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Anomalous quantum glass of bosons in a random potential in two dimensions

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We present a quantum Monte Carlo study of the “quantum glass” phase of the 2D Bose-Hubbard model with random potentials at filling \( \rho = 1 \). In the narrow region between the Mott and superfluid phases the compressibility has the form \( \kappa \sim \exp(-b/T^\alpha) + c \) with \( \alpha < 1 \) and \( c \) vanishing or very small. Thus, at \( T = 0 \) the system is either incompressible (a Mott glass) or nearly incompressible (a Mott-glass-like anomalous Bose glass). At stronger disorder, where a glass reappears from the superfluid, we find a conventional highly compressible Bose glass. On a path connecting these states, away from the superfluid at larger Hubbard repulsion, a change of the disorder strength by only 10% changes the low-temperature compressibility by more than four orders of magnitude, lending support to two types of glass states separated by a phase transition or a sharp cross-over.

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There are two types of ground states of interacting lattice bosons in the absence of disorder: the superfluid (SF) and the Mott-insulator (MI). In the Bose-Hubbard model (BHM) with repulsive on-site interactions [1, 2] an MI state has an integer number of particles per site and there is a gap to states with added or removed particles. The gapless SF can have any filling fraction. These phases and the quantum phase transitions between them are well understood [1–6] and have been realized experimentally with ultracold atoms in optical lattices [7, 8].

If disorder in the form of random site potentials is introduced in the BHM (which can also be accomplished [9, 10]) a third state appears—an insulating but gapless quantum glass. This state has been the subject of numerous studies [1–3, 11–27] but many of its properties are still not well understood. Two types of glass states are known: the compressible Bose glass (BG) and the incompressible Mott glass (MG), with the latter commonly believed to appear only at commensurate filling fractions in systems with particle-hole symmetry [18–20, 26–29]. The currently prevailing notion is that the glass state in the 2D BHM with random potentials is always of the compressible BG type [20–22, 25].

We here present quantum Monte Carlo (QMC) results for the two-dimensional (2D) site-disordered BHM, showing that there is actually an extended parameter region in which the BG is either replaced by an MG or has an anomalously small (in practice undetectable) compressibility. The system is described by the Hamiltonian

\[
H = -t \sum_{\langle ij \rangle} (b_i^+ b_j + b_j^+ b_i) + U/2 \sum_{i=1}^{N} n_i (n_i - 1) + \sum_{i=1}^{N} \epsilon_i n_i, \tag{1}
\]

where \( \langle ij \rangle \) are nearest neighbors on the square lattice, \( b_i^+ \) (\( b_i \)) are boson creation (destruction) operators, \( n_i = b_i^+ b_i \) site occupation numbers, and \( \epsilon_i \) random potentials uniformly distributed in the range \([-\Lambda - \mu, \Lambda - \mu]\) about the average chemical potential \( \mu \). We study the model using the stochastic series expansion (SSE) QMC method with directed loop updates [30]. We adjust the chemical potential so that the mean filling-fraction \( \rho = \langle n_i \rangle = 1 \) (to within \( < 10^{-5} \)) when averaged over sites \( i \), disorder realizations, quantum and thermal fluctuations. To speed up the simulations, we impose a cut-off \( n_i \leq 2 \) (some times \( n_i \leq 3 \)) which does not change the nature of the states. We study sufficiently large inverse temperatures \( \beta = t/T \) and lattice sizes \( L (N = L^2 \) sites) to address the ground state in the thermodynamic limit.

In the plane \((\mu/U, t/U)\), for fixed disorder strength \( \Lambda \), there are characteristic “Mott lobes” inside which the filling is integer, while outside \( \rho \) changes with \( \mu, U \). At fixed integer filling, in the plane \((U, \Lambda)\) there is a narrow “finger” of the glass phase intervening between the MI and SF, shrinking to a point \( U_c \) at \( \Lambda = 0 \). Most studies have focused on \( \rho = 1 \) and the phase diagram in this case is qualitatively very similar in two [25] and three [22] dimensions. We show a schematic phase diagram in Fig. 1.

