Superfluid-Insulator Transition in Commensurate Disordered Bosonic Systems: Large-Scale Worm Algorithm Simulations

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We report results of large-scale Monte Carlo simulations of superfluid-insulator transitions in disordered commensurate 2D bosonic systems. In the off-diagonal disorder case, we find that the transition is to a gapless incompressible insulator, and its dynamical critical exponent is $z = 1.5(2)$. In the diagonal-disorder case, we prove the conjecture that rare statistical fluctuations are inseparable from critical fluctuations on the largest scales and ultimately result in crossover to the generic universality class (apparently with $z = 2$). However, even at strong disorder, the universal behavior sets in only at very large space-time distances. This explains why previous studies of smaller clusters mimicked a direct superfluid–Mott-insulator transition.

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Quantum phase transitions in disordered systems remain a poorly understood phenomenon despite enormous interest in this field. The $T = 0$ transition between the superfluid (SF) and insulating (I) phases is believed to determine properties of various condensed matter systems: ^{4}He in porous media, aerogels, and various substrates [1], thin superconducting films [2], Josephson-junction arrays [3], disordered magnets [4], etc.

There are strong arguments that the basic Hamiltonian which captures the physics of the SF-I transition is the bosonic Hubbard model with disordered chemical potential [5–7]. In the limit of large occupation numbers, the bosonic Hubbard Hamiltonian is equivalent to the system of coupled Josephson junctions. Fermionic systems map to this Hamiltonian under the assumption that Cooper pairs are preformed at finite temperature, and the transition is driven only by quantum fluctuations of the phase of the complex order parameter. To deal with granular superconductors one may also introduce disorder to hopping amplitudes.

It was suggested in Ref. [6] that one has to consider only two competing insulating phases—the incompressible (gapped) Mott-insulator phase (MI) and the compressible gapless Bose glass (BG) phase. However, more recently it was argued that apart from the BG phase characterized as a compressible insulator with variable-range-hopping conductivity at finite temperature [6], there may exist other phases such as a Bose metal with finite conductivity in the $T \to 0$ limit [8] and an incompressible Mott glass with the conductivity pseudogap [9]. Theoretical calculations for the strongly coupled SF-I critical point are notoriously difficult and are not based on well controlled approximations since localization and interaction effects cannot be separated [10]. Thus, even the qualitative understanding of the phase diagram is still under debate. In particular, it was argued in [6,7,11,12] that MI and SF phases are always separated by the BG phase at any finite disorder. However, experiments [1], most Monte Carlo simulations [13,14], and other theories [15] present evidence in favor of a direct transition between MI and SF phases (in the case of commensurate filling of the lattice and not so strong disorder).

In this Letter, we numerically address the problem of the SF-I transition in a disordered commensurate 2D system. Our large-scale simulations based on the classical worm algorithm [16] demonstrate the absence of the direct SF-MI transition. We clearly see, however, that—even at strong disorder—the universal asymptotic long-range behavior sets in only at large space-time distances. This result, on one hand, explains previous observations of the direct SF-MI transitions in simulations of much smaller clusters, and, on the other hand, implies that the superfluid stiffness and compressibility should obey generic scaling laws only in a very close vicinity of the phase transition point which may be hard to study experimentally.

The worm algorithm (WA) [16] is a high-performance universal Monte Carlo scheme applicable to any model with the configuration space of continuous paths [16,17]. If one is interested in generic properties of quantum phase transitions, then the best model to simulate is a $(d + 1)$-dimensional *classical* scheme, which is algorithmically superior from all points of view. This approach was advocated in Ref. [7], and, most recently, using WA, in Ref. [18]. One of the many mappings between the quantum model (in the path integral representation of particle trajectories) and the classical model of closed-loop (or zero-divergence) "J currents" was suggested in Ref. [7](see also [19]). Let us denote by $J_{\mathbf{x},\alpha}$ the integer bond current where $\mathbf{x} = (\mathbf{r}, \tau)$ are discrete space-time coordinates, and index $\alpha = \hat{\boldsymbol{r}}_1, \ldots, \hat{\boldsymbol{r}}_d, \hat{\boldsymbol{\tau}}$ stands for unit vectors of axis directions, so that $(\mathbf{x}, \alpha)$ defines a bond in the direction α, adjacent to the site $\mathbf{x}$. Then the model of Ref. [7] reads

