

Berezinskii-Kosterlitz-Thouless Renormalization Group Flow at a Quantum Phase Transition

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We present a controlled numerical study of the Berezinskii-Kosterlitz-Thouless (BKT) transition in the one-dimensional Bose-Hubbard model at unit filling, providing evidence of the characteristic logarithmic finite-size scaling of the BKT transition. Employing density matrix renormalization group and quantum Monte Carlo simulations under periodic boundary conditions, together with a systematic finite-size scaling analysis of bipartite particle number fluctuations, we resolve boundary-induced complications that previously obscured critical scaling. We demonstrate that a suitably chosen central region under open boundaries reproduces universal renormalization group signatures, reconciling earlier discrepancies. Finally, leveraging a nonparametric Bayesian analysis, we determine the critical interaction strength with high precision to be $U_c/J = 3.275(2)$, establishing a benchmark for BKT physics in one-dimensional quantum models.

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Introduction—The Berezinskii-Kosterlitz-Thouless (BKT) transition [1,2] is a remarkable infinite-order topological phase transition, originally discovered in the classical two-dimensional (2D) XY model. The low-temperature phase is characterized by algebraically decaying spin correlations, and the transition to a high-temperature disordered phase is driven by the unbinding of topological defects (vortex-antivortex pairs) due to thermal fluctuations. The location of the critical point is known from Monte Carlo [3–7] and tensor network simulations [8–10]. BKT physics has been found in a variety of systems, including the 2D Coulomb gas [11], superconducting films [12–17], Josephson junction arrays [18,19], superconductor-ferromagnetic-superconductor junctions [20], and lattice models at zero temperature [21,22]. Near the transition, all these systems are expected to follow a renormalization group (RG) flow characteristic of the BKT universality class. Although this RG flow has been numerically demonstrated in the classical XY

model [10,23–27], its observation in quantum systems (with the transition driven by quantum instead of thermal fluctuations) remains a major challenge. This is due to a signature feature of BKT scaling—logarithmic system size dependence at criticality—necessitating costly large-scale numerical simulations of quantum systems.

The transition between superfluid (SF) and Mott insulator (MI) in the one-dimensional (1D) Bose-Hubbard model with dynamical critical exponent of one is a paradigmatic example of quantum BKT physics, corresponding to a 2D classical BKT transition via the quantum-to-classical mapping [28]. The transition is governed by a competition between the kinetic energy of the bosons and the on-site repulsive interaction U . For small interactions, the system is in a superfluid phase, while it is in a Mott-insulating phase when the on-site repulsion is dominant. This quantum phase transition has been experimentally observed in cold-atom systems [29,30] and due to its intrinsic interest, a variety of theoretical studies have attempted to locate the critical point in the 1D Bose-Hubbard model [31]. This includes approximate analytical approaches [32], numerically solving a Bethe ansatz [33], exact diagonalization [34–38], density matrix renormalization group (DMRG) [39–49], infinite matrix product state simulations [50,51], quantum Monte Carlo (QMC) [52–56], Green function Monte Carlo [57], time evolving

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block decimation [58–62], and entanglement-based techniques [63]. While these studies have reported a range of critical interaction strengths with varying degrees of accuracy and precision, the expected BKT RG flow behavior remains unobserved.

A key difficulty in pinpointing the BKT RG flow in quantum simulations arises from boundary conditions. For open boundary conditions (OBC), a position-dependent vortex fugacity and superfluid stiffness must be introduced to account for “image vortices” induced by the system’s edges [64–66], complicating direct comparisons to RG predictions developed for infinite or periodic systems. This is a nontrivial boundary effect, with the emergent low-energy description taking on the form of a nonlocal Sine-Gordon model [64]. The logarithmic interaction between vortices and image vortices gives rise to corrections on the same order as the logarithmic finite-size scaling. Capturing these subtleties is essential for extracting BKT scaling, and their neglect may explain the spread in critical parameters observed in DMRG studies with OBC [39–44].

In this Letter, we perform an analysis of the BKT transition in the 1D Bose-Hubbard model by combining periodic boundary conditions (PBC) DMRG with a systematic finite-size scaling analysis of bipartite particle number fluctuations [44]. Our main contributions are (i) an observation of the BKT RG flow at a quantum phase transition, overcoming the boundary-related issues

that affected previous studies; (ii) when using OBC, identifying the small fraction of the system near the center that can be used to extract observables compatible with infinite-size RG predictions; and (iii) a high-precision determination of the critical interaction strength in the Bose-Hubbard model at unit filling with uncertainty quantification via a nonparametric Gaussian process model.

