Critical Exponents of the Superfluid–Bose-Glass Transition in Three Dimensions

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Recent experimental and numerical studies of the critical-temperature exponent ϕ for the superfluid–Bose-glass universality in three-dimensional systems report strong violations of the key quantum critical relation, $\phi = \nu z$, where z and ν are the dynamic and correlation-length exponents, respectively; these studies question the conventional scaling laws for this quantum critical point. Using Monte Carlo simulations of the disordered Bose-Hubbard model, we demonstrate that previous work on the superfluid-to-normal-fluid transition-temperature dependence on the chemical potential (or the magnetic field, in spin systems), $T_c \propto (\mu - \mu_c)^{\phi}$, was misinterpreting transient behavior on approach to the fluctuation region with the genuine critical law. When the model parameters are modified to have a broad quantum critical region, simulations of both quantum and classical models reveal that the $\phi = \nu z$ law [with $\phi = 2.7(2)$, $z = 3$, and $\nu = 0.88(5)$] holds true, resolving the ϕ-exponent "crisis."

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The disordered Bose-Hubbard (DBH) model is frequently employed as a key prototype system to discuss and understand a number of important experimental cases, such as ^{4}He in porous media and on various substrates, thin superconducting films, cold atoms in disordered optical lattice potentials, disordered magnets (see [1,2] and references therein), and so forth.

The pioneering work [3,4] on the DBH model has established that at $T = 0$ an insulating Bose-glass (BG) phase will emerge as a result of localization effects in disordered potentials. On a lattice, this phase will intervene between the Mott-insulator (MI) and superfluid (SF) phases at arbitrary weak disorder strength [4,5], and will completely destroy the MI phase at strong disorder. In contrast with the gapped incompressible MI phase, the BG phase has finite compressibility, κ, due to the finite density of localized gapless quasiparticle and quasihole excitations. Using scaling arguments, and the fact that $\kappa = \text{const}$ at the critical point of the quantum SF-BG transition, it was predicted that the dynamic critical exponent, z, always equals the dimension of space; i.e., $z = d$ [4]. The decrease of the normal-to-superfluid transition temperature, T_c, on approach to the quantum critical point (QCP) is characterized by the ϕ exponent, $T_c \propto (g_c - g)^{\phi}$, where g is the control parameter used to reach the QCP. Standard scaling analysis of the quantum critical free-energy density predicts that ϕ has to satisfy the relation $\phi = \nu z$. Therefore, taking into account the Harris criterion $\nu \geq 2/d$ [6] for the correlation-length exponent in disordered systems, it is expected that $\phi \geq 2$, which is within the standard picture of quantum critical phenomena.

Despite substantial research efforts in the last two decades, some aspects of the universal critical behavior described above remain controversial (see, e.g., Ref. [7]). For instance, Ref. [8] argues that finite κ at the SF-BG critical point might come from the regular analytic (rather than singular critical) part of the free energy, and, thus, $z < d$ should be considered as an undetermined critical exponent. Moreover, recent experiments on magnetic systems [1], as well as quantum Monte Carlo simulations of related disordered $S = 1$ antiferromagnets with single-ion anisotropy [9], which use a magnetic field (equivalent to the chemical potential in the bosonic system) as a control parameter to drive the system to quantum criticality, report compelling evidence that the values $\phi \approx 1.1(1)$ and $\nu \approx 0.75(10)$ are in strong violation of the key relation $\phi = z\nu$ and the bound $\phi \geq 2$. As a result, finite-temperature scaling relations that have been used to describe SF-BG criticality for decades are challenged.

In this Letter, we address the ϕ-exponent "crisis" in the three-dimensional SF-BG universality class by performing accurate studies of quantum and classical model; we use Monte Carlo simulations based on a worm algorithm [10,11] and established protocols of measuring critical points using finite-size scaling (FSS) plots of mean-square winding number fluctuations (see, e.g., Ref. [12]) averaged over disorder realizations (typically 5000–20 000 realizations). Regarding previous studies, we find that they were performed away from the quantum critical region, and the genuine critical behavior was simply out of reach—the transition temperature drops below the detection limit before the data become suitable for extraction of ϕ. However, the low-T_c problem is avoided when the SF-BG transition is approached by increasing the disorder strength at constant particle density. In this regime, simulations of the $(d+1)$-dimensional classical J-current model (in the same universality class) reveal that $z = d = 3$, $\phi = 2.7(2)$, and $\nu = 0.88(5)$ are fully consistent with the $\phi = \nu z$ relation. This conclusion is further confirmed by quantum Monte Carlo simulations of the hard-core DBH, putting an end to the controversy.