$$H/T = \sum_{\mathbf{x}\alpha}\left[\frac{1}{2}J^2_{\mathbf{x},\alpha} - \delta_{\alpha,\hat{\tau}}\mu_{\mathbf{r}}J_{\mathbf{x},\hat{\tau}}\right]\Big/K \qquad (1)$$

with the zero-divergence constraint $\sum_\alpha J_{\mathbf{x},\alpha} + \sum_\alpha J_{\mathbf{x},-\alpha} = 0$, where, by definition, the direction $-\alpha$ is understood as opposite to α and $J_{\mathbf{x},-\alpha} = -J_{\mathbf{x}-\alpha,\alpha}$.

In terms of the underlying bosonic system, K represents the particle hopping amplitude in units of the on-site repulsion, and $\mu_{\mathbf{r}} = \mu_0 + \tilde{\mu}_{\mathbf{r}}$ consists of the chemical potential μ_0 and the uncorrelated diagonal-disorder $\tilde{\mu}_{\mathbf{r}}$ uniformly distributed on the interval $[-\Delta, \Delta]$. In this study we are concerned with the commensurate filling of the lattice, i.e., $n = \langle\langle J_{\mathbf{x},\hat{\tau}}\rangle\rangle =$ integer, where $\langle\langle\cdots\rangle\rangle$ stands for the average over all lattice points, statistical and disorder fluctuations, and thus set $\mu_0 = 0$. (An accurate study of the half-integer n case has been reported recently by Alet and Sørensen [18]). We also consider a model (1) with the off-diagonal disorder introduced by letting K be dependent on $\mathbf{r}$ and spatial direction, and confine ourselves to the case of a broken-bond disorder, where for some randomly chosen $\mathbf{r}$ and $\alpha' = \hat{r}_1, \ldots, \hat{r}_d$ we set $K_{\mathbf{r}\tau\alpha'} \to 0$ (equivalent to a rigid constraint $J = 0$ on the corresponding bond).

We start with the off-diagonal disorder case, and consider a system with a quarter of all bonds being broken. Typically, we include about 10^3 disorder realizations in the statistics for system sizes $L \le 40$, and $4 \times 10^4/L$ for larger L. The critical point, K_c, and the dynamical exponent, z, may be obtained from the study of the Green function, $G(\mathbf{r}, \tau)$, naturally evaluated within the WA approach [16]. At the critical point one should see a power-law decay: $G(r, 0) \to r^{-(z+\eta)}$ as $r \to \infty$, and $G(0, \tau) \to \tau^{-(1+\eta/z)}$ as $\tau \to \infty$. This way we find (see Fig. 1, as well as Figs. 2 and 3)

$$K_c = 0.3810(5), \qquad (2)$$

$z + \eta = 1.20(1)$, $1 + \eta/z = 0.80(6)$, i.e.,

$$z = 1.5(2), \qquad \eta = -0.3(1). \qquad (3)$$

It is clear in Fig. 1 that the asymptotic behavior sets in only at sufficiently large space-time distances > 10 lattice periods. Moreover, the short-range behavior of G mimics the critical point of the SF-MI transition in the regular system, where $z = 1$. This peculiar behavior implies that the curves for the superfluid stiffness, ρ_s, and compressibility, κ, will acquire their universal forms only in a very narrow region around the critical point. Away from this region, $\rho_s(K - K_c)$ and $\kappa(K - K_c)$ curves should be essentially different, as suggested by the extended transient evolution of z from ≈ 1 to its true critical value. In Figs. 2 and 3 we, indeed, observe such a behavior. The anomalously narrow critical region makes it virtually impossible—even with our large cluster sizes—to reliably determine the correlation radius critical exponent ν. Along with the dynamical exponent z, it is supposed to determine the critical behavior of the