RG flow finite-size scaling—The famous BKT RG flow is depicted by the solid lines in Fig. 1 [67,68]. Each line is defined by a constant of flow ζ , and following such a line describes how the Luttinger parameter K (stiffness) and lattice potential strength V (prefactor of a $2k_F$ Umklapp term) flow when increasing the system size $L = e^l$, where $d\zeta/dl = 0$. The critical flow at the BKT transition corresponds to $\zeta = 1$ (black, dashed line), while $\zeta > 1$ in the SF and $\zeta < 1$ in the MI phase. Based on the RG flow, we can approximate the finite-size scaling form of the Luttinger parameter K analytically in three regions of the BKT phase diagram,

$$K_{\text{SF}} \sim K^* + \kappa_0 \left(\frac{L_0}{L} \right)^{2(K^*-2)}, \quad (1)$$

$$K_{\text{sep}} \sim 2 + \frac{1}{1/\kappa_0 + \ln L/L_0}, \quad (2)$$

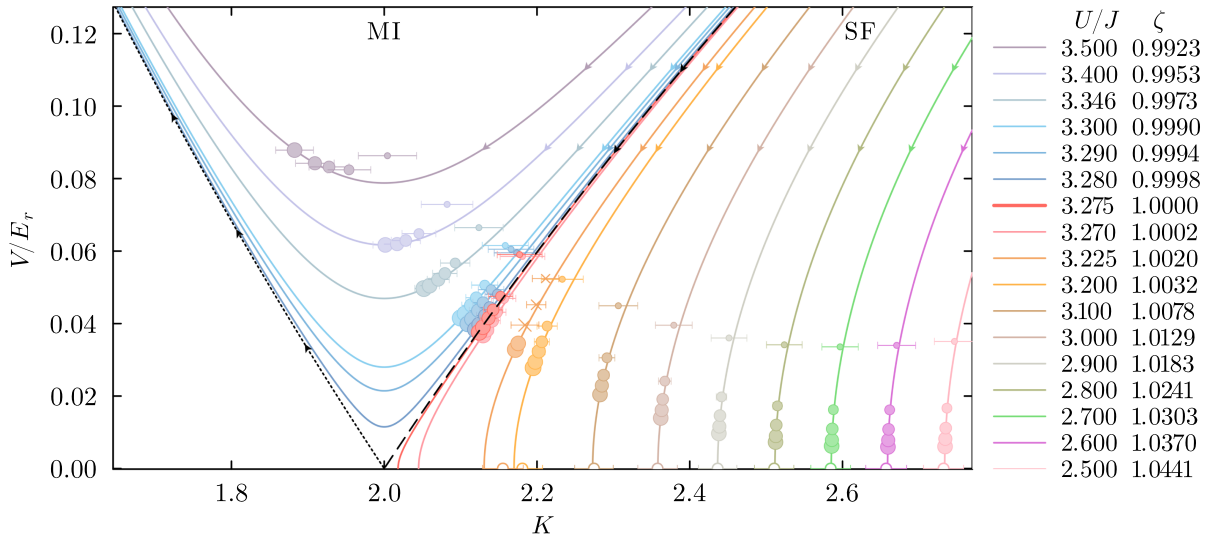


FIG. 1. RG flow close to the BKT phase transition constructed from the numerical DMRG simulations for periodic boundary conditions [using Eq. (A2)]. Here, K is the Luttinger parameter, V the strength of the periodic lattice potential, $E_r = u\pi/a$ a characteristic energy scale, and U the interacting strength of the Bose-Hubbard model, Eq. (4), considered in the numerical simulations. The dashed black line is the separatrix marking the critical line of the phase transition with $\zeta(U_c/J) = 1$. To the right of the separatrix, the system is in the superfluid (SF) phase, and to the left it is in the Mott-insulating (MI) phase. Each colored line corresponds to one value of $\zeta(U/J)$ obtained from the numerical results for the largest two system sizes for each U/J . Circles show the points for individual system sizes (larger circles correspond to larger L , $L \in \{16, 32, 48, 64, 96, 128\}$). Open circles are obtained by fits of the $L \rightarrow \infty$ limit of Eq. (5) to data obtained for infinite boundary conditions using the variational uniform matrix product state algorithm [69]. Crosses are obtained from QMC. We estimate error bars on K by varying the fit intervals. We find excellent agreement of the DMRG data with the predicted RG flow and between the different methods.

