Phase Diagram of the Commensurate Two-Dimensional Disordered Bose-Hubbard Model

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We establish the full ground state phase diagram of the disordered Bose-Hubbard model in two dimensions at a unity filling factor via quantum Monte Carlo simulations. Similarly to the three-dimensional case we observe extended superfluid regions persisting up to extremely large values of disorder and interaction strength which, however, have small superfluid fractions and thus low transition temperatures. In the vicinity of the superfluid-insulator transition of the pure system, we observe an unexpectedly weak—almost not resolvable—sensitivity of the critical interaction to the strength of (weak) disorder.

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Disordered systems keep attracting attention as they reveal the rich and nontrivial physics of the interplay between interaction effects and localization [1,2]. Bosons are particularly interesting because noninteracting particles are always localized in the region of space which corresponds to the deepest bound state in the disorder potential; i.e., the limit of weak disorder and weak interactions is singular. The study of the so-called "dirty boson problem" was first prompted by the disappearance of superfluidity of ^{4}He in porous media (vycor) [3]. Other condensed matter systems of interest include thin superconducting films [4], Josephson junction arrays [5], superfluid helium films on substrates [6], etc.

More recently, the realization of ultracold atoms in optical lattices [7,8] paved the road to studies of strongly correlated systems in a controlled way, and to using them as emulators for condensed matter models. In the presence of disorder, most cold atomic systems are described by the Bose-Hubbard model (BHM) with disorder in the on-site potential. Control over disorder has been implemented in optical lattices in several ways such as using bichromatic lattices, a laser speckle field, and by loading a second (heavy) component into the system [9–13]. Both weakly interacting and strongly interacting limits have been realized in these experiments.

Considerable amount of theoretical effort has been dedicated in the past to understanding the phases and phase transitions in the system [14–25]. In addition to the Mott insulator (MI) and superfluid (SF) states present in the pure case, disordered ground states feature a third, nonconducting but compressible, Bose glass (BG) phase. Whether there exists a direct transition between the MI and SF states has been the subject of a long debate. Fisher *et al.* [2] argued that such a transition is unlikely; i.e., for finite disorder MI and SF phases are always separated by BG, but alternative possibilities were not ruled out rigorously. This resulted in a controversy since, on one hand, mean-field type theories are inadequate in capturing the physics of rare statistical fluctuations driving the MI-BG transition, and, on the other hand, various numerical techniques are severely limited by finite-size effects [16,18,19]. The controversy has been resolved in Refs. [26,27], which proved the theorem of inclusions and concluded that all transitions between the fully gapped and gapless ground states in disordered systems are of the Griffiths type and thus the resulting gapless phase is insulating. Moreover, the original conjecture [2,14] that the MI-BG boundary corresponds to the disorder bound Δ equal to the MI gap in a pure system turns out to be a rigorous result by the same theorem. Here it is important that disorder is bounded since otherwise the MI phase is eliminated altogether. [We note that proofs based on rare statistical fluctuations are valid only in the thermodynamic limit; in finite experimental systems phase boundaries are replaced by crossovers, including complete elimination of the BG state for weak enough disorder.]

Theorems fix the overall topology of the phase diagram but say nothing about its shape and quantitative features. For example, we are not aware of any rigorous argument in dimensions $d > 1$ for why weak disorder would favor SF versus insulating states in the vicinity of the MI transition. By simulations it was found to be the case in $d = 3$; what happens in $d = 2$ remains unanswered. This question is particularly interesting because all existing considerations regarding relevance of weak disorder (see also below) point out that $d = 2$ is a special dimension. In the present work we study a two-dimensional disordered BHM and present the first accurate results for its ground state phase diagram at unity filling factor [28]. The numerical method of solution is based on the lattice path integral Monte Carlo calculations using the worm algorithm [30]. We pay special attention to the critical behavior of the system in the limit of weak disorder in proximity to the SF-MI transition in the homogeneous system.

