings significantly expand the current understanding of E-Log criticality.

The study for 3D and 4D plane-defect systems is a remarkable step toward exploring E-Log criticality in generic O(n) systems with effective interactions. The hints for such a generalization also come from the logarithmic forms of correlators in certain 2D O(n) loop models [37,38].

Our findings can be realized with *emergent* O(n) symmetry or O(n)-symmetric Hamiltonian with $n \geq 2$. Because of classical-quantum correspondence, our results further indicate the E-Log universality for the line defects in 2D and 3D quantum O(n) systems [39–44]. Besides, the conformal field theory of plane-defect criticality is currently a subject of intensive research [45–48].

This work was supported by the National Natural Science Foundation of China (Grants No. 12275002, No. 12275263, No. 11975024), Innovation Program for Quantum Science and Technology (Grant No. 2021ZD0301900), Natural Science Foundation of Fujian province of China (under Grant No. 2023J02032), and National Key R&D Program of China (Grant No. 2018YFA0306501).

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