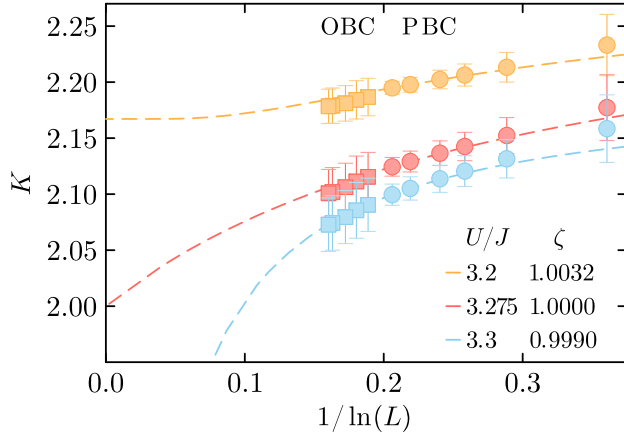


FIG. 2. Finite-size scaling of the Luttinger parameter as a function of system size L according to the RG flow. The circles depict the results obtained from high precision DMRG calculations with periodic boundary conditions. Dashed lines show fits of the corresponding scaling form to the data. We show the three scaling regimes (i) in the superfluid phase according to Eq. (1) (upper orange curve), (ii) for the value of U closest to the separatrix using Eq. (2) (center red curve), and (iii) in the insulating phase according to Eq. (3) (bottom blue curve). Squares depict data obtained for open boundary conditions using a fine-tuned fitting interval for extraction of K [70].

$$K_{\text{MI}} \sim 1 + (1 + \kappa_0) \left(\frac{L_0}{L} \right)^{8(1-\zeta)}. \quad (3)$$

For weak lattice potential strength V in the SF phase, we expand $K_{\text{SF}} = K^* + \kappa$ for small κ resulting in the scaling Eq. (1). Here, $K(L_0) = K^* + \kappa_0$ for some system finite-size L_0 with distance κ_0 from K^* . For the critical flow on the separatrix (sep), $\zeta = 1$ and $K^* = 2$, yielding the finite-size scaling Eq. (2). In the insulating phase, as K flows to zero, one cannot expand for the asymptotic L dependence. However, $K(V)$ has a minimum at $K = 2$ close to which the scaling form is given by Eq. (3).

This shows that the finite-size scaling is logarithmic on the separatrix and nearly logarithmic, i.e. of power-law type with small exponent, close to it. Thus the functional form of the finite-size scaling (even asymptotically) depends on the exact point in the phase diagram. This renders typical empirical $1/L$ extrapolations for $L \rightarrow \infty$ inaccurate, and requires utilization of the RG flow to produce accurate predictions of the thermodynamic limit behavior from finite-size numerical simulations. Examples of the scaling forms in Eqs. (1)–(3) are shown in Fig. 2 (dashed lines), together with numerical data obtained for the Bose-Hubbard model (circles PBC; squares OBC) as described below.

Bose-Hubbard model—As an example system, we study the Bose-Hubbard model at zero temperature,

$$H = -J \sum_{i=1}^L \left(b_i^\dagger b_{i+1} + b_{i+1}^\dagger b_i \right) + \frac{U}{2} \sum_{i=1}^L n_i(n_i - 1), \quad (4)$$

on a one-dimensional lattice of length L . Here, J is the nearest neighbor hopping strength, $U > 0$ the repulsive on-site interaction, $b_i(b_i^\dagger)$ annihilates (creates) a boson on site i , and $n_i = b_i^\dagger b_i$ is the number operator for site i . For PBC, we identify $b_{L+1} = b_1$, while for OBC, $b_{L+1} = 0$. We consider unit filling where $\langle n_i \rangle = N/L = 1$.

The low-energy sector of Eq. (4) can be described by the Luttinger liquid Hamiltonian [see End Matter Eq. (A1)] via bosonization, which allows for the relation of the interaction strength U to the Luttinger parameter K . Here, the density pinning term with prefactor V/E_r is related to Umklapp processes on the lattice [72] and becomes interaction-dependent. The Bose-Hubbard model exhibits a BKT phase transition between a Mott-insulating phase for $U > U_c$ ($K < 2$) and superfluid phase for $U < U_c$ ($K > 2$) and falls under the universality class of models following the RG flow described above [73] and depicted in Fig. 1. The critical point can then, in principle, be determined by inverting the unknown function $K(U/J)$.