Consider the hard-core DBH on the simple cubic lattice (equivalent to the spin-$1/2$ XY ferromagnet in a magnetic field) with the Hamiltonian

$$H = -t\sum_{\langle ij\rangle}(a_i^\dagger a_j + \text{H.c.}) - \sum_i \mu_i n_i, \tag{1}$$

where a_j is the bosonic annihilation operator, t is the hopping amplitude, $n_i = a_i^\dagger a_i$ is the particle-number operator with the hard-core constraint $n_i \leq 1$, $\langle \cdots \rangle$ stands for the summation over the nearest-neighbor sites, and $\mu_i = \mu + \delta\mu_i$. Here μ is the chemical potential and $\delta\mu_i$ is a bounded random potential with uniform distribution on the $[-\Delta, \Delta]$ interval that is uncorrelated in space. The SF-BG transition is induced by fixing disorder strength at $\Delta/t = 16$ and decreasing the chemical potential, similar to the protocol employed in Refs. [1,7,9]. Our data for $T_c(\mu)$ are shown in Fig. 1. They feature an extended region in the parameter space where $T_c(\mu)$ is decreasing by closely following the reported $(\mu - \mu_c)^{1.1}$ law. However, with highly accurate data for T_c (our system sizes are at least an order of magnitude larger than in previous work) we observe that the last point is deviating from this power law well outside of its error bar, see inset in Fig. 1; this indicates that most of the points in Fig. 1 might not be in the critical regime yet. This observation is confirmed by revealing the $n(\mu)$ dependence in Fig. 2. Since density remains finite at

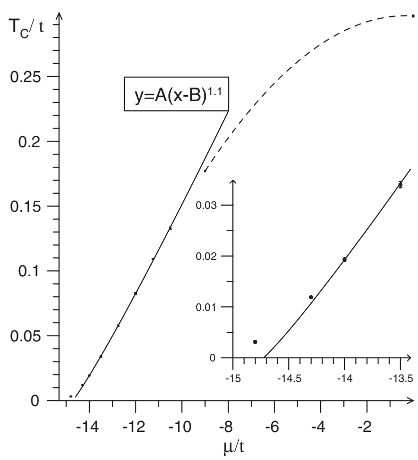

FIG. 1. Critical temperature of the hard-core Bose-Hubbard model as a function of chemical potential for disorder strength $\Delta/t = 16$ fitted to the $T_c = A(\mu - \mu_c)^{1.1}$ power law. The dashed line is to guide the eye.

the QCP, one requirement of being in the quantum critical region is to have $n(\mu) - n(\mu_c) \ll n(\mu_c)$. This condition is clearly violated for most of the points used to establish the $T_c \propto (\mu - \mu_c)^{1.1}$ law in previous studies at low fields.

Because current problems with scaling relations likely originate from strong $n(\mu)$ dependence, when μ is used as a control parameter (leading to the critical region with extremely small T_c values), we radically change the strategy and study the SF-BG criticality as a function of disorder strength Δ at constant density. Universal properties of QCPs in d dimensions can be equally well studied using $(d+1)$-dimensional classical mappings, which are algorithmically superior from the numerical point of view. The simplest classical counterpart of the hard-core DBH in $d = 3$ is the $(3+1)$-dimensional J-current model [13]

$$\beta H = K\sum_{n,\alpha} J_{n,\alpha}^2 - \sum_n \mu_{\vec{r}} J_{n,\tau}, \tag{2}$$

