Many-body localization in the two dimensional Bose-Hubbard model

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When dealing with many-body localization, one of the hardest tasks is the investigation in more than one spatial dimension and for bosons. We investigate the disorder driven localization of the two dimensional Bose-Hubbard model by evaluating the full low energy quasi-particle spectrum via a recently developed fluctuation operator expansion. For any considered (local) interaction we find a mobility edge that terminates at sufficiently large disorder strength, implying the existence of a many-body localized phase. The finite size scaling is consistent with a Beresinskii-Kosterlitz-Thouless scenario. A direct comparison to a recent experiment yields an excellent match of the predicted transition point and scaling of single particle correlations.

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In the last decade the study of disorder-driven localization of quantum particles has received considerable interest, following the suggestion that Anderson localization for non-interacting models \cite{1,2} can be generalized to interacting ones \cite{3,4} in the framework of the so-called many-body localization (MBL). One of the most prominent features of MBL is its incompatibility with the eigenstate thermalization hypothesis (ETH) resulting from an extensive number of local integrals of motion \cite{8,9}. A complete demonstration of MBL would in principle require knowledge of the whole spectrum, limiting the use of exact diagonalization techniques to small system sizes, especially when bosonic particles are considered \cite{10,11}. The existence of MBL has been rigorously proven in one-dimensional spin-chains \cite{12,13}, while early perturbative arguments \cite{14,15} and numerical evidence \cite{16,17} have also supported its existence in two dimensions - involving a mobility edge (ME) separating mobile from localized states in the spectrum. However, recent numerical evidence has challenged the existence of MBL both in 1D \cite{18} and 2D \cite{19,20} in the thermodynamic limit. Experimental realizations of bosonic systems have already been achieved in cold atom setups where a disorder potential can be imprinted onto an (confined) optical lattice in one \cite{21,22} and two dimensions \cite{21}, showing strong signs of localization in both cases.

Here, we investigate the quantum phases of the two-dimensional Bose-Hubbard model (BHM) in the presence of disorder utilizing a recently developed fluctuation operator expansion (FOE) method \cite{23,24}, which gives access to the complete spectrum of quasiparticle (QP) excitations for system sizes comparable to experiments. Our results are summarized in Fig. 1. For all interaction strengths disorder induces (at least) one ME. We find that the finite-size scaling at these critical points is consistent with a Beresinskii-Kosterlitz-Thouless (BKT) scenario \cite{25,26}. Importantly, for each interaction strength and low enough energy, the ME is an exponentially decreasing function of the disorder strength up to a critical disorder strength, which marks the transition to a MBL phase. In its vicinity the ME shows reentrant behavior consistent with predictions of the Bose glass phase \cite{27,28,29,30,31}. For the case of particles confined by a harmonic potential, we compute correlation functions and extract the inverse decay length, finding excellent agreement with recent experiments \cite{26}.

The Hamiltonian of the BHM with on-site disorder and in the grand canonical ensemble reads

\[ \hat{H} = \sum_{\ell} \left( \mu_{\ell} \hat{b}_{\ell}^\dagger \hat{b}_{\ell} + \frac{U}{2} \hat{b}_{\ell}^\dagger \hat{b}_{\ell}^\dagger \hat{b}_{\ell} \hat{b}_{\ell} + t \sum_{\langle \ell, \ell' \rangle} \langle \ell' \rangle \hat{b}_{\ell}^\dagger \hat{b}_{\ell'} + \text{h.c.} \right), \]

where \( \hat{b}_{\ell} \) (\( \hat{b}_{\ell}^\dagger \)) are bosonic creation (annihilation) operators at the site \( \ell \), \( t \) is the tunneling rate between near-
est neighbor sites \((\ell, \ell')\) on a square lattice of spacing \(a\) and linear size \(L\), while \(U\) is the local on-site Hubbard interaction. The energy \(\mu_{\ell}\) reads \(\mu_{\ell} = -\mu + \epsilon_{\ell}\), with \(\mu\) the chemical potential and \(\epsilon_{\ell}\) a local energy shift due to disorder or an external harmonic potential. With Ref. [21] in mind we choose a Gaussian probability distribution \(P(\epsilon_{\ell}) = (2\pi W^2)^{-1/2} \exp(-\epsilon_{\ell}^2/2W^2)\) with \(W\) and \(\Delta = 2\sqrt{2}naW\) the standard deviation (SD) and the full width at half maximum, respectively [32]. In this work we analyze this model over a range of interactions \(U/t\in [1, 2.5]\) and disorder strengths \(W/t\in [1, 15]\). We furthermore investigate the effect of an external trapping potential in order to compare with the recent experiment [21] for \(U = 24.4t\) and \(W/t \in [0, 4, 7]\).