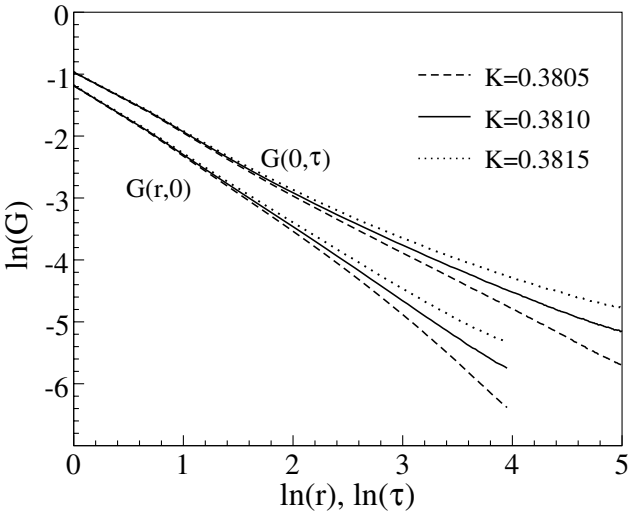

FIG. 1. Correlation functions $G(r, 0)$ and $G(0, \tau)$ for $K = 0.3805, 0.3810, 0.3815$ and system size $L \times L \times L_\tau = 160 \times 160 \times 500$. Error bars are comparable to the linewidths.

compressibility, $\kappa \propto (K - K_c)^{\nu(2-z)}$, and superfluid stiffness, $\rho_s \propto (K - K_c)^{\nu z}$ [6]. The data in Figs. 2 and 3 at best guarantee only the inequalities $\nu(2 - z) < 1$ and $\nu z > 1$, but do not allow us to test the Harris criterion [20] $\nu > 2/d = 1$.

The finite-size scaling of the data for compressibility demonstrates no sign of saturation below K_c and thus strongly suggests that in the insulating state the compressibility vanishes. Though the insulating state is incompressible, i.e., $\kappa = dn/d\mu\,|_{\mu=0} = 0$, it is easy to prove that it is *gapless,* i.e., $dn/d\mu\,|_{\mu\neq 0} \neq 0$ with no plateau on the $n(\mu)$ curve, and thus is qualitatively different from the conventional MI and BG states.

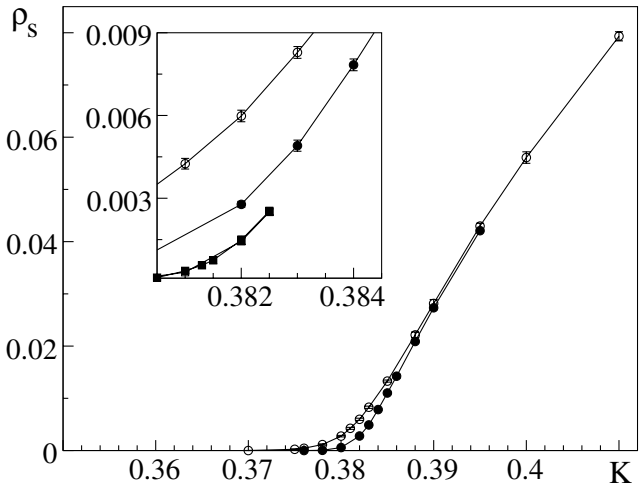

FIG. 2. Superfluid stiffness of the broken-bond model as a function of K at different system sizes: $40 \times 40 \times 40$, open circles; $80 \times 80 \times 80$, filled circles; $160 \times 160 \times 160$, open squares; $160 \times 160 \times 500$, filled squares.