We extract K from the fluctuations of the particle number in an interval $A = [0, \ell]$ defined as $\mathcal{F}(\ell) = \langle (\hat{N}_A - \langle \hat{N}_A \rangle)^2 \rangle$ [44], where the particle number operator is related to the density via $\hat{N}_A = \int_0^\ell dx \rho(x)$. Particle number fluctuations are proportional to the Luttinger parameter, and for PBC are given by

$$\mathcal{F}_{\text{pbc}}(\ell; K, \alpha) = \frac{K}{2\pi^2} \ln \left[1 + \frac{\sin^2(\pi\ell/L)}{\sinh^2(\pi\alpha/L)} \right], \quad (5)$$

with α a short-distance cutoff. The OBC case is discussed in Supplemental Material (SM) [70]. For the region $\ell \sim L/2$ in the case of sufficiently large systems, such that $\ell/L \gg \alpha/L$, we can write $\mathcal{F}_{\text{pbc}}(\ell; K, \alpha) \approx (K/\pi^2) \ln \sin(\pi\ell/L) + \mathcal{A}$ with constant $\mathcal{A} \in \mathbb{R}$, allowing us to extract K as the slope of a linear fit to $\mathcal{F}_{\text{pbc}}$ plotted against $(1/\pi^2) \ln \sin(\pi\ell/L)$ as seen in Fig. 3.

Microscopic simulations—To numerically demonstrate the BKT RG flow for the Bose-Hubbard model, we perform high-precision numerical DMRG simulations for periodic chains of sizes up to $L = 128$ sites using the ITensors.jl software library [74]. For OBC, we perform simulations up to $L = 512$. We restrict the local site occupancy of bosons by $n_{\text{max}} = 6$, which is larger than those typically used but may not be sufficient when considering fluctuations [75]. Because of the nonperiodic nature of the matrix product states used for the DMRG algorithm, the description of periodic systems requires large bond dimensions, which makes simulating large periodic systems challenging. Therefore, we carefully ensure the convergence of the DMRG algorithm by the following criteria: (i) no change in energy larger than 10^{-12} for consecutive sweeps, (ii) no change in the bond dimension for at least four sweeps using a truncation cutoff of 10^{-12} , and (iii) a final energy variance satisfying

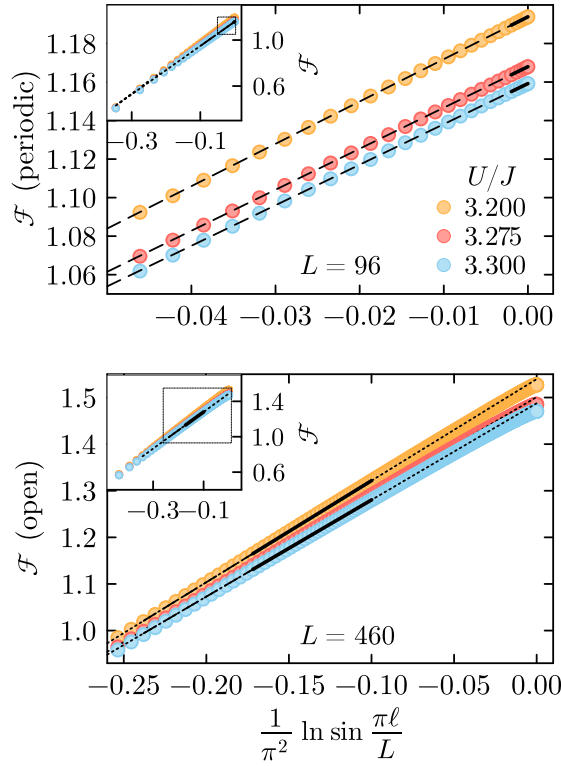


FIG. 3. Extracting the Luttinger parameter K from the particle number fluctuations for different interaction strengths U/J . We fit Eq. (5) to the periodic boundary condition DMRG data (upper panel) for intervals close to $\ell = L/2$, i.e., $\ell \in [L/2 - L/16, L/2]$, with the extracted value of K being insensitive to the choice of fitting region. The bottom panel shows fits to the open boundary condition data, where we fit to a small center region $\ell \in [L/8.2 - L/16, L/8.2]$ such that ℓ covers the same absolute range as in the top panel. This restriction is necessary to mitigate the strong boundary effects for ℓ approaching $L/2$, which leads to a strong dependence of K on the fitting region, ultimately causing a large uncertainty in the extracted value.

$\langle (H - E)^2 \rangle / E^2 < 10^{-11}$. We allow the bond dimension to be large enough to fulfill the cutoff criterion (ii), which results in values on the order of 10 000 for the largest systems with PBC.