We focus first on a vertical line in the phase diagram in Fig. 1 at moderate \( U \). With increasing \( \Lambda \) we can go from the MI, transition into the glass state in the finger region, then into the SF, and finally re-enter a glass state at much larger \( \Lambda \). We also consider a line to the right of the SF phase in Fig. 1, studying the evolution of the glass with increasing disorder when the SF is not crossed but (as we will show) the properties change dramatically.

We compute two observables characterizing the states: the compressibility \( \kappa \) and the superfluid stiffness \( \rho_s \) (obtained with SSE using, respectively, particle-number and
winding number fluctuations [30]). The results were averaged over \(500 \sim 1000\) realizations of the random potentials. Fig. 2 shows the evolution with \(\Lambda\) of these quantities for a fixed system size at a low temperature.

Before discussing the results, we recall the reasons for the existence of a glass phase and its expected nature. In disordered systems in general, one can expect Griffiths phases where statistically rare large regions of some phase inside another phase lead to singularities not present in the absence of disorder [31–33]. For the integer-\(\rho\) BHM with site disorder, the Griffiths argument states the following [2, 3]: Once the width \(2\Lambda\) of the disorder distribution exceeds the Mott gap \(\Delta_M\), there can be arbitrarily large domains of SF inside the MI. Until \(\Lambda\) exceeds some larger critical value these domains are not percolating through the lattice, and the state is therefore insulating [34]. In the standard scenario (discussed further in supplementary material), fluctuations of the overall chemical potential within the SF domains lead to near degeneracies of different particle-number sectors and, therefore, nonzero compressibility (a BG) [21, 22, 25]. With these notions in mind, we now discuss our results.

Looking first at the superfluid stiffness in Fig. 2, the sharp increase at \(\Lambda \approx 8\) signals the entry into the SF phase. A finite-size scaling analysis, presented below, shows that the transition takes place at \(\Lambda_c \approx 8.3\), which is in reasonable agreement with the result by Söyler et al., \(\Lambda_c(U = 22) \approx 7.8\) [25]. Here we note that our model is slightly different, because of the cut-off \(n_i \leq 2\) (while there was no cut-off in Ref. [25]). When we increase the cut-off to \(n_i \leq 3\) the critical point moves to a value consistent with that of Söyler et al. Increasing \(\Lambda\) further in Fig. 2, the superfluid stiffness eventually again decreases to zero at \(\Lambda \approx 30\). This transition point is much smaller than that of Söyler et al., \(\Lambda_c \approx 70\), as would be expected in this region where the probability of site occupations beyond our cut-off is substantial. Since the cut-off does not alter any symmetries of the system there is no reason to believe that it will affect our conclusions regarding the nature of the phases and transitions.

Turning to the compressibility, it is substantial in the SF phase and when the glass is re-entered at large \(\Lambda\). However, it is very small below the SF transition, not only in the Mott phase (which extends up to \(\Lambda \approx 4.3\) in our system, based on the Mott gap of the clean MI as discussed in supplementary material) but also in the region \(\Lambda \approx 5 \sim 7\), where the system is in a glass phase. The \(L \to \infty\) compressibility as a function of temperature is shown in Fig. 3. At \(\Lambda = 0\) and 3, we observe the normal exponential decay with \(\beta\) expected in the gapped MI phase. At \(\Lambda = 6\) and 7 we instead find the form

\[
\kappa \sim \exp(-b/T^\alpha) + c, \tag{2}
\]

where \(\alpha < 1\) and \(c = 0\) (to within statistical errors). This form has previously been found in random quantum spin systems [29, 35], where \(\kappa\) corresponds to the magnetic susceptibility and one expects it to vanish as \(T \to 0\) because of spin-inversion symmetry (corresponding to particle-hole symmetry for bosons). Such an incompressible and insulating quantum glass is called an MG [13] and has also been shown to exist in variants of the 2D random BHM where particle-hole symmetry is explicitly built in [27, 28] (and Ref. [13] argued for its possible existence also more generally). To our knowledge, \(\kappa(T)\) was not computed for these systems and there is no theoretical prediction for its form. In the presence of random potentials there is no explicit particle-hole symmetry (but in principle there could be emergent particle-hole symmetry, as in the clean BHM at the tips of the Mott lobes [2]). It had been argued that the glass state of the BHM should then always be a clearly compressible BG [21, 22, 25], contrary to our findings.