The FOE [23, 24] is a quasiparticle method based on a Gutzwiller expansion of \(\|\) in terms of eigenstates \(|i\rangle_{\ell}\) of the local mean-field Hamiltonians \(\hat{H}^{(i)}_{\text{MF}} = H_{\ell} - t \sum_{\ell',\ell}(\hat{b}_{\ell'}\hat{\phi}_{\ell} + \text{h.c.})\). Here we introduce the fluctuation operators \(\delta b_{\ell} = \hat{b}_{\ell} - \phi_{\ell}\) and the fields \(\phi_{\ell} = \langle 0|\hat{b}_{\ell}|0\rangle \) are determined self-consistently. Drawing from variational concepts [33, 34] the FOE allows for a systematic improvement over standard Bogoliubov theory [36] by considering in principle general local fluctuations, giving access to the complete QP spectrum of \(\hat{H} = \sum_{\ell} \hat{H}^{(i)}_{\text{MF}} - t \sum_{\ell,\ell'} \left(\delta b_{\ell'}\hat{\phi}_{\ell} - \delta\phi_{\ell'}\hat{\phi}_{\ell} + \text{h.c.}\right)\).

In the limit \(N \to \infty\), the FOE expansion \(\delta b_{\ell} = \sum_{i=0}^{N} \epsilon_{i}|\hat{b}_{\ell}|i\rangle_{\ell}\langle i| + \text{c.c.}\) constitutes an exact quadratic map onto a complete basis set of the local Gutzwiller raising (lowering) operators \(\sigma_{\ell}^{(i)}\) \(\equiv |i\rangle_{\ell}\langle 0|\) \((\sigma_{\ell}^{-1}\) \(\equiv |0\rangle_{\ell}\langle i|\)). These generate arbitrary local fluctuations \(\kappa_{\ell} = \sum_{i,j} \sigma_{\ell}^{(i)}\sigma_{\ell}^{(i)}\) of any self-consistent MF state \(|\psi_{\text{MF}}\rangle = \prod_{\ell} |\psi_{\ell}\rangle\). The quality of the approximation is ascertained for \(\kappa = L^{-2}\sum_{\ell} \kappa_{\ell} \leq 1\), which is always fulfilled below [37]. We consider terms of second order in the Gutzwiller operators, leading to an approximate representation of \(\hat{H} \approx \sum_{\gamma} \omega_{\gamma}\beta_{\gamma}^{\dagger}\beta_{\gamma} + \Delta E_{\text{QP}}\) in terms of non-interacting QP modes \(\gamma\) with corresponding energies \(\omega_{\gamma}\) [35]. \(\beta_{\gamma} \equiv \langle u(\gamma)|\sigma + v(\gamma)\sigma \rangle\) are the generalized Bogoliubov-type operators, with \(u(\gamma)\) and \(v(\gamma)\) the corresponding eigenvectors, and \(\sigma = \left(\sigma_{1}^{(1)}, \ldots, \sigma_{L_{x}}^{(1)}\right)^{T}\).

Analogous to standard Bogoliubov theory we require the normalization condition \(|u(\gamma)|^2 - |v(\gamma)|^2 = 1\) preserving the approximately bosonic commutation relations of the Gutzwiller operators. \(v(\gamma)\) and \(u(\gamma)\) can be interpreted as dual wave-functions analogous to particle and hole fluctuations. Normal ordering of the operators results in a scalar correction \(\Delta E_{\text{QP}}\), irrelevant to the present discussion [39].

To characterize the degree of localization we consider the following two observables, computed within FOE: (i) The gap ratio \(r_{\gamma} \equiv \langle \min[\Delta\omega_{\gamma+1} - \Delta\omega_{\gamma}] / \max[\Delta\omega_{\gamma+1} - \Delta\omega_{\gamma}]\rangle_{d}\), with \(\Delta\omega_{\gamma} = \omega_{\gamma+1} - \omega_{\gamma}\) the quasiparticle energy gaps and \(\langle \cdot \rangle_{d}\) the disorder average. The observable \(r_{\gamma}\) is known from random matrix theory [6, 10] to have the mean value \(r_{\gamma} \approx 0.5307\) and \(r_{p} = 2\ln 2 - 1 \approx 0.3863\) in the delocalized and localized phases, respectively, resulting from level statistics belonging to the Gaussian orthogonal and Poisson ensembles. The second observable is (ii) the fractal dimension \(D_{L}^{(\gamma)}\) of the QP fluctuation wave-functions \(v(\gamma)\). Analogous to the definition for many-body eigenstates [11, 43] we define

