Quantum extraordinary-log universality of boundary critical behavior

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The recent discovery of extraordinary-log universality has generated intense interest in classical and quantum boundary critical phenomena. Despite tremendous efforts, the existence of quantum extraordinary-log universality remains extremely controversial. Here, by utilizing quantum Monte Carlo simulations, we study the quantum edge criticality of a two-dimensional Bose-Hubbard model featuring emergent bulk criticality. On top of an insulating bulk, the open edges experience a Kosterlitz-Thouless-like transition into the superfluid phase when the hopping strength is sufficiently enhanced on edges. At the bulk critical point, the open edges exhibit the special, ordinary, and extraordinary critical phases. In the extraordinary phase, logarithms are involved in the finite-size scaling of two-point correlation and superfluid stiffness, which admit a classical-quantum correspondence for the extraordinary-log universality. Thanks to modern quantum emulators for interacting bosons in lattices, the edge critical phases might be realized in experiments.

I. INTRODUCTION

Scaling and universality are pillars of modern critical phenomena [1]. In the paradigm of criticality, the two-point correlation \( g(r) \) decays as the power law [1–4]

\[ g(r) \sim r^{2-(d+z)-\eta} \]  

with the spatial distance \( r \), where \( d \), \( z \) and \( \eta \) are respectively spatial dimension, dynamic critical exponent and anomalous dimension.

Boundary critical behavior (BCB) refers to the critical phenomena occurring on boundaries of a critical bulk [5–16] and relates to a rich variety of state-of-the-art concepts [17–23]. Recently, in the context of BCB, the extraordinary-log universality (ELU) was predicted by Metlitski for the classical three-dimensional (3D) O(N) model with \( 2 \leq N < N_c \), where \( N_c \) is an upper bound [24]. For ELU the boundary two-point correlation \( g(r) \) decays logarithmically with \( r \) as [24]

\[ g(r) \sim [\ln(r)]^{-\hat{\eta}}, \]

where \( \hat{\eta} \) is only dependent on \( N \). Shortly afterwards, much attention was devoted to the BCB in classical [25–31] and quantum [32–36] systems.

Evidence for classical ELU was obtained from the Monte Carlo simulations of Heisenberg and XY models [25, 26, 28]. Inspired by the studies using magnetic fluctuations at different Fourier modes to explore precise finite-size scaling (FSS) [37, 38] as well as the two-length scenarios for high-dimensional Ising models [39–44] and deconfined criticality [45], an alternative scaling formula of \( g(r) \) was conjectured for ELU [26]. This conjecture was based on the fact that the critical magnetic fluctuations at zero and smallest non-zero modes scale as \( L^2[\ln(L)]^{-\hat{\eta}} \) and \( L^2[\ln(L)]^{-\hat{\eta}} \), with the critical exponents \( \hat{\eta} \) and \( \hat{\eta} = \hat{\eta} + 1 \), respectively. This observation can be related to the FSS of \( g(r) \) as [26]

\[ g(r) \sim \begin{cases} [\ln(r)]^{-\hat{\eta}}, & \ln(r) \leq O[(\ln(L))^{\hat{\eta}/\eta}], \\ [\ln(L)]^{-\hat{\eta}}, & \ln(r) \geq O[(\ln(L))^{\hat{\eta}/\eta}]. \end{cases} \]  

With the concept “unwrapping” [40, 46, 47], a geometric explanation of two-length scenario was introduced based on unwrapped correlation length [40, 44, 48]. The two exponents \( \hat{\eta} \) and \( \hat{\eta} \) were also observed in the classical ELU at an emergent O(2) critical point [30]. Eq. (3) formally agrees with (2) on the FSS of \( g(r) \) in the \( r \to \infty \) limit.

Quantum edge criticality (QEC) has been extensively studied in the two-dimensional dimerized antiferromagnetic quantum (2D-DAQ) Heisenberg and XXZ models, which are prototype models for O(3) and O(2) criticality [13–16, 32–34], respectively. On one hand, the dangling edges of 2D-DAQ spin-1/2 and spin-1 Heisenberg models harbor the non-ordinary criticality [14–16, 32], where the critical exponents in magnetic sector are almost compatible with O(3) special transition [14, 15]. The numerical results for scaling dimension \( \Delta_n \) of Néel (valence bond solid) order were compared [32] to the field-theoretic prediction [49]

\[ \Delta_n - 1/2 = \epsilon_n \text{ and } \Delta_v - 1/2 = -3\epsilon_n \]  

with \( \Delta_v - 3/2 = -\epsilon_n \), where \( \Delta_v \approx 1.187 \) [10] is the scaling dimension of spin order in O(3) ordinary universality. For the spin-1/2 case, the results do not agree with Eq. (4) but conform with the scaling relation \( 3\Delta_n + \Delta_v = 2 \). For the spin-1 case, the estimate \( \Delta_v \approx -2 \) is roughly compatible with the theory of extraordinary-power phase [24], hence in sharp contrast to Eq. (4) and the theory of ELU. On the other hand, the non-dangling edges of 2D-DAQ spin-1/2 Heisenberg model host the ordinary phase, special transition and long-range ordered extraordinary phase [14, 15, 33]. Moreover, the 2D-DAQ spin-1 XXZ model may exhibit the extraordinary-log criticality, yet this observation does not hold for the spin-1/2 case [34].