with the $J_{n,\alpha=\tau} = 0, 1$ and $J_{n,\alpha\neq\tau} = -1, 0, 1$ constraints. Here, index α enumerates space-time directions $\hat{x}, \hat{y}, \hat{z}$, and $\hat{\tau}$, $n = (\vec{r}, \tau)$ is the site index in the hypercubic space-time lattice, and $\mu_{\vec{r}} = \mu + \delta\mu_{\vec{r}}$ is the chemical potential plus bounded random potential energy that depends on the space coordinate only. The random potential $\delta\mu_{\vec{r}}$ is uncorrelated in space and is uniformly distributed on the $[-\Delta, \Delta]$ interval. An integer-valued current $J_{n,\alpha}$ is defined on lattice bonds $\langle n, n+\alpha\rangle$ and satisfies the divergence-free condition; i.e., $\sum_\alpha (J_{n,\alpha} + J_{n,-\alpha}) = 0$, where it is understood that $J_{n,-\alpha} = -J_{n-\alpha,\alpha}$. Graphically, the configuration space is composed of J-current loops mimicking path-integral trajectories of bosonic particles. In terms of the underlying bosonic system, $\{J_{n,\alpha=\tau}\}$ and $\{J_{n,\alpha\neq\tau}\}$ represent the on-site occupation numbers and hopping transitions, respectively, while $K \propto 1/t$.

An accurate determination of the critical exponent ϕ ultimately rests on the precise location of the QCP, or critical disorder strength Δ_c, where the power law

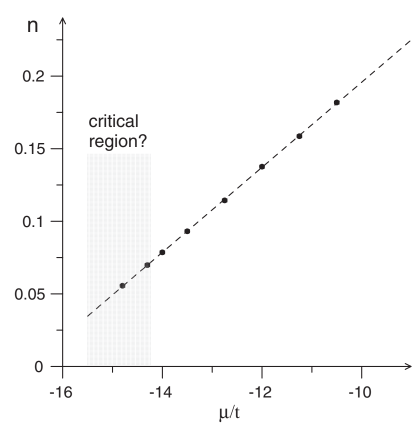

FIG. 2. Density at the thermal critical point of model 1 as a function of chemical potential for $\Delta/t = 16$. The dashed line is a linear fit.

originates. [Otherwise, one can be easily misled by the transient behavior (similar to that shown in Fig. 1). Likewise, all data points for the J-current model can be fit nearly perfectly with the power law based on $\phi \approx 3.3$, if Δ_c is kept as a free parameter.] To determine Δ_c along with the correlation-length exponent ν, we employ FSS of scale-invariant mean-square winding number fluctuations,

$$\langle W^2 \rangle = (1/d) \sum_{\alpha=x,y,z} \langle W_\alpha^2 \rangle, \tag{3}$$

where $W_\alpha = (1/L_\alpha)\sum_n J_{n,\alpha}$ is the winding number in α direction. If a small detuning from the QCP is characterized by $\delta = (\Delta_c - \Delta)/\Delta_c$, then the correlation lengths in space and time directions, ξ and ξ_τ, diverge as $\xi_\tau \propto \xi^z \propto |\delta|^{-\nu z}$, and $\langle W^2 \rangle$ is a universal function of length-scale ratios

$$\langle W^2 \rangle = f(L/\xi, L_\tau/\xi_\tau) = \tilde{f}(L^{1/\nu}\delta). \tag{4}$$

In the last equality, we assume that the ratio L_τ/L^z is fixed. By plotting $\langle W^2 \rangle$ for different system sizes, one determines the critical parameter from the crossing point of $\tilde{f}$ curves (if z was guessed correctly). We argue that $z = d$ is an exact relation. Indeed, in the vicinity of QCP the compressibility can be formally decomposed into critical and regular (nonsingular) parts $\kappa(\Delta) = \kappa_s(\delta) + \kappa_{\text{reg}}(\delta)$, with $\kappa_s \propto |\delta|^{\nu(d-z)}$ [4]. One may speculate that finite $\kappa(\delta = 0)$ is due to the regular part, while the critical part vanishes at $\delta = 0$. However, this possibility is immediately ruled out by the observation that finite κ in the BG phase is due to localized single-particle modes, while such modes do not exist in the superfluid phase. Thus, finite $\kappa(0)$ is entirely due to critical modes and $z = d$ (our FSS data are in perfect agreement with this conclusion, see Fig. 3).

Our simulations of model 2 were done with $K = 2$ at half-integer filling factor, when $\mu = K$. For FSS at the QCP we fix $L_\tau/L^3 = 2$ and consider only large system sizes, from $N = 2\times 12^6$ to $N = 2\times 20^6$ sites. (We hit the limit of what a modern computer cluster can handle in reasonable time, given that every parameter point has to be averaged over 5000–20000 disorder realizations.) The crossing of $\tilde{f}$ curves shown in Fig. 3 pinpoints the critical disorder strength to be at $\Delta_c = 9.02(5)$.

