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

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(Dated: February 25, 2014)

PACS numbers: 67.85.Hj, 67.85.-d,64.70.Tg

Recent experimental and numerical studies of the critical-temperature exponent $\phi$ 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 $\nu$ are the dynamic and correlation length exponents, respectively, and question the fundamental concepts underlying quantum critical phenomena. 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 chemical potential (or 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 $\phi$-exponent “crisis”.

For instance, Ref. [8] argues that finite $\kappa$ 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 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 $\nu \approx 0.75(10)$ and $\phi \approx 1.1(1)$ are in strong violation of the key relation $\phi = z\nu$ and the bound $\phi \geq 2$. As a result, scaling relations that form the basis of our understanding of quantum critical phenomena for decades are challenged.

In this Letter, we address the $\phi$-exponent “crisis” in the three-dimensional SF-BG universality class by performing accurate studies of quantum and classical models using Monte Carlo simulations based on 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 5000-20000 realizations). With regard to 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 $\phi$. However, the low-$T_c$ problem is avoided when the SF-BG transition is approached by increasing 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 $z = d = 3$, $\phi = 2.7(2)$, $\nu = 0.88(5)$ 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 magnetic field) with the Hamiltonian

$$H = -t \sum_{\langle ij \rangle} \left( a_i^\dagger a_j + h.c. \right) - \sum_1^\mu \mu_i n_i , \quad (1)$$

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 summation over the nearest-neighbor sites, and $\mu_i = \mu + \delta \mu_i$. Here $\mu$ is the chemical potential and $\delta \mu_i$ is a bounded random potential with uniform distribution on the $[-\Delta, \Delta]$ interval and uncorrelated in space. The SF-BG transition is induced by fixing disorder strength $\Delta$ 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

$$\beta H = K \sum_{n,\alpha} J_{n,\alpha}^\mu - \sum_{\bar{n}} \mu_{\bar{\tau}} J_{n,\bar{\tau}} , \quad (2)$$

with the $J_{n,\alpha=\bar{\tau}} = 0, 1$ and $J_{n,\alpha=\bar{\tau}} = -1, 0, 1$ constraints. Here index $\alpha$ enumerates space-time directions $\hat{x}, \hat{y}, \hat{z}, \hat{\tau}$, $n = (\hat{r}, \tau)$ is the site index in the hyper-cubic space-time lattice, $\mu_{\bar{\tau}} = \mu + \delta \mu_{\bar{\tau}}$ is the chemical potential plus bounded random potential energy that depends on space coordinate only. The random potential $\delta \mu_{\bar{\tau}}$ 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., $\sum_\alpha \left( J_{n,\alpha} + J_{n, -\alpha} \right) = 0$, where it is understood that $J_{n, -\alpha} = -J_{n, -\alpha}$. Graphically, the configuration space is composed of $J$-current loops mimicking path-integral trajectories of bosonic particles. In terms of the underlying bosonic system, $\{ J_{n,\tau} \}$ and $\{ J_{n,\hat{x},\hat{y},\hat{z}} \}$ represent the on-site occupation numbers and hopping transitions, respectively, while $K \propto 1/t$.

Accurate determination of the critical exponent $\phi$ ultimately rests on precise location of the QCP, or critical disorder strength $\Delta_c$, were the power law originates. [Otherwise, one can be easily mislead by the transient behavior (similarly to one shown in Fig. 1). Likewise, all data points for the $J$-current model can be fit nearly perfectly with the power law based on $\phi = 3.25$ if $\Delta_c$ is kept as a free parameter.] To determine $\Delta_c$ along with the

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 an eye.

Since current problems with scaling relations are likely originating from strong $n(\mu)$ dependence when $\mu$ 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 $\Delta$ 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.

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.
correlation length exponent $\nu$, we employ FSS of scale-invariant mean-square winding number fluctuations,

$$\langle W^2 \rangle = \frac{1}{d} \sum_{\alpha=x,y,z} \langle W^2_\alpha \rangle,$$

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

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

In the last equality we assume that the ratio $L_\tau/L^2$ is fixed. By plotting $\langle W^2 \rangle$ for different system sizes, one determines the critical parameter from the crossing point of $f$ curves (if $\nu$ was guessed correctly). We argue that $\nu = d$ is an exact relation. Indeed, in the vicinity of QCP the compressibility can be formally decomposed into critical and regular (non-singular) parts $\kappa(\Delta) = \kappa_c(\delta) + \kappa_{reg}(\delta)$ with $\kappa_c \propto |\delta|^{|d-z|}$.

One may speculate that finite $\kappa(\delta = 0)$ is due to regular part, while the critical part vanishes at $\delta = 0$. However, this possibility is immediately ruled out by observation that finite $\kappa$ 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 $\nu = d$ (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 $N = 2 \times 10^6$ to $N = 2 \times 10^8$ sites (we hit the limit of what 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 $f$-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

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

enabling one to determine the correlation length exponent $\nu$ 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 $f$ derivatives. This result is in full agreement with previous findings.

We now proceed to the evaluation of the critical-temperature exponent $\phi$ from accurate measurements of $T_c(\Delta)$ (using similar FSS analysis) and the power-law $T_c = A_0^5$ 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 nearly two orders in magnitude! If $\Delta_c$ 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 $\phi$ 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 $\nu = 0.88(5)$.

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 4 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 normal-to-superfluid transition temperature as a function of disorder strength are shown in Fig. 6 (W²) plots with 8 ≤ L ≤ 64). Given that simulations of quantum models are more challenging numerically, we did not attempt to determine Δc and averaged results over smaller number of disorder realizations, from 5000 at high temperature to 5000 at low temperature. The lowest transition temperatures can be perfectly fitted to the Tc ∝ (Δc - Δ)².7 law with exponent 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 Δc ≈ 24.64. Error bars are shown but are smaller than the symbol size. Inset: Zoom in to the tail of the main plot.

We thank Y. Deng for help with simulations. MK appreciates fruitful discussions with A. Zheludev. This work was supported by the National Science Foundation under the grant PHY-1314735, the MURI Program “New Quantum Phases of Matter” from AFOSR; K. P. C. da Costa’s work was supported by FAPESP. We also thank ICTP (Trieste), the Aspen Center for Physics and the NSF Grant # 1066293 for hospitality during the crucial stages of this work.

In summary, we addressed the current φ-exponent “crisis” for the superfluid-to-Bose Glass universality class in three dimensions. Previous work questioned the cornerstone relations z = d and φ = zν with ν > d/2, putting the established physical picture of quantum critical phenomena in doubt. Using extensive Monte Carlo simulations of the hard-core DBH and its classical J-current counterpart we were able to identify problems with previous analysis (strong dependence of density/magnetization on chemical potential/external magnetic field on approach to quantum criticality). We argued that z = d as an exact relation, and used it to determine the critical-temperature exponent φ from simulations of the J-current model. Our final result φ = 2.7(2) is in good agreement with the quantum critical prediction φ = zν = dν based on ν = 0.88(5), putting the controversy to an end. We verified universality of our findings and determined under what conditions the φ exponent can be studied experimentally.

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 known location of the quantum critical point. Dashed line is a power-law originating from Δ = 8.83.

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(Δc - Δ)φ law with exponent 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 Δc ≈ 24.64. Error bars are shown but are smaller than the symbol size. Inset: Zoom in to the tail of the main plot.

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