\[
D_{L}^{(\gamma)} = \log_{L} \left[ \frac{\sum_{\ell} |v_{\ell}^{(\gamma)}|^2}{\max_{\ell} |v_{\ell}^{(\gamma)}|^2} \right],
\]

with \(|v_{\ell}^{(\gamma)}|^2 = \sum_{i>j} |v_{i\ell}^{(\gamma)}|^2\) the local amplitudes of the wave-function. We note that the fluctuation wave-function preserves real-space information in its amplitudes, so \(D_{L}^{(\gamma)} \in [0, 2]\) characterizes the spatial extension of each QP mode in relation to the system size [see examples in Fig. 3(a)].

Delocalized states with \(r_{\gamma} \approx r_{C}\) appear primarily at low QP energies \(\omega_{\gamma}/t\) and for sufficiently weak disorder \(W/t\), as shown in the contour plots Figs. 2(c, e) for weak \((U = 3t)\) and strong \((U = 20t)\) interactions, respectively. For \(U/t > 20\) and small \(W/t \lesssim 1\), we find a band of additional delocalized states for energies \(\omega_{\gamma} < U\), reflecting the presence of typical Hubbard subbands. In all cases, increasing \(W/t\) drives a transition to localized states with \(r_{\gamma} > r_{C}\), implying the existence of (multiple) MEs. We find similar behavior for the fractal dimension \(D = D_{L}^{(\gamma)}\), as shown in Figs. 4(b, d) for the same cases. There, black dots marking the ME are determined either from data crossing the critical values \(D_{c}\) or \(r_{C}\) [see Fig. 2(a)] [44], or by finite size scaling as discussed next.

We determine the position of the (lowest energy) ME via finite size scaling for the case \(U = 20t\), with linear sizes \(L \in \{10, 20, 24, 32, 40\}\) and corresponding numbers of realizations \(N_{r} \in \{480, 240, 240, 95, 48\}\). In qualitative agreement to recent RG arguments [23, 27] we find the data to be consistent with the scaling relations \(r_{L,W}(\omega) = \tilde{r}(|\omega - \omega_{c}(W)|L)\) and \(D_{L,W}(\omega) = L^{-n/2}\hat{D}_{W}\left(|\omega - \omega_{c}(W)|L\right)\). Here \(\hat{L} = \ln(L/L_{\alpha})\) with \(\alpha \in \{r, L\}, \) valid for \(L \gg L_{\alpha}\). \(\eta_{s}\) and \(L_{\alpha}\) are universal exponents and characteristic lengths, respectively, to be determined self-consistently in combination with the critical energies \(\omega_{c}(W)\) corresponding to the ME. Furthermore, \(\tilde{r}(\cdot)\) and \(\hat{D}_{W}(\cdot)\) are non-universal scaling functions.

Figures 3 show the data collapse of \(D\) [panel (a)] and \(r\) [panel (b)] over a wide range of energies \(\omega_{\gamma}\), disorder strengths \(W/t\) [corresponding to the region within the black boxes in Figs. 2(d, e)] and all system sizes \(L\). As a result of the collapse we find \(\eta_{s}/2 = 0.100(4), s = 0.84(5), L_{D} = 0.89(16)\) and \(L_{r} = 4.0(2)\) [35]. While for individual disorder values we get a full collapse within the errorbars...
In Fig. 2 (a), bright grey area], deviations from a single line imply a weak dependency of $D_W$ on $W$, while the decay of $r$ away from $r_G$ is nearly exponential [see Fig. 2 (c), solid line]. From the collapsed data we extract the critical values of the observables $\tilde{D}_W(0) = 1.26(2)$ and $r_c = \tilde{r}(0) = 0.528(3)$.