From Eq. (4), it follows that at the critical point

$$\partial\langle W^2 \rangle/\partial\Delta = \text{const} \times L^{1/\nu}, \tag{5}$$

enabling one to determine the correlation-length exponent ν from the slopes of universal curves at the crossing point. The corresponding analysis is shown in Fig. 4, where $\nu = 0.88(5)$ is deduced from the log-log plot of $\tilde{f}$ derivatives. This result is in full agreement with previous findings [9,14].

We now proceed to the evaluation of the critical-temperature exponent ϕ from accurate measurements of $T_c(\Delta)$ (using similar FSS analysis) and the power-law $T_c = A\delta^\phi$ fit to the lowest transition temperatures, see Fig. 5. In striking contrast to Fig. 1 and previously reported results [1,9], all data points nicely follow the power-law curve $T_c \propto (8.83 - \Delta)^{3.27}$, as T_c decreases by nearly 2 orders of magnitude. If Δ_c were left undetermined, we would have to conclude that $\phi \approx 3.3$. However, if the power-law fit is performed with the known value of QCP (i.e., with $\Delta_c = 9.02$), the prediction is different: The ϕ exponent decreases from 2.9 to 2.7 as we reduce the number of the lowest-temperature points to be included in the fit, from $T_c < 0.1$ to $T_c < 0.01$. We thus claim our final result as $\phi = 2.7(2)$, which is in good agreement with the prediction based on the quantum critical relation $\phi = z\nu$ with $z = 3$ and $\nu = 0.88(5)$. [The order parameter exponent deduced from the constant-density approach,

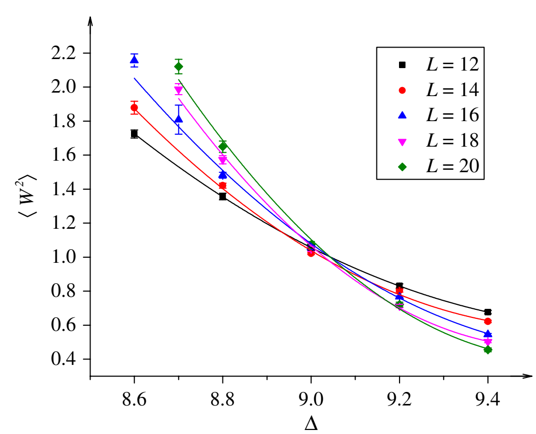

FIG. 3 (color online). Finite-size scaling plots for $\langle W^2 \rangle = \tilde{f}(L^{1/\nu}\delta)$ for system sizes $L = 12$ (black), $L = 14$ (red), $L = 16$ (blue), $L = 18$ (magenta), and $L = 20$ (green) with fixed ratio $L_\tau = 2L^3$. Data points are fitted with second-order polynomials. We do not observe corrections to scaling within our error bars.

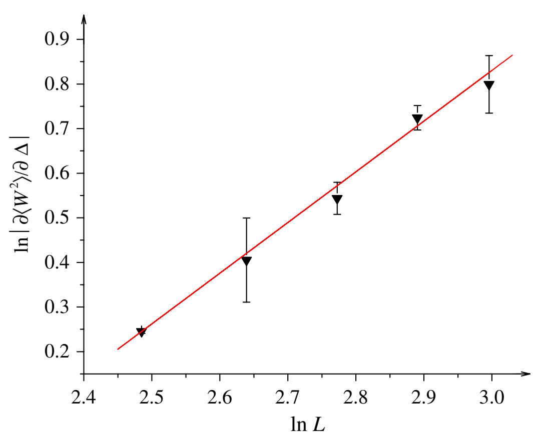

FIG. 4 (color online). Deducing $1/\nu$ from the linear fit of $\ln|\partial\langle W^2 \rangle/\partial\Delta|$ as a function of $\ln L$ using four points near the critical point, $\Delta = 8.8, 9.0, 9.2,$ and 9.4. Error bars are based on the uncertainty of the fitting procedure, given the data points and their statistical error bars in Fig. 3.