We perform DMRG calculations for many different values of the interaction U/J in both the superfluid and Mott-insulating phases for different system sizes L . Next, we compute the particle number fluctuations $\mathcal{F}$ as a function of the subsystem size ℓ in the ground state. We then extract the Luttinger parameter as described below [Eq. (5)] (see Fig. 3) for each value of U/J and L . We linearly fit to the region $\ell \in [L/2 - \lfloor L/16 \rfloor, L/2]$ and obtain an error bar by varying the number of included points up to $\ell \in [L/4, L/2]$. As a consistency check, a similar procedure is performed using ground state lattice worm quantum Monte Carlo [71] with details provided in SM [70].

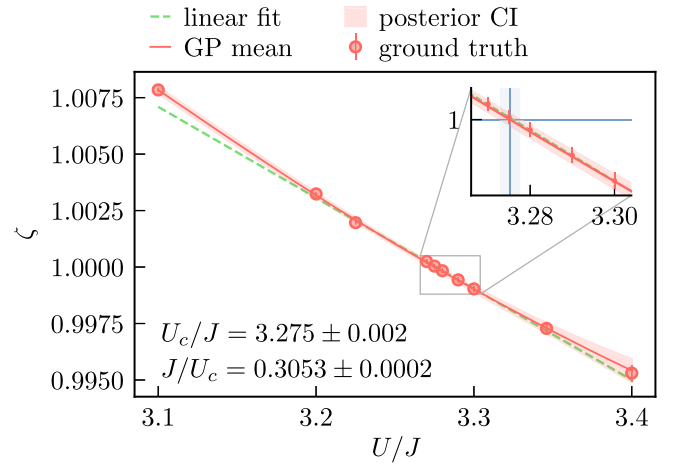


FIG. 4. Dependence of the flow parameter ζ on the interaction strength U/J (ground truth, red circles). A Gaussian process (GP) is used to perform a nonparametric fit to the data, with the predicted posterior mean [Eq. (6)] shown as a solid red line, accompanied by a red shaded region indicating the posterior confidence interval [CI, Eq. (7)]. The critical point occurs when $\zeta = 1$, yielding $U_c/J = 3.275 \pm 0.002$ indicated by the vertical blue line, and a shaded region of uncertainty in the inset. Near the transition, a linear fit to $U/J \in \{3.275, 3.280, 3.290, 3.300\}$ (green dashed line) yields the same critical point and uncertainty, but away it deviates outside of error bars.

For OBC, the bipartite fluctuations in Eq. (5) computed for the Luttinger model depend on the location of the bipartition [70]. Near the center of the interval, the PBC and OBC expressions agree with each other. However, in the OBC case, the Luttinger parameter K acquires a strong spatial dependence due to the formation of image vortices at the boundaries [64]. This is in striking contrast to the assumption of a spatially constant K used in the derivation of the Luttinger liquid prediction for bipartite fluctuations, which is valid only for a very small center interval in the presence of OBC. Extracting physically consistent values of K requires extensive fine-tuning of this region, which may be responsible for the scatter of previously reported critical points discussed in the introduction. For this reason, PBC offer advantages for studying the phase transition, despite their increased computational cost in DMRG.

Finally, approximate infinite matrix product state calculations can be performed directly in the thermodynamic limit using the ITensorsInfiniteMPS.jl software implementing the variational uniform matrix product state algorithm [69]. We find excellent agreement with the infinite system extrapolation of K (see open circles in Fig. 1) deep in the superfluid phase where $V = 0$. However, close to the phase transition there is a discrepancy between the infinite matrix product state approach and that extrapolated from finite L , which is plausible as the growth in entanglement [75] cannot be captured at finite bond dimension [76].

Demonstration of BKT flow—For each U/J , the extracted values of K for PBC at two consecutive system sizes can be used to determine the flow line, $\zeta(U/J)$, and thus $K(V)$ by solving the RG flow equations between these two points (for details see End Matter). Using the two largest values of L , this process gives the flow lines shown in Fig. 1 as well as their V values. We obtain error bars by additionally computing ζ using values of the Luttinger parameters varied within their error bars and taking the maximum deviation. Thus, the observed agreement between flow lines and data points for smaller system sizes represents a stringent consistency check of BKT flow. We only observe deviations from the RG flow for the smallest system sizes deep in the Mott-insulator phase, where the Luttinger liquid description of the low-energy sector of the Bose-Hubbard model begins to break down. Moreover, near the transition, we find excellent agreement with the predicted analytic scaling forms in Eqs. (1)–(3) as seen in Fig. 2. While, as shown, the results for OBC agree with the scaling, this requires fine-tuning of the fit window to determine K and comes with large systematic uncertainty due to the presence of boundary effects giving rise to corrections on the order of the differences between the points shown [70]. These problems are absent for PBC, and no fine-tuning is required.