The disordered BHM reads as

$$H = -t\sum_{\langle ij\rangle} a_i^\dagger a_j + \frac{U}{2}\sum_i n_i(n_i - 1) + \sum_i (\varepsilon_i - \mu) n_i, \quad (1)$$

where $a_i^\dagger(a_i)$ is the boson creation (annihilation) operator, $\langle ij\rangle$ denotes nearest neighbor sites, and $n = a_i^\dagger a_i$ is the density operator. In what follows we use the hopping matrix element t as a unit of energy, U is the on-site repulsion between atoms, and μ is the chemical potential. Random disorder ε_i is uniformly distributed on the $[-\Delta, \Delta]$ interval with no correlations between the sites of a square lattice. In our numerical study, we work at filling factor $n = 1$ and, for definiteness, choose the chemical potential in the middle of the MI gap when appropriate; i.e., gaps for creating particle and hole excitation in the MI phase are both equal to $E_{g/2}$.

To construct the phase diagram we employ standard procedures. The SF-BG transition lines are determined from finite-size scaling of the superfluid stiffness calculated from the statistics of winding numbers squared, $\langle W^2\rangle$, using formula $\Lambda_s = \langle W^2\rangle L^{2-d}/Td$ [31]. According to the theorem of inclusions, the BG-MI line is determined by the $\Delta = E_{g/2}$ criterion (recall that it is impossible to detect this boundary directly in finite-size simulations).

Figure 1 shows $\langle W^2\rangle/2$ vs Δ/t curves at $U/t = 22$ for different system sizes averaged over 500 disorder realizations with error bars dominated by sample-to-sample fluctuations. In this case we scale space and imaginary time dimensions according to the dynamical critical exponent $z = 2$ predicted in Ref. [2] (strictly speaking, in the thermodynamic limit any value of $z > 0$ can be used for determination of the critical point). A barely measurable flow of intersection points with the system size allows us to estimate transition points with relatively high accuracy. From the data in Fig. 1 we deduce $\Delta_c/t = 7.76 \pm 0.06$. The full ground state phase diagram in the (U, Δ) plane is shown in Fig. 2. The boundary between the MI and BG phases at $\Delta/t = E_{g/2}$ was constructed using data for the MI gap in a pure system calculated in Ref. [32].

Reentrant behavior, similar to that observed in $d = 1$ and $d = 3$ phase diagrams, is also present in $d = 2$ in agreement with earlier observations at finite disorder [16,29]. In compliance with the theorem of inclusions, BG always separates SF and MI states which meet only at the MI-SF transition point of the clean system at $U_c/t = 16.7424(5)$. As we move away in the vertical direction, weak disorder always works in favor of the SF phase shifting the transition points to the right—this appears to be a common behavior in all physical dimensions. The mechanism, however, is not universal and only in $d = 1$ it can be explained theoretically by the destructive interference of the vortex instanton contributions to the partition function [20].

In the weak interaction limit $U \to 0$, the transition line goes to zero with an infinite slope $\Delta_c \propto \sqrt{U}$ [33]. In this region, the interaction is very efficient in screening deep potential wells and stabilizing superfluidity. Numerically, it is extremely hard to study [34] and we were not able to clearly resolve the square-root law though our data provide an estimate for the prefactor in $\Delta \approx 20\sqrt{Ut}$.

Remarkably, superfluidity persists up to extremely large values of disorder and interactions. For intermediate interactions, superfluidity survives when disorder potential is about 10 times larger than the bandwidth, $\Delta/t = 72$. Likewise, the superfluid "finger" at $\Delta/t = 30$ extends all the way to $U/t = 49$. However, superfluid properties of the system in the large disorder and large interaction limits are not robust. In Figs. 3 and 4 we plot the superfluid stiffness calculated along two representative cuts of the phase diagram, one at fixed interaction $U/t = 26$ and the other at fixed disorder $\Delta/t = 35$. Small values of Λ_s for $\Delta > 30t$