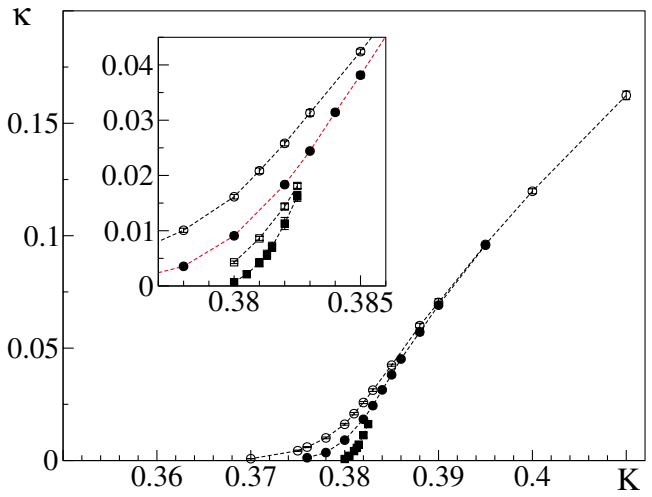

FIG. 3 (color online). Compressibility of the broken-bond model as a function of K at different system sizes: $40 \times 40 \times 40$, open circles; $80 \times 80 \times 80$, filled circles; $160 \times 160 \times 160$, open squares; $160 \times 160 \times 500$, filled squares.

Indeed, in an infinite system it is always possible to find an arbitrarily large cluster that is nearly uniform (in the sense that fluctuations of K away from its cluster average value are arbitrarily small/rare). Taking into account that K_c in the disordered system is larger than the ideal-system critical value [18] $K_c^{(0)} = 0.333\,05(5)$, we conclude that such clusters are nothing else but finite-size *superfluid* lakes. Hence, the gap associated with adding one more particle to the cluster scales as $1/l^d$, where l is the cluster size. The absence of an upper bound on l immediately implies the absence of the global gap in the system spectrum and finite optical conductivity.

The diagonal-disorder case is different. Previously reported data [14] for small clusters $L \times L \leq 12 \times 12$ and disorder strength $\Delta = 0.2$ were interpreted as a direct SF-MI transition with $z = 1$. We extended the study of the $\Delta = 0.2$ case to system sizes $L \times L \leq 160 \times 160$ and did not find any deviations from the direct transition picture at $K_c(\Delta = 0.2) = 0.325(1)$. However, the value of the MI gap in the ideal system, E_{gap}, is almost 3 times smaller than Δ at $K = K_c$ (for the ideal-system phase diagram see Ref. [19]). According to the argument/theorem of Refs. [6,12], the state with $\Delta > E_{\text{gap}}$ is a compressible (gapless) insulator, or BG, because in the infinite system one can always find arbitrary large regions with the chemical potential being nearly homogeneously shifted downwards or upwards by Δ which are doped with particles or holes. Since the distance between such regions is exponentially large for $\Delta \to 0$, their effect is simply undetectably small for $\Delta = 0.2$.

Even if the state right below K_c is a compressible insulator, the question remains whether Griffiths-McCoy singularities are inseparable from critical fluctuations and ultimately result in the crossover to the generic SF-BG transition, or they merely provide a regular background contribution to κ on which a singular contribution κ_{sing} is superimposed. The latter scenario implies a cusp on the compressibility curve and criticality different from SF-BG. To answer this question, we performed simulations for disorder strength $\Delta = 0.4$. As before, the ideal MI gap at the transition point $K_c = 0.2910(5)$ is about 2 times smaller than Δ, and κ has to be finite at K_c.

In Figs. 4 and 5 we present the data for ρ_s and κ which away from the critical point mimic the ideal-system behavior (with the correlation length exponent $\nu \approx 0.7$ and $z \approx 1$), but close to K_c show a spectacular crossover to another universality class. Strong finite-size corrections to κ for system sizes $L \leq 20$ saturate for $L > 20$, and the thermodynamic curve clearly demonstrates *finite* and *nonsingular* dependence $\kappa(K - K_c)$. At the same time, we observe a crossover in the $\rho_s(K - K_c)$ dependence, and see that ρ_s approaches zero with zero derivative, i.e., $\nu z > 1$. From the decay of the Green function at the critical point we obtain

$$z = 2.0(2), \qquad \eta = 0.11(2). \tag{4}$$

Unfortunately, the large-scale crossover did not allow us to determine the critical exponent ν from this set of data. Recent data for half-integer n are best fit with $\nu = 1.15$, but they also suffer from large finite-size corrections [18]. Apparently, the best strategy in the future is to search for a classical model with the smallest crossover scale.