Gaussian-process-based extraction of the critical point—Because no analytic expression is available for the interaction dependence of the flow parameter ζ , we infer the function $\zeta(U/J)$ directly from the data by Gaussian-process (GP) regression. We then invert the learned relation numerically to locate the critical coupling U_c defined by $\zeta(U_c/J) = 1$.

A GP is a nonparametric Bayesian regression method. Given N measurements $(U_n, \zeta_n \pm \delta\zeta_n)$, with $\zeta_n = \zeta(U_n)$ and uncertainties $\delta\zeta_n$, we introduce a kernel function $k_\theta(U, U')$ and treat the vector $\boldsymbol{\zeta} = (\zeta_1, \dots, \zeta_N)$ as drawn from a multivariate Gaussian with covariance $\mathcal{C}_{nm} = k_\theta(U_n, U_m) + \delta\zeta_n^2 \delta_{nm}$ [77]. All energies are expressed in units of J . The kernel hyperparameters θ are determined by maximizing the marginal-log-likelihood $\mathcal{L}(\theta) = \ln[(2\pi)^{-N/2} |\mathcal{C}|^{-1/2} \exp(-\boldsymbol{\zeta}^\top \mathcal{C}^{-1} \boldsymbol{\zeta}/2)]$ using standard gradient methods (see End Matter).

For predicting a function value ζ_{N+1} for a new coupling U_{N+1} , we define a kernel vector $\mathbf{k}$ with entries $k_n = k_\theta(U_n, U_{N+1})$. The prediction and quantified uncertainty is then given by

$$\zeta_{N+1} = \mathbf{k}^\top \mathcal{C}^{-1} \boldsymbol{\zeta}, \quad (6)$$

$$\delta\zeta_{N+1}^2 = k_\theta(U_{N+1}, U_{N+1}) - \mathbf{k}^\top \mathcal{C}^{-1} \mathbf{k}. \quad (7)$$

Figure 4 shows the resulting function $\zeta(U/J)$. The condition $\zeta = 1$ yields $U_c/J = 3.275(2)$, $J/U_c = 0.3053(2)$, where the uncertainty reflects the 68% confidence interval of the GP posterior [70]. Very close to the transition we

observe the empirical linearity $\zeta \propto U/J$ with significant deviations outside the narrow critical window.

Conclusions—Finite-size scaling is derived from the renormalization group (RG), making it essential to obtain numerical data consistent with a given RG description. For the Berezinskii-Kosterlitz-Thouless transition, the RG framework for open boundary conditions is qualitatively different and significantly more complex than that for periodic boundary conditions. To ensure a robust data analysis, we have therefore obtained numerical data for periodic boundary conditions. We observed finite-size scaling behavior at the quantum phase transition in the one-dimensional Bose-Hubbard model consistent with the standard BKT RG flow, and obtained a high-precision estimate for the critical interaction strength at unit filling. Knowing its precise value may be important to quantify the effects of gapless modes and particle number fluctuations on entanglement [75,78,79]. We expect this approach to be useful in pinpointing critical points in other microscopic models where vortex proliferation is the dominant driver of the quantum phase transition. In such systems, we advise avoiding open boundary conditions, where systematic uncertainty can be introduced by boundary effects, even for large system sizes.

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Data availability—The data that support the findings of this article are openly available [80,81].

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End Matter

Sine-Gordon model and BKT RG flow—We consider a one-dimensional system of interacting quantum particles at zero temperature described by the Luttinger liquid (LL) Hamiltonian [67]

$$H_{\text{LL}} = \int_0^L dx \frac{u}{2\pi} \left[K(\partial_x \theta)^2 + \frac{1}{K}(\partial_x \phi)^2 \right] + \frac{V}{2\pi a} \cos(2\phi), \quad (\text{A1})$$

with bosonic phase field $\theta(x)$, displacement field $\phi(x)$, and a pinning term due to a periodic lattice potential of strength V . Here, u is the velocity of excitations, a the lattice spacing, and $K > 1$ is the Luttinger parameter determined by the strength of repulsive interparticle interactions. In the low-energy limit under the assumption of an average density ρ_0 and excitations causing small fluctuations around ρ_0 , the particle field operator $\psi(x)$ is related to the phase field via $\psi(x) \approx \sqrt{\rho(x)}e^{i\theta(x)}$, and the density profile is given by $\rho(x) \approx \partial_x \phi(x)/\pi \equiv \rho_0 + \partial_x \tilde{\phi}(x)/\pi$ [67,82–84].