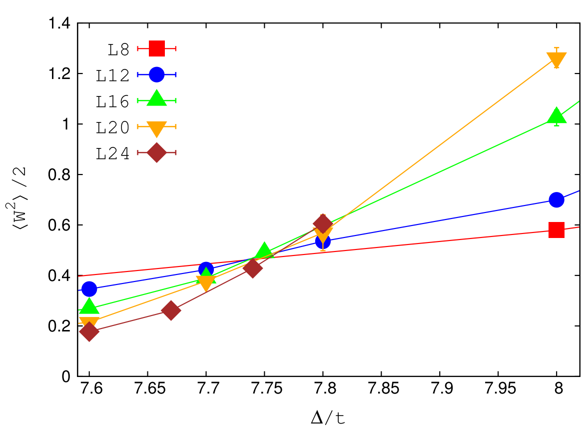

FIG. 1 (color online). Finite-size scaling of winding number fluctuations as a function of disorder bound Δ for interaction strength $U/t = 22$ and dynamical exponent $z = 2$. Data are shown for $\beta = (L/4)^2$.

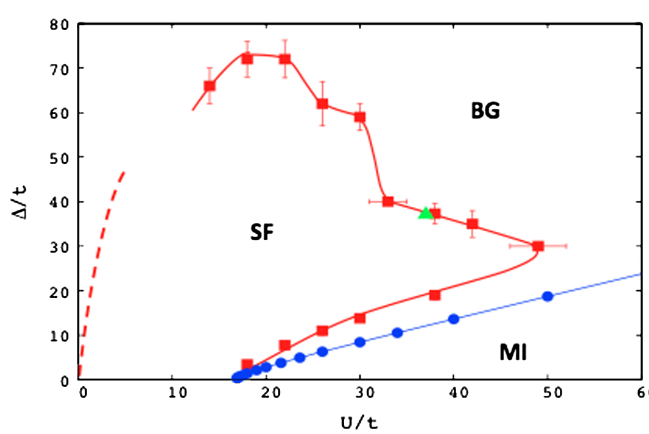

FIG. 2 (color online). Zero temperature phase diagram of the two-dimensional BHM at filling factor $n = 1$. The MI-BG transition at $\Delta = E_{g/2}$ is obtained using gap data from Ref. [32]. The green triangle point on the SF-BG boundary was obtained in Ref. [29]. The dashed line is the square-root law predicted for the $\Delta, U \to 0$ limit in Ref. [33].

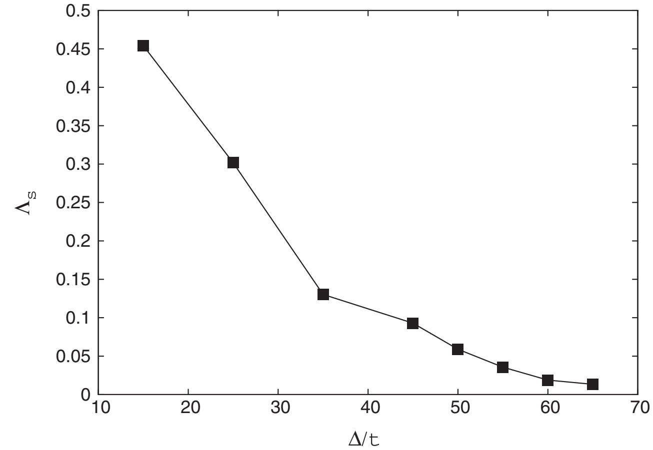

FIG. 3. Superfluid stiffness as a function of disorder bound Δ at fixed interaction strength, $U/t = 26$, and temperature, $T/t = 0.042$, for system size $L = 12 \times 12$.

ensure small superfluid-normal transition temperatures according to the Nelson-Kosterlitz relation $T_c/t = (\pi/2)\Lambda_s(T_c)$. Note that Figs. 3 and 4 can be used to determine upper bounds on T_c because $\Lambda_s(T_c) < \Lambda_s(0)$. For example, numerical simulations of the SF-normal transition temperature at $U/t = 26$ and $\Delta/t = 35$ yielded $T_c/t = 0.07 \pm 0.012$ below the upper bound estimate $T_c/t = 0.2$.