Hence, despite the tremendous efforts devoted to the BCB of quantum antiferromagnets, the existence of quantum ELU
remains extremely controversial. Moreover, as indicated in Ref. [24], the existing results cannot form a self-contained picture for the classical-quantum correspondence of BCB and failed to realize quantum ELU. Here, we switch to interacting bosons and show that the open-edge Bose-Hubbard model hosts quantum ELU. This conclusion is based on the logarithmic FSS of two-point correlation and superfluid stiffness for extraordinary phase as well as an overall classical-quantum correspondence for various critical phases. The sharp difference from the BCB of XXZ antiferromagnet [34] reflects the sensitivity of BCB to geometric settings and local operators. In the following, we focus on the open-edge Bose-Hubbard model and explore the quantum O(2) BCB of the model. Section II defines the open-edge Bose-Hubbard model and presents its ground-state phase diagram. Section III introduces the methodology adopted throughout present study. Section IV presents Monte Carlo data and scaling analyses. A summary is finally given in Sec. V.

II. MODEL AND GROUND-STATE PHASE DIAGRAM

We consider the square-lattice Bose-Hubbard model at unit boson filling with the Hamiltonian

\[ \hat{H} = - \sum_{\langle ij \rangle} t_{ij} (\hat{b}^+_i \hat{b}_j + \hat{b}^+_j \hat{b}_i) + \hat{U} \sum_i \hat{n}_i (\hat{n}_i - 1), \]

where \( \hat{b}^+_i \) and \( \hat{b}_i \) are respectively bosonic creation and annihilation operators at site \( i \), and \( \hat{n}_i = \hat{b}^+_i \hat{b}_i \). \( t_{ij} \) denotes the amplitude of the nearest-neighbor hopping between \( i \) and \( j \), and \( \hat{U} > 0 \) represents onsite repulsion. The first summation runs over pairs of nearest neighboring sites while the second summation is over sites. We set \( \hat{U} = 1 \) as energy unit.

As illustrated by Fig. 1(a), we define our model for BCB by setting open and periodic boundary conditions along [01] and [10] directions, respectively. Hence, a pair of open edges are specified. The hopping amplitude \( t_{ij} = t' \) on open edges is distinguished from \( t_{ij} = t \) in bulk. The edge hopping enhancement is parameterized by \( \kappa = (t' - t)/t \).

At \( \kappa = 0 \), model (5) reduces to the standard Bose-Hubbard model at unit boson filling [50], which has an emergent O(2) quantum critical point separating the Mott insulating and superfluid phases. This critical point features Lorentz invariance with \( z = 1 \). The present authors and coworkers have given an estimate for the quantum critical point as \( t_c = 0.0597291(8) \) [51], which agrees with the literature result \( t_c = 0.05974(3) \) [52].

We explore quantum phases of model (5) by FSS and the results are summarized as a ground-state phase diagram in Fig. 1(b). There is a phase, dubbed SE-MIB, that features superfluid edges on top of Mott insulating bulk. Moreover, there are three critical edge phases at \( t_c \): the ordinary, special and extraordinary-log phases. Scaling behaviors of edge critical phases are described in Table I [53].

Table I. Leading scaling behaviors of the edge two-point correlation \( g(L/2) \) and the superfluid stiffness \( \rho_s \) in critical phases.

| Critical phase | \( g(L/2) \) | \( \rho_s \) |
|----------------|-------------|------------|
| special        | \( L^{-\eta}, \eta \approx 0.65 \) | \( L^{-1} \) |
| KT-like        | \( L^{-\eta}, \eta = 1/4 \) | \( L^{-1} \) |
| SE-MIB         | \( L^{-\eta}, \eta \in (0, 1/4) \) | \( L^{-1} \) |
| ordinary       | \( L^{-\eta}, \eta \approx 2.438 \) | \( L^{-1} \) |
| extraordinary   | \( [\ln(L)]^{-\eta}, \eta \approx 0.59 \) | \( L^{-1}\ln(L) \) |

III. METHODOLOGY

We apply the Prokof’ev-Svistunov-Tupitsyn worm quantum Monte Carlo algorithm [54, 55] to simulate model (5) in the imaginary-time path integral representation. The maximum side length of the square lattice is up to \( L = 192 \). The inverse temperature is set as \( \beta = L \), which is in line with \( z = 1 \). We study the special, ordinary and extraordinary phases at \( t_c = 0.0597291 \) by varying \( \kappa \), and explore the KT-like transition for \( t < t_c \). In particular, we analyze the extraordinary phase in a broad parameter regime.

Analyses of the FSS involving \( \ln(L) \) may be "notoriously difficult" [56]. We perform the analyses using least-squares fits. Following standard criterion, we prefer the fits with \( \chi^2/DF \sim 1 \), where \( \chi^2 \) is the Chi squared and DF denotes the degree of freedom. We also examine the stability against varying \( L_{\min} \), which represents the minimum side length involved in fitting.
IV. RESULTS