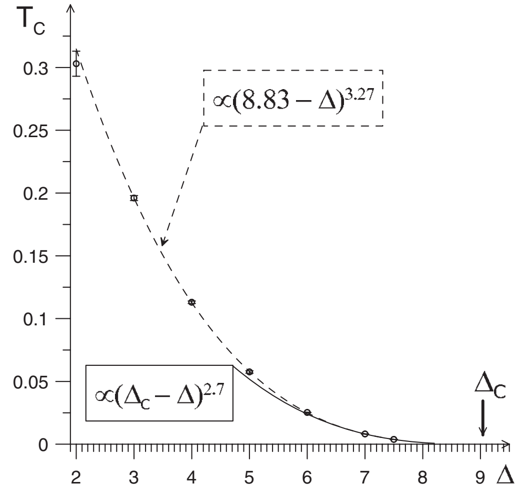

FIG. 5. Critical temperature of the J-current model as a function of disorder strength. Solid line is the power-law fit to the lowest transition temperatures assuming a known location of the quantum critical point. Dashed line is a power law originating from $\Delta = 8.83$.

$\beta = 1.5(2)$, also differs significantly from the value $\beta \approx 0.6(1)$ characteristic of the transient $\mu/t \geq -14$ interval.]

To verify the universality of our findings and to shed light on what to expect if a similar study is attempted experimentally using magnetic or cold-atom systems, we performed quantum Monte Carlo simulation of model 1 at half-integer filling factor (i.e., at $\mu = 0$, or zero external magnetic field in the case of spin-$1/2$ XY ferromagnet). Our data for the normal-to-superfluid transition temperature as a function of disorder strength are shown in Fig. 6 [$T_c(\Delta)$ was determined from FSS analysis of $\langle W^2 \rangle$ plots with $8 \leq L \leq 64$]. Given that

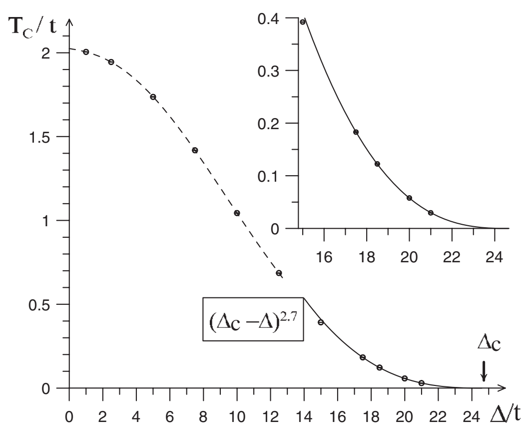

FIG. 6. Critical temperature dependence on disorder strength in the hard-core DBH at half-integer filling factor. The solid line is a fit of the last five points to the $A(\Delta_c - \Delta)^{\phi}$ law, with exponent $\phi = 2.7$ fixed at the value determined from simulations of the J-current model. From this fit we predict that the quantum critical point is located at $\Delta_c \approx 24.67$. Error bars are shown, but they are smaller than the symbol size. Inset: Zoom in on the tail of the main plot.

simulations of quantum models are more challenging numerically, we did not attempt to determine Δ_c, and instead averaged results over a smaller number of disorder realizations, from 5000 at high temperature to 500 at low temperature. The lowest transition temperatures can be perfectly fitted to the $T_c \propto (\Delta_c - \Delta)^{2.7}$ law with $\Delta_c/t = 24.67$. This critical behavior starts at temperatures as high as $T_c/t < 0.5$; we were able to verify it down to $T_c/t \approx 0.03$, see Fig. 6 inset. There is no doubt that the $\phi > 2$ condition is satisfied at the SF-BG transition.

In summary, we addressed the current ϕ-exponent crisis for the superfluid-to-Bose-glass universality class in three dimensions. Previous work questioned conventional scaling relations $z = d$ and $\phi = z\nu$ with $\nu > d/2$ for the SF-BG quantum critical point. Using extensive Monte Carlo simulations of the hard-core DBH and its classical J-current counterpart, we were able to identify problems with previous analyses [strong dependence of density (magnetization) on chemical potential (external magnetic field) on approach to quantum criticality]. We argued that $z = d$ is an exact relation, and used it to determine the critical-temperature exponent ϕ from simulations of the J-current model. Our final result, $\phi = 2.7(2)$, is in good agreement with the quantum critical prediction $\phi = z\nu = d\nu$ based on $\nu = 0.88(5)$, putting the controversy to an end. We verified the universality of our findings and determined under what conditions the ϕ exponent can be studied experimentally.

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