While \(c = 0\) in (2) may not hold strictly, the very
In terms of the unknown exponents theory [36] (but may be different in a quantum system). $b$ can in principle be computed using classical percolation.

The lattice size $L = 32$ in all cases, which is sufficient to eliminate finite-size effects at these temperatures. The curves are fits to the form (2) with $\alpha = 1$ for $\Lambda = 0.3$ (MI state) and $\alpha = 0.78$ and 0.53 for $\Lambda = 6$ and 7, respectively (MG state). For $\Lambda = 9$ (SF state) $\kappa$ is essentially constant.

small $\kappa(T \rightarrow 0)$ at the very least shows that the system is an anomalous BG, with exceedingly small (essentially undetectable) compressibility in a large part of the phase diagram. We here use the term MG because, as we will argue below, even if $c > 0$ but small the physics behind the anomalous BG is very similar to a true MG.

The form (2) of $\kappa(T)$ with $c = 0$ can be understood heuristically as follows: Consider non-Mott domains below the percolation point inside an MI. At temperature $T$ there is some size $m$ such that for $T \lesssim m^{-a}$ all domains of size $s < m$ are effectively in their ground states and do not contribute to the compressibility. The exponent $a$ depends on the low-energy level spectrum of the domains, which should be related to the fractal nature of the domains. Domains with $s > m$ should contribute essentially independently of $T$ and $s$. The probability of a site belonging to a domain of size $s > m$ is $\propto \exp(-dm^b)$, where $b$ can in principle be computed using classical percolation theory [36] (but may be different in a quantum system). In terms of the unknown exponents $a$ and $b$ the compressibility due to non-Mott domains is $\kappa \propto \exp(-dT^{-b/a})$, which is Eq. (2) with $\alpha = b/a$.

The above scenario neglects the arbitrarily close degeneracy of different particle-number sectors due to fluctuations of the average chemical potential of the domains, which lead to $\kappa(T = 0) > 0$ in the standard BG scenario (where the non-Mott domains are superfluid). How can these degeneracies be avoided? By studying isolated domains with a different chemical potential embedded in an MI, we have found (see supplementary material) that there are finite-size effects due to which particle-number degeneracies in the region of interest here only occur when the domains are large (with the critical size diverging at the Mott phase boundary). All domains below a critical size (which depends on the domain shape) have vanishing $T \rightarrow 0$ compressibility and should not be regarded as superfluid—they are insulating because of finite size and effectively possess particle-hole symmetry at low energy. One still expects rare domains exceeding the critical size to contribute when $T \rightarrow 0$. However, we will show below that typical large domains should also have an altered spectral structure due to quantum-criticality when the SF boundary is approached. Thus, both small and large typical domains (the latter of which are fractals) may not contribute to the $T = 0$ compressibility.

Within the standard scenario, there should still exist rare large compressible domains in the Mott background, but in reality the domains are never completely isolated from each other and the picture of degenerate single-domain levels may ultimately not be valid away from the atomic limit (large $U$ and $\Lambda$). Whether or not strictly $c = 0$ in Eq. (2), in practice the compressibility is undetectably small and the system is effectively an MG in the finger region (and, as we will see, also at larger $U$ in a substantial region along the Mott boundary).

We do find a compressible BG in the re-entrance region at large $\Lambda$ (above the SF in Fig. 1), as illustrated by results at $\Lambda = 60$ in Fig. 4. There should then be a phase transition or a cross-over separating the MG and the BG phases. We have identified a dramatic variation in the compressibility along a vertical line at $U = 60$. As shown in the inset of Fig. 2, at $\beta = 8$, $\kappa$ increases rapidly with $\Lambda$ between 28 to 31 (which is far away from the Mott boundary at $\Lambda \approx 24$), before flattening out. The enhancement is more than four orders of magnitude, $\kappa$ being very small before the sharp increase. We do not find any significant finite-size effects in this region for $L > 8$, and also the behavior does not change substantially upon further increasing $\beta$ (and the $n_i$ cut-off also does not play a role here). The behavior therefore indicates a sharp cross over, not a phase transition, though in principle $\kappa$ could still vanish exponentially at some point away from the Mott boundary. As a function of $U$, the cross-over most likely occurs on a line extending out from the right-side SF tip (“nose”) in Fig. 1 and can be interpreted as a change from a state where typical non-Mott domains are not superfluid to a BG where the domains are superfluid but do not form a coherent global state.