A. Special transition

We detect the special transition by tuning $\kappa$ at $t = t_c$. We sample the winding probability $R_{[10]} = \langle R_{[10]} \rangle$, where $R_{[10]} = 1$ if there exists at least a particle line winding around the periodic [10] direction of square lattice. The winding probability is dimensionless and obeys the FSS $R_{[10]} = \tilde{R}_{[10]}(\epsilon L^{\nu})$, where $\epsilon = \kappa - \kappa_c$ represents the deviation from the critical point $\kappa_c$, and $y_t$ relates to the correlation length exponent $\nu$ by $y_t = 1/\nu$. $\tilde{R}_{[10]}$ is useful for locating critical points [51]. Expanding $\tilde{R}_{[10]}$ and incorporating corrections to scaling, we obtain

$$R_{[10]} = R^c_{[10]} + \sum_j a_j \epsilon^j L^{y_t} + \sum_m b_m \epsilon^{\omega_m}, \quad (6)$$

where $R^c_{[10]}$ is somewhat universal, $a_j$ ($j = 1, 2, \ldots$) and $b_m$ ($m = 1, 2, \ldots$) are non-universal, and $\omega_m$ represents exponents for corrections. We show $R_{[10]}$ versus $\kappa$ in Fig. 2(a), where a scaling invariance point is nearly at $\kappa \approx 1.2$. We fit $\tilde{R}_{[10]}$ data with $L = 48, 64, 96, 128$ and 192 to Eq. (6). We observe $\omega_1 \approx 1.4$, which is larger than $\omega_1 \approx 0.789$ of 3D O(2) value [57] and $\omega_1 = 1$ from boundary irreducible fields [25]. The correction with $\omega_1 \leq 1$ is either absent or weak. Hence, we also perform fits without correction term and monitor the effects of corrections by examining the stability of fits upon gradually increasing $L_{\min}$. We obtain $\kappa_c = 1.206(7)$ and $y_t = 0.44(8)$ with $\chi^2/DF \approx 4.6$ for $L_{\min} = 64$, $\kappa_c = 1.184(6)$ and $y_t = 0.4(1)$ with $\chi^2/DF \approx 0.9$ for $L_{\min} = 96$, as well as $\kappa_c = 1.175(5)$ and $y_t = 0.8(3)$ with $\chi^2/DF \approx 0.2$ for $L_{\min} = 128$. Next, by fixing $y_t$ at the estimate $y_t = 0.608$ for the special transition of classical O(2) model [10], we obtain $\kappa_c = 1.197(2), 1.180(3)$ and 1.175(7) with $\chi^2/DF \approx 4.6, 1.1$ and 0.3, for $L_{\min} = 64, 96$ and 128, respectively. When $y_t = 0.58$ is fixed, we obtain close estimates, which are detailed in Appendix C. By comparing all these fits, we finally estimate $\kappa_c = 1.18(2)$. For illustrating the single-variable function $R_{[10]}$ together with the estimates of $\kappa_c$ and $y_t$, we plot $R_{[10]}$ versus $\epsilon L^{y_t}$ in Fig. 2(a) with $\kappa_c = 1.18$ and $y_t = 0.608$, where finite-size corrections are already negligible for large systems.

Further evidence comes from the FSS of the superfluid stiffness $\rho_s$, which is defined as [58] $\rho_s = \langle W_{[10]}^2 \rangle/(2t^3)$ through the fluctuations of the winding number $W_{[10]}$ along the [10] direction of square lattice. At $\kappa_c$, $\rho_s$ should scale as $\rho_s \sim L^{2-2(d+z)}$. This scaling behavior is verified by Fig. 2(b) with $d = 2$ and $z = 1$: as $L \to \infty$, $\rho_s L$ is asymptotically a constant for $\kappa \leq \kappa_c$, but bends upwards for $\kappa > \kappa_c$.

We consider the two-point correlation $g(L/2)$ at the largest distance $r_{[10]} = L/2$ along an open edge, which is estimated from the random walks of the two defects in worm quantum Monte Carlo simulations. More descriptions and benchmarks for this estimator are presented in Appendix B. Figure 2(c) shows that the result at $\kappa_c$ is compatible with the critical scaling behavior $g(L/2) \sim L^{-0.65}$, yet deviates when $\kappa \neq \kappa_c$.

B. KT-like criticality

Figure 3(a) shows $R_{[10]}$ versus $t$ for $\kappa = 10$. Around $t_x \approx 0.023$, $R_{[10]}$ varies drastically. For $t > t_x$, $R_{[10]}$ extrapolates to a nontrivial value in the $L \to \infty$ limit, which is dependent on $t$. Meanwhile, the superfluid stiffness scales as $\rho_s \sim L^{-1}$. These observations indicate a regime of critical phase.

The KT-like criticality is evidenced by the anomalous dimension $\eta$. Figure 3(b) demonstrates that, at $t_{K_T} \approx t_x$, $g(L/2)$ scales as $g(L/2) \sim L^{2(d+z)-\eta}$ with $d = 1, z = 1$ and $\eta = 1/4$. The value 1/4 is consistent with that of the KT transition in 2D XY model [60]. For $t > t_{K_T}$, we fit $g(L/2)$ to the formula $g(L/2) \sim L^{-\eta}$ of leading scaling. The fits are illustrated by Fig. 3(c) and detailed in Appendix C. In particular, for $t = 0.027$ and 0.05, we obtain $\eta = 0.150(2)$ and 0.058(4) respectively, with $\chi^2/DF \approx 0.1$ and $L_{\min} = 96$. The continuously varying exponent $\eta$ is reminiscent of the low-temperature critical phase of 2D XY model [61].
Figure 3. KT-like criticality ($\kappa = 10$). (a) Winding probability $R_{[10]}$ versus $t$. The inset displays the scaled superfluid stiffness $\rho_s L$. (b) Scaled two-point correlation $g(L/2)L^{1/4}$ versus $t$. (c) Log-log plot of $g(L/2)$ versus $L$.