In summary, we have performed large-scale simulations of the superfluid-insulator transition in the $(2 + 1)$-dimensional classical analog of the commensurate disordered 2D bosonic system. For diagonal-disorder, our results suggest that commensurability is not relevant in the long-range limit. We unambiguously resolved finite

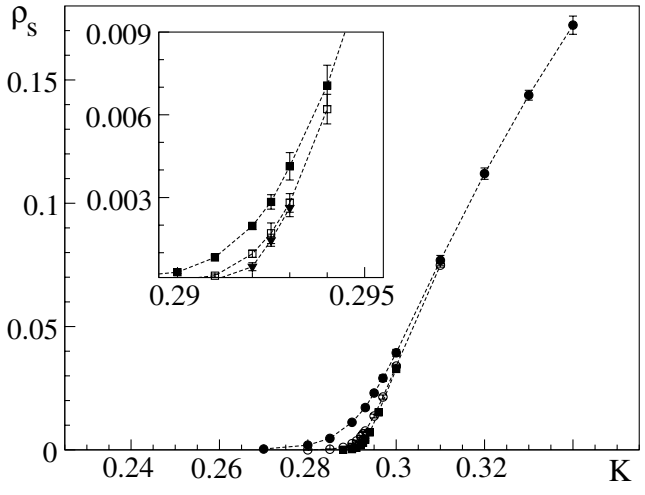

FIG. 4. Superfluid stiffness for the diagonal disorder case as a function of K at different system sizes: $10 \times 10 \times 20$, filled circles; $20 \times 20 \times 49$, open circles; $40 \times 40 \times 121$, filled squares; $80 \times 80 \times 298$, open squares; $160 \times 160 \times 733$, triangle down.

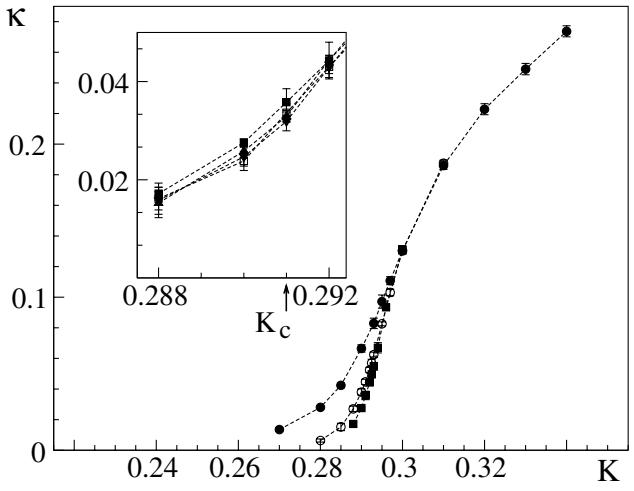

FIG. 5. Compressibility for the diagonal disorder case as a function of K at different system sizes: $10 \times 10 \times 20$, filled circles; $20 \times 20 \times 49$, open circles; $40 \times 40 \times 121$, filled squares; $80 \times 80 \times 298$, open squares; $160 \times 160 \times 733$, triangle down; $160 \times 160 \times 160$, triangle up. The data for $L \geq 80$ collapse on each other within the error bars.

and nonsingular κ at the critical point, and rule out the earlier-reported direct superfluid–Mott-insulator transition in this model. In the off-diagonal disorder case, the compressibility vanishes at the critical point. The incompressible insulating phase, however, is gapless, and its universality class is characterized by the dynamical critical exponent $z = 1.5(2)$. For smaller values of K one has to observe transitions to the MI phase which are governed by statistically rare fluctuations discussed above [6,21]. The rare-region scenario implies that the corresponding critical points, K_{MI}, are obtained from exact relations: $E_{\text{gap}}(K_{MI}) = \Delta$ (for diagonal disorder) and $K_{MI} = K_c^{(0)}$ (for the broken-bond model).

A general observation is that even for large disorder, the universal long-range behavior sets in only at large space-time distances (~ 20 lattice periods). This circumstance explains previous observations of the direct superfluid–Mott-insulator transition in small-size clusters and implies that the superfluid stiffness and compressibility should obey generic scaling laws only in a very close vicinity of the phase transition point.

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