Low transition temperatures have important consequences for current cold-atom experiments. Though the ($U/t = 26$, $\Delta/t = 35$) point is chosen to be far from the edges of the SF-BG boundaries in Fig. 2, the value of T_c is well below typical experimental temperatures which are still at (or above) the tunneling amplitude t. Thus observing the ground state phase diagram remains a challenging task. In current experimental setups, only a small fraction of the superfluid region will survive finite temperature effects.

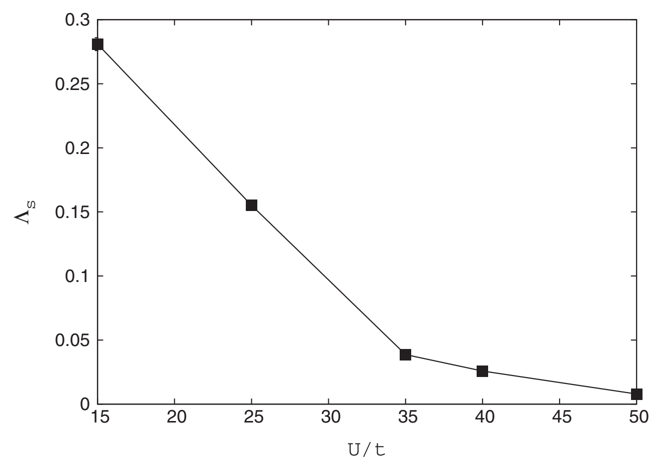

FIG. 4. Superfluid stiffness as a function of interaction strength U/t at fixed disorder bound, $\Delta/t = 35$, and temperature, $T/t = 0.042$, for system size $L = 12 \times 12$.

Let us now focus on the weak disorder case at the tip of the Mott lobe in the pure system. Similar to the one-dimensional case (see Refs. [2,20,35]), the *qualitative* aspects of the effect of disorder can be described within Popov's superfluid hydrodynamic action ($\hbar = 1$)

$$S = \int d\vec{r} \int d\tau \left\{ i\langle n\rangle \dot{\Phi} + \frac{\kappa}{2}\dot{\Phi}^2 + \frac{\Lambda_s}{2}[\nabla\Phi]^2 \right\}, \quad (2)$$

where κ is the compressibility, τ is the imaginary time, $\Phi(\vec{r}, \tau)$ is the superfluid phase field, and $\langle n(\vec{r})\rangle$ is the average density at the lattice point $\vec{r}$ (the integral over $d\vec{r}$ is understood as a discrete lattice sum, and the gradient as a finite difference). Since the first term contains a full time derivative of the phase variable, we observe that (i) the integral $\int \dot{\Phi} d\tau$ can be only a multiple of 2π, (ii) in a pure system with $\langle n(\vec{r})\rangle = 1$ this term is irrelevant and the effective action (after rescaling of the time variable with the sound velocity) is that of the classical 3D XY model, (iii) in a disordered system this term is of any importance (not a multiple of 2π) only in the presence of topological defects in the phase field. More precisely, its value is purely imaginary and for the (2 + 1)-dimensional space-time vortex loop with projected (on the space plane) d-dimensional algebraic area A is given by a simple formula

$$S_{\rm loop} = 2\pi i \int_A d\vec{r} \langle \delta n(\vec{r})\rangle, \quad (3)$$

where $\delta n(\vec{r}) = n(\vec{r}) - 1$ is the local density fluctuation about the mean value.

The nature of the SF-MI transition in a clean system described by the 3D XY model is linked to the proliferation of large vortex-loop instantons which disorder the phase field. In the absence or irrelevance of the phase term all vortex-loop instantons act in "unison," in other words their contributions interfere constructively in the partition function. This is no longer the case in the disordered system since an area integral in Eq. (3) is now a random variable. When random vortex phases become large, their contributions to the partition function cancel each other making them inefficient in destroying phase coherence across the system. Let us estimate the typical phase of a vortex loop of size ξ where ξ is the correlation length. It is proportional to the total particle number fluctuation in the area $A \sim \xi^2$ in response to the random chemical potential fluctuation in this region, $\delta\mu_A = A^{-1}\int \epsilon_r d^2 r$, which, by the central limit theorem, scales as Δ/ξ. Using the system's compressibility, $\kappa = \partial n/\partial\mu$, we then find

$$\mathrm{Im}\, S_{\rm loop} \sim 2\pi A\kappa\Delta/\xi \sim 2\pi\xi\kappa\Delta. \quad (4)$$