C. Ordinary critical phase

Corresponding to classical O(2) BCB, the small-$\kappa$ side of special transition may fall into the ordinary critical universality class. For $\kappa = 0.4$, Fig. 4 demonstrates that $g(L/2)$ scales as $L^{2-(d+z)-\eta}$ with $\eta \approx 2.438$, $d = 1$ and $z = 1$. The value of $\eta$ relates to $\eta_b = 0.781(2)$ [10] of the O(2) BCB by $\eta = 4 - 2\eta_b$. As $L \to \infty$, $\rho_s L$ and $R_{[10]}$ tend to be independent of $L$. These scaling behaviors indicate the existence of the O(2) quantum ordinary universality.

D. Extraordinary-log critical phase

To explore the extraordinary phase, we make use of a broad parameter regime in the large-$\kappa$ side of special transition. In the ELU, $g(L/2)$ scales as [24]

$$g(L/2) = a[\ln(L/l_0)]^{-\hat{q}},$$

where $l_0$ is a reference length and $a$ denotes a non-universal constant. For the classical XY model, this scaling form was verified and $\hat{q} = 0.59(2)$ was estimated [26]. Close values of $\hat{q}$ were obtained for the classical ELU of O(2) model [28] and emergent O(2) criticality [30, 31]. We perform fits for $g(L/2)$ according to Eq. (7) and obtain $0.3 \lesssim \hat{q} \lesssim 0.7$ for $\kappa = 2, 3, 5$ and 7. We observe that $l_0$ decreases significantly as $\kappa$ increases. These features conform to the observations for classical ELU in Ref. [26]. When $\hat{q} = 0.59$ is fixed, we achieve, for each $\kappa$, stable fitting results for $l_0$ and $a$. Instance results of $l_0$ include $l_0 = 0.31(3), 0.21(1), 0.04(4), 0.0108(5)$ and $0.002(1)$ with $\chi^2/DF \approx 0.3, 1.8, 0.9, 0.7$ and $0.5$, for $\kappa = 2, 3, 5, 7$ and 10, respectively. The power-law dependence of $g(L/2)$ on $\ln(L/l_0)$ is illustrated by Fig. 5(a).

From Fig. 5(b), we find that $\rho_s L$ roughly obeys the loga-
with universal $b \approx 1.1$ and non-universal $c$. Preferred fits are achieved in deep extraordinary regime. With $L_{\text{max}} = 192$, we obtain $b = 1.14(3)$, $1.15(3)$ and $1.1(1)$ with $\chi^2/DF \approx 0.9$, 2.8 and 0.7, for $\kappa = 5$, 7 and 10, respectively. We also perform fits to $\sum_\kappa \rho_\kappa L = 5b\ln(L) + C$ ($C$ is a fitting parameter) where the summation runs over the set $\{2, 3, 5, 7, 10\}$ of $\kappa$. For $L_{\text{min}} = 64$, we obtain reasonably good results as $5b = 5.8(2)$ and $C = -5.3(7)$ with $\chi^2/DF \approx 2.0$ and $L_{\text{max}} = 192$, as well as $5b = 5.6(2)$ and $C = -4.6(8)$ with $\chi^2/DF \approx 0.8$ and $L_{\text{max}} = 128$. These fits are consistent and finally yield $5b = 5.7(3)$, which relates to $b = 1.14(6)$. By contrast, the logarithmic divergence of $\rho_\kappa L$ is absent in the paradigm of criticality, as illustrated for special transition [Fig. 2(b)] and ordinary critical phase [Fig. 4(b)], and does not emerge in the KT-like criticality [Fig. 3(a)]. The logarithmic FSS (8) with unit exponent and universal coefficient resembles that of the helicity modulus in classical XY and Heisenberg models [24–26].

V. SUMMARY

The extensive ongoing activities in the search for quantum ELU are restricted to dimerized antiferromagnets, for which conclusive evidence remains unavailable. Here, we switch to interacting bosons by formulating an open-edge Bose-Hubbard model and demonstrate the emergence of quantum ELU. An edge superfluid phase is observed on top of an insulating bulk. When the bulk is at the emergent quantum critical point, the special, ordinary and extraordinary-log critical phases emerge on open edges. In the extraordinary-log critical phase, the leading FSS for the largest-distance two-point correlation and scaled superfluid stiffness are logarithmic. By an overall classical-quantum correspondence of O(2) BCB as well as the universal behavior of logarithmic FSS in the extraordinary phase, we provide complementary evidence for the existence of quantum ELU. As the Bose-Hubbard model can be accessed by quantum emulators with ultracold bosons in optical lattices [62–65], our results indicate a possible experimental scheme for realizing ELU.

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Appendix A: Details of methodology

In the appendices, we present details for Monte Carlo simulations and provide a benchmark for two-point correlation using bulk criticality. We then analyze the data for the quantum critical phenomena on open edges, which include the special transition, the Kosterlitz-Thouless-like criticality, the ordinary critical phase and the extraordinary-log critical phase.

The raw data are all obtained from quantum Monte Carlo simulations, by means of the worm algorithm in the continuous-time path integral representation. The side lengths of square lattices include $L = 16, 32, 48, 64, 96, 128$ and $192$. In the worm simulations, the number of tentative updates for the defects, usually denoted by $Ira$ (I) and $Masha$ (M), ranges from $3.6 \times 10^{12}$ to $3.4 \times 10^{13}$ for $16 \leq L \leq 48$, and from $1.8 \times 10^{13}$ to $3.7 \times 10^{13}$ for $64 \leq L \leq 192$.