We next study the critical $T = 0$ compressibility at the lower glass–SF boundary, where $\kappa \sim (\Lambda - \Lambda_c)^{z(2-z)}$ is expected in the thermodynamic limit. If $z = 2$, as is often assumed [21, 22, 25], $\kappa > 0$ is non-singular at the transition. One would then expect $\kappa > 0$ also close to the transition inside the glass [18]. Then the only plausible scenario is that $\kappa > 0$ throughout the glass phase (and there is no a priori reason to expect a very small $\kappa$). A key question then is whether $z = 2$ or $z < 2$. In the former case divergent SF clusters in the MI background close to the percolation point would be compressible, while in the latter case they should be incompressible. There are arguments for $z = 2$ at the glass-SF transition [2] but...
no rigorous proofs. Some numerical works on models related to the BHM have in fact pointed to $z < 2$ [37, 38]. Calculations suggesting $z = 2$ are affected by large uncertainties [11, 17, 18] and are also consistent with $z < 2$.

We extract $z$ using the following finite-size scaling behaviors [2] expected exactly at the critical point:

$$\kappa(L, \Lambda_c) \propto L^{-d-z}, \quad \rho_s(L, \Lambda_c) \propto L^{-z}. \quad (3)$$

In Fig. 5 we show results using different system sizes and scaling the inverse temperature according to $\beta = L^z$ with three choices of $z$ [39]. Based on Eqs. (3) we expect curves of $\kappa L^{d-z}$ for different $L$ to cross each other at a point (asymptotically for large $L$) if the correct value of $z$ is used, and a similar behavior of $\rho_s L^z$. It should be noted, however, that there are crossings even if a wrong $z$ is used, but the vertical crossing value (e.g., for system sizes $L$ and $2L$) will then drift up or down instead of converging to a constant. One can also expect larger corrections to the horizontal crossing value if an incorrect $z$ is used. The compressibility crossing points in Fig. 5 are very sensitive to the value of $z$, while the stiffness crossings are more stationary. Such behavior has also been observed in certain clean bosonic systems [40]. Based on our result, $z$ should be between 1.5 and 1.75, which implies that the percolating SF cluster is incompressible.

In the above analysis it has been implicitly assumed that any non-singular contributions to $\kappa$ can be neglected. If regular contributions arise from SF domains larger than a critical size, then we would expect these contributions to increase with $L$ and, by Eq. (3), this would lead to an apparent enhancement of $z$. Since we instead find a reduction from $z = 2$ it appears that non-singular background contributions are not responsible for this effect and $z < 2$ should be a robust result. This is also consistent with the drop of $\kappa$ seen in Fig. 2 when approaching the lower SF–glass transition from the right, while at the higher transition point there are no strong variations, suggesting $z = 2$ there.

Along with a large critical size needed for non-Mott domains to become superfluid, even far away from the Mott boundary, a dynamic exponent $z < 2$ provides an explanation for an anomalously small, or possibly vanishing, $T = 0$ compressibility in the finger region of the phase diagram between the Mott and SF phases. The sharp cross-over from anomalously small to normal compressibility away from the SF phase at larger $U$ also shows that there are two distinct types of glass phases in the BHM, one being either an MG or an anomalous BG with physics similar to an MG, and the other one a standard BG with isolated non-coherent superfluid domains.

The scenario discussed here applies only to integer filling fractions, since a compressible state follows trivially from a non-constant $\rho(U, \Lambda)$ for incommensurable systems. Differences between integer and non-integer fillings were found in a recent renormalization-group study [23], although it is not clear whether the state is the MG or anomalous BG identified in our work.

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