The Hamiltonian (A1) has the form of a sine-Gordon model [67], which is known to host a Berezinskii-Kosterlitz-Thouless (BKT) phase transition [1,2] at $K(L \rightarrow \infty) = 2$ close to which the RG flow is governed

by the flow equations $(dK/dl) = -(\pi V/E_r)^2(K^2/4)$ and $(dV/dl) = (2 - K)V$ [67,68] with a characteristic energy scale $E_r = u\pi/a$ and $l = \ln L$ sets the RG scale.

The flow equations can be solved by the introduction of $\zeta(K, V)$ with $d\zeta/dl = 0$ [85,86], resulting in

$$2 \ln \left(\frac{L_2}{L_1} \right) = \int_{K_2}^{K_1} \frac{dK}{K^2(\ln(K/2) - \zeta) + 2K}, \quad (\text{A2})$$

$$\zeta \equiv \frac{2}{K} + \ln \left(\frac{K}{2} \right) - \frac{\pi^2}{8} \left(\frac{V}{E_r} \right)^2. \quad (\text{A3})$$

Given the values of (K_1, K_2) for two system sizes (L_1, L_2) , solving Eq. (A2) for ζ determines a line in the flow diagram $K(V; L)$ describing how K and V change when increasing the system size L (solid lines in Fig. 1). For each U/J , the extracted values of K for PBC at two consecutive system sizes are used in conjunction with Eq. (A2) to determine a value of $\zeta(U/J)$. Then, Eq. (A3) gives the associated value of V corresponding to the K of the smaller system size. Knowledge of the flow line allows for the finite-size scaling of K to the thermodynamic limit $L \rightarrow \infty$. In the superfluid phase, $\zeta > 1$, the Luttinger parameter K flows to a line of fixed points $K^*(\zeta) > 2$ and V to zero. The separatrix

(dashed black), i.e., the critical flow line of the quantum phase transition, corresponds to $\zeta = 1$. For strong interactions, $\zeta < 1$, the system is in the MI phase, where K flows to zero and V to infinity.

Estimation of the critical point via Bayesian optimization—The simultaneous solution of the RG equations (A2), (A3) allows us to numerically evaluate $\zeta(U/J)$ in the thermodynamic limit for the Bose-Hubbard model through the dependence $K(U/J)$. The critical coupling U_c/J can then be determined by identifying when $\zeta(U_c/J) = 1$. However, as described throughout this Letter, obtaining a reliable and accurate value of $K(U/J)$ is costly, requiring the use of PBC simulations (either DMRG or QMC) with considerable computational effort. A precise grid search is thus not feasible. We also have no access to analytical derivatives of this function, limiting the ability to use gradient based approaches.

While we empirically observe that near the transition $\zeta \propto U/J$, deviations outside the critical region are large, and an assumption of linearity could introduce bias and/or systematic error to the extraction of U_c . To mitigate the need for any assumptions on the functional form of $\zeta(U/J)$ and reduce the computational cost of identifying U_c/J , we employ a surrogate nonparametric GP model [87] for ζ as described in the main text,

$$\zeta(\mathbf{x}) \sim \text{GP}(\mathbb{E}[\zeta(\mathbf{x})], k(\mathbf{x}, \mathbf{x}')), \quad (\text{B1})$$

where we define $\mathbf{x} \equiv U/J$ to ease notation. We assume a constant mean function $\mathbb{E}[\zeta(\mathbf{x})] = (1/N) \sum_{n=1}^N \zeta_n$ and correlations between the ground truth data, ζ_n , along with their fixed uncertainties, $\delta\zeta_n$, are expressed through a covariance matrix computed using a Matern kernel function

with smoothness parameter $\nu = 5/2$ (chosen via manual tuning),

$$k(\mathbf{x}, \mathbf{x}') = \theta_0 \left(1 + \sqrt{5} \frac{|\mathbf{x} - \mathbf{x}'|}{\theta_1} + \frac{5}{3} \frac{(\mathbf{x} - \mathbf{x}')^2}{\theta_1^2} \right) \times \exp \left(-\sqrt{5} \frac{|\mathbf{x} - \mathbf{x}'|}{\theta_1} \right). \quad (\text{B2})$$

The scale (θ_0) and length (θ_1) hyperparameters were optimized via a gradient based method, and the GP model was fit using the GPyTorch library [88] using $x_n \in \{3.1, 3.2, 3.225, 3.27, 3.28, 3.3, 3.346, 3.4\}$. The results, including multiple draws from the posterior distribution and the resulting GP mean, are shown in the left panel of Fig. 5. As described in the main text, we identify the critical point as the value of U/J where the predictive mean of the GP yields $\mu = 1$ and its associated uncertainty can be quantified through the confidence interval corresponding to a single standard deviation σ of the surrogate model.