We perform FSS analyses by using least-squares fits. To this end, we utilize the function NonlinearModelFit in Mathematica, as adopted in Ref. [66]. According to standard criterion, we prefer the fits with $\chi^2/\text{DF} \sim 1$, where $\chi^2/\text{DF}$ represents the Chi squared per degree of freedom. We draw conclusions by comparing the fits that are stable against varying $L_{\text{min}}$, which is the minimum side length incorporated in fitting. In certain situations, we also include a cutoff $L_{\text{max}}$ for larger sizes.

Appendix B: Benchmark for two-point correlation using bulk criticality

We use an estimator of equal-imaginary-time correlations, which avoids reweighting along imaginary-time axis and turns out to be computationally cheap. The estimator correctly captures the asymptotic behavior in the $L \to \infty$ limit. Specifically speaking, in the worm quantum Monte Carlo simulations, we trace the trajectories of the defects $I$ and $M$ on an edge. If the imaginary-time distance between the defects is less than the $1/L$ fraction of entire axis, the distance $r$ of two defects along the edge is recorded. The follow-up treatment is similar to the measurement of two-point correlations in a classical model [43] which was based on the original idea in Ref. [67]. We use the $r = 1$ result to normalize the two-point correlation and concentrate on the $r \neq 0$ domain of correlation function. Hence, the results do not suffer from the biased allocations of statistical weight between original and Green function state spaces. Finally, we obtain the two-point correlation $g(r)$ as a function of $r$ along the edge.

We proceed to benchmark the above-mentioned methodology for correlation function using the bulk criticality. Particularly, we apply periodic conditions for both [10] and [01] directions to eliminate the open edges and sample the correlation functions at $t_c$. We analyze the $r$ dependence of $g(r)$ as well as the $L$-dependent behavior of $g(L/2)$. We quote a precise estimate $\eta = 0.03853(48)$ for the anomalous dimension of the $(2+1)$-dimensional O(2) criticality [51]. As shown in Fig. 6(a), the $r$-dependent behavior converges to the power law $g(r) \sim r^{2-\eta}$, with $d = 2, z = 1$ and $\eta = 0.03853$. From Fig. 6(b), we verify that $g(L/2)$ scales as $g(L/2) \sim L^{-\xi}$.

More quantitative verification can be achieved by least-squares fits. We fit $g(L/2)$ to

$$g(L/2) = aL^b,$$  \hspace{1cm} (B1)

where $a$ is a constant and $b = 1 - \eta$. The results are summarized in Table II. We obtain $b = -1.027(6)$ and $\chi^2/\text{DF} \approx 1.2$ for $L_{\text{min}} = 48$, $b = -1.03(1)$ and $\chi^2/\text{DF} \approx 1.5$ for $L_{\text{min}} = 64$, as well as $b = -1.06(3)$ and $\chi^2/\text{DF} \approx 1.4$ for $L_{\text{min}} = 96$. The estimates of $b$ are consistent with $1 - \eta = 0.03853(48)$ of the $(2+1)$-dimensional O(2) universality.

Appendix C: Details of the FSS analyses for BCB

In this appendix, we perform FSS analyses for the special transition, the Kosterlitz-Thouless-like criticality, the ordinary critical phase and the extraordinary-log critical phase. Special transition. We locate the special transition point $t_c$ for correlation function using the bulk criticality. Partic-

$$R_{[10]} = R_{[10]}^c + \alpha_1 (\kappa - \kappa_c) L^{\nu_1} + b_1 L^{-\omega_1},$$  \hspace{1cm} (C1)

where $\kappa = 1$ for $\kappa = 2/3$ for $\kappa = 1$ for $\kappa = 2$ for $\kappa = 3$.
ble IV, we also perform fits without incorporating correction
ω and flow [59], respectively. For each situation for
being free or fixed at
We perform least-squares fits with
ν denotes the exponent for leading finite-size corrections.
(a) log-log plot of
= 48
(b) log-log plot of
= 128

![Figure 6. Bulk criticality. (a) Log-log plot of \( g(r) \) vs. \( r \). (b) Log-log plot of \( g(L/2) \) versus \( L \).](image)

| \( L_{\text{min}} \) | \( \chi^2/\text{DF} \) | \( a \) | \( b \) |
|------------------|------------------|-------|-------|
| 32               | 20.62/4          | 2.65(3) | -1.009(3) |
| 48               | 3.45/3           | 2.86(6) | -1.027(6) |
| 64               | 3.04/2           | 2.9(1)  | -1.03(1)  |
| 96               | 1.41/1           | 3.4(4)  | -1.06(3)  |

Table II. Fits of \( g(L/2) \) to Eq. (B1) at the bulk critical point.

where \( R_{10}^{c} \) is the critical dimensionless ratio, \( a_1 \) and \( b_1 \) represent fitting parameters, \( \kappa_c \) denotes the transition point, \( y_t \) relates to the correlation length exponent \( \nu \) by \( y_t = 1/\nu \), and \( \omega_1 \) denotes the exponent for leading finite-size corrections. We perform least-squares fits with \( \kappa = 1.16, 1.18, 1.2 \) and \( L = 48, 64, 96, 128, 192 \). We consider the situations with \( y_t \) being free or fixed at 0.608 and 0.58, which were estimated for the special transition of classical O(2) model in spin [10] and flow [59] representations, respectively. For each situation, we obtain reasonably good results for large \( L_{\text{min}} \). When the leading correction term is present, the best estimate of \( \omega_1 \) is \( \omega_1 \approx 1.4 \) (Table III), which is larger than \( \omega_1 = 0.789 \) of 3D O(2) value [57] and \( \omega_1 = 1 \) originating from boundary irrelevant fields [25], indicating that the correction term with \( \omega_1 \leq 1 \) is either absent or weak. Hence, as shown in Table IV, we also perform fits without incorporating correction term, which have a reduced number of fitting parameters, and examine the stability of fitting results by varying \( L_{\text{min}} \). By comparing the fits, our final estimate of \( \kappa_c \) is \( \kappa_c = 1.18(2) \).