Next, we determine two independent estimates of $\omega_c(W)$ for other $U/t$ at fixed $L = 32$ by taking the crossing points of $D_c = L^{-\gamma/2} \sum W D_W(0)/13 = 0.89(2)$ with $D$-data [Fig. 2(b), black dots] and of $r_c$ with exponential fits [compare Fig. 3(b)] to $r$-data [Fig. 2(c), black dots]. Figs. 2 show the $D_c$ contours of binned $D$-data [4 values per bin, panels (b, d)] and binned $r$-data [6 values per bin, panels (c, e)] in the vicinity of $r_c$ for $U/t \in \{3, 20\}$ respectively. Excitingly, this procedure leads to consistent values for $\omega_c(W)$ for all considered values of $W$ and $U$. Interestingly, we find that for all data sets and $W$ large enough, the dependence of $\omega_c(W)$ on $W$ is approximately consistent with

$$\omega_c(W) = \omega_0 \exp(-W/\Omega).$$

Individual exponential fits are shown as continuous black lines in Figs. 2(b-e) and the obtained parameters are summarized in the inset of Fig. 1(b), showing amplitudes $\omega_0$ (left-pointing triangles) and decay constants $\Omega$ (right-pointing triangles) as a function of $U/t$. At a critical $W_c$ the exponential decay of the ME is always truncated by a reentrant behavior [see e.g. Fig. 2(d)], which for vanishing $\omega_c$ extrapolates to the Bose glass ground state [28–31]. This implies the existence of a transition point from a thermal to fully QP localized MBL phase at $W_c(U)$, which is a central result of this work shown in Fig. 1(b). Our results suggest that the thermal phase reaches its maximum extension $W_c(U)$ at $U/t \approx 15$.

We end our discussion with the analysis of the added effect of a harmonic trap as realized in [21], only approximating the skewed Gaussian disorder used therein by an exact Gaussian. All other parameters of [1] are taken directly from the reference, so $U = 24.4t$, the total particle number is 133 and we set $L = 32$ with $N_r = 95$. In Fig. 4(a) we show the gap ratio of the QP spectrum related to a mean-field ground state with a Mott-core
surrounded by a condensate ring, contrary to the experiment which used a purely Mott-type initial state. The considered QP states localize at roughly the same energy scale as in the experiment, which we quantify by an exponential fit of $r$ for the least localized states at $\omega_c/t \approx 0.1$ [see Fig. 4(b)] resulting in $\Delta^{(r)}/t = 7.8(1.5)$ [46].

To get further insight we consider the scaling of connected single particle correlations as given by $G_c(\ell, \ell') \equiv \langle \hat{b}_\ell \hat{b}_{\ell'} \rangle_{\text{QP}} - \phi_\ell \phi_{\ell'}$. Here $\langle \cdot \rangle_{\text{QP}}$ is the QP ground state expectation value implicitly defined via $\beta_\gamma |\psi_{\text{QP}}\rangle = 0$ for all $\gamma$ [23, 24], thus best fulfilling the original approximation of neglected QP interactions. We then consider the radial correlations of the four central sites averaged for each unique distance from the trap center [see Fig. 4(c)]. Due to the vicinity to a localization transition and the inhomogeneous nature of the system we expect an interplay of algebraic and exponential correlations which we summarize in the fit function

$$G_c(d) = a_1 \exp(-\lambda d) + a_2 d^{-b}. \quad (4)$$

In Fig. 4(d) we show the various obtained inverse localization lengths $\lambda$ of these fits together with one SD (68% confidence) of the fitting error. Below a certain disorder strength we find no exponential contribution. A linear fit for all nonzero $\lambda$ yields the theoretical critical disorder strength $\Delta_c^{(\lambda)}/t = 5.82(95)$ well matching the experimental value of $\Delta_c/t = 5.3(2)$, which, to our knowledge, is the first theoretical prediction. The different slope compared to experiment likely stems from the slightly different nature of the considered observables. We note that the localization happens at a much smaller disorder strength than predicted for the unconfined system. This is most likely due the trap enhanced variance of the local potential.

We have performed a detailed analysis of the two dimensional BHM with Gaussian disorder at half filling by discussing gap ratios and fractal dimensions of generalized (beyond Bogoliubov) QP eigenstates. For any considered interaction strength we find a MBL transition at sufficiently strong disorder, signified by a truncation of the low energy ME. Finite size scaling in the vicinity of these critical lines is consistent with a BKT scenario, while the MEs are directly related to the band structure in the clean system. Furthermore, our method predicts a scaling of correlations almost identical to that observed in experiment, predicting the transition point without requiring any empirical fit parameter.

As we show in this work, the FOE is a very promising tool for the analysis of extended systems with strong correlations, which could also be used to clarify the interplay between MBL and the Bose glass. As the FOE can easily be extended to the time domain, it furthermore opens up an exciting direction of future research into disorder-driven dynamical effects.

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