To understand the robustness of this prediction, we transform our data via $y_n = (1 - \zeta_n)^2$ for the same inputs as shown in the middle panel of Fig. 5. This allows us to recast finding the critical point as a convex optimization problem that can be accelerated via sample efficient Bayesian optimization methods [89–91]. In particular, we employ the combined power of the GPyTorch and BoTorch [92] software libraries using the same constant mean and covariance kernel as in Eq. (B2). Implementation details are included in an associated repository [80]. To choose the next sample guided by Bayesian optimization, we used the expected improvement (EI) acquisition function

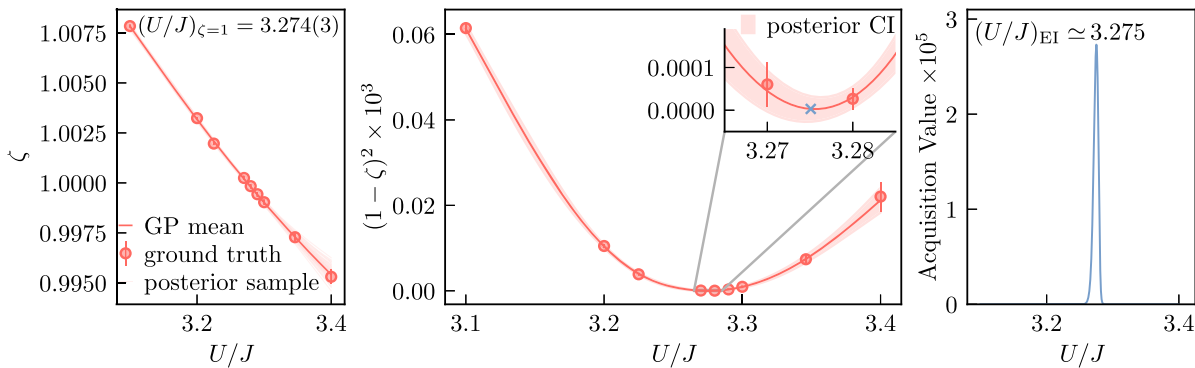


FIG. 5. Gaussian-process (GP) surrogate and Bayesian optimization (BO) approach to determine the critical point. Left: data points represent ground truth values for ζ while the faint pink lines are 100 draws from the posterior distribution for the GP model in Eq. (B2) along with its associated mean. The critical point can be identified by determining the value of U/J , which corresponds to $\zeta = 1$ as shown in the top of the panel along with its associated uncertainty in the last digit shown in parenthesis. Middle: a fit GP model for the transformed data $(1 - \zeta)^2$ allowing us to recast finding the critical point as an optimization problem. The enlargement in the inset shows the posterior distribution confidence interval (CI) as well as a $\times$ at the parametric value of U/J where the expected improvement (EI) function is maximized (right panel).

$$\begin{aligned} \text{EI}(x) = & (\mu_y(x) - y_{\min} - \epsilon) \Phi\left(\frac{\mu_y(x) - y_{\min} - \epsilon}{\sigma(x)}\right) \\ & + \sigma_y(x) \phi\left(\frac{\mu_y(x) - y_{\min} - \epsilon}{\sigma_y(x)}\right), \end{aligned} \quad (\text{B3})$$

where $\mu_y(x)$ and $\sigma_y(x)$ are a GP predictive mean and standard deviation of the transformed data, $y_{\min}$ is the minimal value of the target y_n in the training set, $\Phi(\cdot)$ is the cumulative normal distribution function, and $\phi(\cdot)$ is the normal probability distribution function. A slack parameter $\epsilon = 0.01$ was added for numerical stability and

balancing between exploration and exploitation [93]. A single Bayesian optimization iteration identified the optimal next sampling point as $U/J = 3.275$ via a localized maximum of the acquisition function shown in the right panel of Fig. 5. The small peak value $\text{EI} \approx 3 \times 10^{-5}$ signifies near convergence (rare likelihood that any new better or improved solution can be found compared to the last suggested). We then performed one additional set of DMRG calculations at the identified $U/J = 3.275$ allowing us to pinpoint the critical point with a small and well quantified error $\sim O(10^{-3})$, as shown in Fig. 4 of the main text.