**Kosterlitz-Thouless-like critical phase.** We explore the critical phase on the large-\( t \) side of Kosterlitz-Thouless-like transition for \( \kappa = 10 \). For each \( t \) in the set \{0.027, 0.03, 0.035, 0.04, 0.045, 0.05\}, we perform scaling analyses for \( g(L/2) \) according to Eq. (B1) with \( b = -\eta \), which corresponds to the leading FSS. The results are summarized in Table V, which demonstrates that the fits are precise only at large sizes. Moreover, as \( t \) increases, the exponent \( \eta \) decreases.

**Ordinary critical phase.** We analyze the ordinary critical phase at \( \kappa = 0.4 \) and \( t = t_c \). We fit \( g(L/2) \) to Eq. (B1) with \( b = 2y_t - 4 \). The results are presented in Table VI. For \( L_{\text{min}} = 48, 64 \) and 96, we find \( b = -2.41(2), -2.45(4) \) and \( -2.5(1) \) with \( \chi^2/\text{DF} \approx 1.3, 1.1 \) and 1.4, respectively. These results are compatible with the exponent \( 2y_t - 4 \) with \( y_t = 0.781(2) \) of the classical O(2) ordinary surface criticality [10]. If a correction term is included and the fitting ansatz becomes \( g(L/2) = L^y(a + cL^{-\hat{\omega}}) \), the effects from corrections decrease rapidly with \( L \) as \( L^\hat{\omega} \). It is practically difficult to estimate the amplitude of finite-size corrections.

**Extraordinary critical phase.** We analyze the FSS for the extraordinary phase. We fit \( g(L/2) \) to

\[
 g(L/2) = a[\ln(L/l_0)]^{-\hat{q}}. \tag{C2}
\]

The results are given in Table VII. If \( \hat{q} \) is free, we obtain \( 0.3 \lesssim \hat{q} \lesssim 0.7 \) and find that \( l_0 \) drastically decreases upon increasing \( \kappa \). When \( \hat{q} = 0.59 \) is fixed, we obtain stable fitting results of \( a \) and \( l_0 \) for each considered \( \kappa \). For \( l_0 \), instance results are \( l_0 = 0.31(3), 0.21(1), 0.04(4), 0.0108(5) \) and 0.002(1) with \( \chi^2/\text{DF} \approx 0.3, 1.8, 0.9 \) and 0.5, for \( \kappa = 2, 3, 5, 7 \) and 10, respectively.

Assuming the existence of extraordinary-log critical universality, for each \( \kappa \), we fit the data of \( \rho_s \) to

\[
 \rho_s L = a + b\ln L. \tag{C3}
\]

We obtain preferred fits with \( L_{\text{max}} = 192 \) for the deep extraordinary regime. For \( \kappa = 5 \), we obtain \( b = 1.14(3) \) with \( L_{\text{min}} = 64 \) and \( \chi^2/\text{DF} \approx 0.9 \). For \( \kappa = 7 \), we obtain \( b = 1.15(3) \) with \( L_{\text{min}} = 64 \) and \( \chi^2/\text{DF} \approx 2.8 \). For \( \kappa = 10 \), we obtain \( b = 1.1(1) \) with \( L_{\text{min}} = 96 \) and \( \chi^2/\text{DF} \approx 0.7 \). To obtain a unique estimate of fitting parameters, we analyze the sum of the scaled superfluid stiffness \( \rho_s L \) over \( \kappa = 2, 3, 5, 7 \) and 10 by performing fits to

\[
 \sum_\kappa \rho_s L = A + B\ln L. \tag{C4}
\]

As summarized in Table VIII, we obtain reasonably good fits with \( \chi^2/\text{DF} \sim 1 \) for \( L_{\text{max}} = 192 \) and 128. For \( L_{\text{max}} = 192 \), we obtain \( A = -5.3(7), B = 5.8(2) \) and \( \chi^2/\text{DF} \approx 2.0 \) with \( L_{\text{min}} = 64 \), as well as \( A = -8.8(20), B = 6.5(4) \) and \( \chi^2/\text{DF} \approx 0.5 \) with \( L_{\text{min}} = 96 \). For \( L_{\text{max}} = 128 \), we obtain \( A = -4.6(8), B = 5.6(2) \) and \( \chi^2/\text{DF} \approx 0.8 \) with \( L_{\text{min}} = 64 \).
### Table III. Fits of $R_{[10]}$ to Eq. (C1) for the special transition.