As long as disorder remains perturbative (i.e., $S_{\rm loop} \ll 1$), we have $\xi \sim (1 - U_c(\Delta)/U)^{-\nu}$ where $\nu = 0.671\,55$ is the correlation length exponent and $U_c(\Delta)$ is the critical interaction for a given Δ. Equation (4) extrapolated to $\mathrm{Im} S_{\rm loop} \sim 1$ predicts how close U should be to $U_c(\Delta)$ to

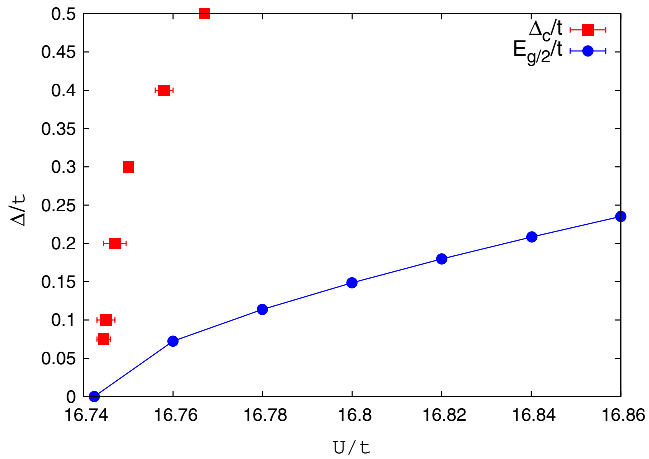

FIG. 5 (color online). Phase diagram in the vicinity of the Mott lobe for weak disorder. Note extremely weak dependence of the SF-BG critical point on disorder for small Δ.

start seeing relevance of disorder, provided the system size is *exponentially* large, $L > \xi \propto \exp(U/\Delta)$; see Eq. (5) below.

One might think that Eq. (4) implies linear scaling of phase with the correlation length. However, in the vicinity of the particle-hole symmetric SF-MI transition point, the renormalized compressibility itself vanishes as $\kappa \sim 1/U\xi$, canceling dependence on ξ in Eq. (4). It means that each length scale contributes equally to the vortex-loop phase; i.e., the final dependence is only logarithmic:

$$\mathrm{Im}\, S_{\mathrm{loop}} \propto (\Delta/U)\ln\xi. \tag{5}$$

We thus conclude that $d = 2$ is the "critical dimension" starting from which the relevance of weak disorder cannot be seen by assuming that compressibility follows the Josephson relation, $\kappa \propto \xi^{1-d}$; i.e., the shape of the critical line $U_c(\Delta)$ is determined by the nonuniversal microscopic physics. [Finite κ in Eq. (4) clearly implies relevance of disorder on length scales $>(\kappa\Delta)^{-2/d}$.] This is to be contrasted to $d = 1$ where relevance of weak disorder defines the critical line; see [20].

In Fig. 5 we show the phase diagram close to the tip of the Mott lobe. Critical points were determined using finite-size scaling with $z = 1$. Clearly, critical points for the SF-BG transition are at disorder values much larger than the $E_{g/2}$ boundary for the MI phase. Surprisingly enough, the first data points for the SF-BG line are indistinguishable from the critical value in the clean system $U_c/t = 16.742\,4(5)$ within the error bars. This was unfortunate because even though critical points were determined with accuracy better than four digits we still did not have enough parameter range to make an unambiguous case for the form of the line $U_c(\Delta)$.

Summarizing, we have presented the full ground state phase diagram of the disordered BHM at unity filling factor. Interestingly, while the superfluid phase is remarkably stable against strong interactions and disorder it is rather fragile with regards to finite temperature effects. Our numerical data feature an essentially vertical SF-BG line for weak disorder; understanding physics behind this phenomenon in $d \geq 2$ remains a challenge.

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