| $L_{\text{min}}$ | $\chi^2$/DF | $\kappa_c$ | $y_t$ | $R_{[10]}$ | $a_1$ | $b_1$ | $\omega_1$ |
|------------------|-------------|------------|------|------------|-------|-------|----------|
| 48               | 5.14/9      | 1.12(7)    | 0.50(5) | 0.02(22)   | 0.06(1) | 0.4(2) | 0.4(7)   |
| 64               | 4.47/6      | 1.1(1)     | 0.55(8) | 0.1(3)     | 0.05(2) | 0.7(5.2)| 0.7(3.0) |
| 96               | 2.92/3      | 1.15(3)    | 0.4(1)  | 0.09(3)    | 0.09(6) | 6.24(1)| 1.4(2)   |
| 48               | 8.83/10     | 1.13(5)    | 0.608   | 0.03(18)   | 0.0390(9)| 0.4(2) | 0.4(7)   |
| 64               | 5.03/7      | 1.1(1)     | 0.608   | 0.1(4)     | 0.038(1)| 0.4(2.3)| 0.5(2.9) |
| 96               | 4.44/4      | 1.16(2)    | 0.608   | 0.10(2)    | 0.038(1)| 8.900(6)| 1.5(2)   |
| 48               | 7.09/10     | 1.13(5)    | 0.58    | 0.03(19)   | 0.044(1)| 0.4(2) | 0.4(7)   |
| 64               | 4.62/7      | 1.1(1)     | 0.58    | 0.1(3)     | 0.043(1)| 0.5(3.4)| 0.6(3.0) |
| 96               | 3.98/4      | 1.16(2)    | 0.58    | 0.10(2)    | 0.043(2)| 7.903(7)| 1.4(2)   |

### Table IV. Fits of $R_{[10]}$ to Eq. (C1) for the special transition with $b_1 = 0$.

| $L_{\text{min}}$ | $\chi^2$/DF | $\kappa_c$ | $y_t$ | $R_{[10]}$ | $a_1$ |
|------------------|-------------|------------|------|------------|-------|
| 48               | 108.12/11   | 1.25(1)    | 0.29(5) | 0.160(7)   | 0.15(3) |
| 64               | 37.02/8     | 1.206(7)   | 0.44(8) | 0.138(4)   | 0.08(3) |
| 96               | 4.41/5      | 1.184(6)   | 0.4(1)  | 0.123(4)   | 0.10(7) |
| 128              | 0.33/2      | 1.175(5)   | 0.8(3)  | 0.117(4)   | 0.01(2) |
| 48               | 145.25/12   | 1.206(2)   | 0.608   | 0.1398(8)  | 0.0394(9)|
| 64               | 41.39/9     | 1.197(2)   | 0.608   | 0.133(1)   | 0.037(1) |
| 96               | 6.35/6      | 1.180(3)   | 0.608   | 0.121(2)   | 0.038(1) |
| 128              | 0.84/3      | 1.175(7)   | 0.608   | 0.116(5)   | 0.035(2) |
| 48               | 138.73/12   | 1.208(2)   | 0.58    | 0.1407(8)  | 0.045(1) |
| 64               | 40.01/9     | 1.198(2)   | 0.58    | 0.134(1)   | 0.042(1) |
| 96               | 5.84/6      | 1.181(4)   | 0.58    | 0.121(2)   | 0.043(2) |
| 128              | 0.98/3      | 1.175(7)   | 0.58    | 0.116(5)   | 0.040(2) |

### Table V. Fits of $g(L/2)$ to Eq. (B1) for the large-$t$ side of Kosterlitz-Thouless-like transition at $\kappa = 10$.

| $t$   | $L_{\text{min}}$ | $\chi^2$/DF | $a$        | $b$        |
|-------|-----------------|-------------|------------|------------|
| 0.027 | 48              | 208.63/3    | 1.115(3)   | -0.1700(6) |
|       | 64              | 36.28/2     | 1.080(4)   | -0.1628(8) |
|       | 96              | 0.96/1      | 1.01(1)    | -0.150(2)  |
| 0.03  | 48              | 591.62/3    | 1.016(2)   | -0.1264(4) |
|       | 64              | 127.87/2    | 0.980(2)   | -0.1187(5) |
|       | 96              | 6.02/1      | 0.929(5)   | -0.108(1)  |
| 0.035 | 48              | 437.57/3    | 0.990(1)   | -0.0979(3) |
|       | 64              | 119.14/2    | 0.964(2)   | -0.0924(4) |
|       | 96              | 5.54/1      | 0.925(4)   | -0.0841(9) |
| 0.04  | 48              | 96.45/3     | 1.010(2)   | -0.0881(5) |
|       | 64              | 28.96/2     | 0.991(3)   | -0.0839(7) |
|       | 96              | 0.65/1      | 0.950(8)   | -0.075(2)  |
| 0.045 | 48              | 24.06/3     | 1.017(3)   | -0.0788(7) |
|       | 64              | 6.70/2      | 1.003(4)   | -0.076(1)  |
|       | 96              | 1.05/1      | 0.97(1)    | -0.069(3)  |
| 0.05  | 48              | 18.18/3     | 1.017(4)   | -0.070(1)  |
|       | 64              | 9.31/2      | 1.004(6)   | -0.067(1)  |
|       | 96              | 0.98/1      | 0.96(2)    | -0.058(4)  |
Table VI. Fits of $g(L/2)$ to Eq. (B1) for the ordinary critical phase at $\kappa = 0.4$.

| $L_{\text{max}}$ | $L_{\text{min}}$ | $\chi^2$/DF | $a$     | $b$      |
|-----------------|-----------------|-------------|---------|---------|
| 192             | 32              | 7.02/4      | 66.6(1.8) | $-2.374(7)$ |
| 48              | 4.01/3          | 76.5(6.5)   | $-2.41(2)$ |
| 64              | 2.15/2          | 90.9(14.1)  | $-2.45(4)$ |
| 96              | 1.41/1          | 141.2(77.8) | $-2.5(1)$  |
| 128             | 32              | 2.62/3      | 66.2(1.8)  | $-2.373(7)$ |
| 48              | 0.84/2          | 73.9(6.4)   | $-2.40(2)$ |
| 64              | 0.002/1         | 83.7(13.7)  | $-2.43(4)$ |

Table VII. Fits of $g(L/2)$ to Eq. (C2) for the extraordinary phase at $\kappa = 2, 3, 5, 7$ and 10.

| $\kappa$ | $L_{\text{min}}$ | $\chi^2$/DF | $a$     | $l_0$     | $\hat{q}$  |
|----------|-----------------|-------------|---------|-----------|------------|
| 2        | 16              | 1.93/4      | 0.68(1) | 3.5(3)    | 0.32(1)    |
|          | 32              | 0.12/3      | 0.76(8) | 2.2(9)    | 0.38(5)    |
|          | 48              | 0.07/2      | 0.7(2)  | 3.3(4.9)  | 0.3(2)     |
|          | 64              | 0.03/1      | 0.8(9)  | 1.7(8.1)  | 0.4(5)     |
| 3        | 16              | 2.74/4      | 1.11(8) | 1.0(2)    | 0.42(3)    |
|          | 32              | 1.01/3      | 0.9(1)  | 2.3(1.3)  | 0.33(6)    |
|          | 48              | 0.42/2      | 1.5(2.0)| 0.3(1.2)  | 0.5(5)     |
|          | 16              | 16.72/5     | 1.649(3)| 0.257(4)  | 0.59       |
|          | 32              | 7.21/4      | 1.69(1) | 0.21(1)   | 0.59       |
|          | 48              | 0.42/3      | 1.73(2) | 0.16(2)   | 0.59       |
|          | 64              | 0.12/2      | 1.31(4) | 0.25(7)   | 0.59       |
|          | 96              | 0.07/1      | 1.33(8) | 0.2(1)    | 0.59       |
| 5        | 16              | 2.17/4      | 2.7(9)  | 0.03(3)   | 0.7(1)     |
|          | 32              | 1.30/3      | 1.5(6)  | 0.3(5)    | 0.5(2)     |
|          | 48              | 1.14/2      | 2.7(6.5)| 0.02(22)  | 0.7(8)     |
|          | 64              | 0.99/1      | 1.1(1.3)| 1.2(7.4)  | 0.3(5)     |
|          | 16              | 2.57/5      | 2.221(6)| 0.053(1)  | 0.59       |
|          | 32              | 1.72/4      | 2.20(2) | 0.058(5)  | 0.59       |
|          | 48              | 1.15/3      | 2.23(4) | 0.05(1)   | 0.59       |
|          | 64              | 1.08/2      | 2.21(7) | 0.05(2)   | 0.59       |
|          | 96              | 0.85/1      | 2.3(2)  | 0.04(4)   | 0.59       |
| 7        | 16              | 2.29/4      | 4.4(2.7)| 0.001(4)  | 0.7(2)     |
|          | 32              | 1.34/3      | 1.7(9)  | 0.1(3)    | 0.4(2)     |
|          | 16              | 3.31/5      | 2.692(9)| 0.0108(5) | 0.59       |
|          | 32              | 1.67/4      | 2.66(3) | 0.013(2)  | 0.59       |
|          | 48              | 0.83/3      | 2.70(5) | 0.010(3)  | 0.59       |
|          | 64              | 0.06/2      | 2.63(9) | 0.015(7)  | 0.59       |
|          | 96              | 0.001/1     | 2.6(2)  | 0.02(2)   | 0.59       |
| 10       | 16              | 12.53/5     | 3.35(2) | 0.00084(8)| 0.59       |
|          | 32              | 0.93/4      | 3.22(4) | 0.0017(4) | 0.59       |
|          | 48              | 0.91/3      | 3.21(8) | 0.0018(7) | 0.59       |
|          | 64              | 0.91/2      | 3.2(1)  | 0.002(1)  | 0.59       |
|          | 96              | 0.08/1      | 3.0(3)  | 0.01(1)   | 0.59       |
Table VIII. Fits of the summed scaled stiffness $\sum \rho_s L$ over $\kappa = 2, 3, 5, 7$ and 10 to Eq. (C4) for the extraordinary phase.

| $L_{\text{max}}$ | $L_{\text{min}}$ | $\chi^2$/DF | $A$   | $B$   |
|------------------|------------------|-------------|-------|-------|
| 192              | 32               | 95.84/4     | 0.2(2)| 4.47(5)|
|                  | 48               | 28.71/3     | −2.3(4)| 5.10(9)|
|                  | 64               | 3.98/2      | −5.3(7)| 5.8(2) |
|                  | 96               | 0.45/1      | −8.8(2.0)| 6.5(4)|
| 128              | 32               | 64.32/3     | 0.5(2)| 4.41(5)|
|                  | 48               | 16.33/2     | −1.9(4)| 5.0(1) |
|                  | 64               | 0.77/1      | −4.6(8)| 5.6(2)|