Many-body localization from a one-particle perspective in the disordered 1D Bose-Hubbard model

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We numerically investigate 1D Bose-Hubbard chains with onsite disorder by means of exact diagonalization. Consistent with previous studies, we observe signatures of a transition from the ergodic to the many-body localized (MBL) regime when increasing the disorder strength or energy density, implying the existence of an inverted many-body mobility edge. Apart from the entanglement entropy as a conventional but indirect measure for the ergodic-MBL transition, we primarily utilise the one-particle density matrix (OPDM) to characterize the system. We show that the natural orbitals (the eigenstates of the OPDM) are extended in the ergodic phase and real-space localized when one enters into the MBL phase. Furthermore, the distributions of occupancies of the natural orbitals can be used as measures of Fock-space localization in the respective basis. We further demonstrate that the Fock-space localization, albeit weaker, is also evidently present in the distribution of the physical densities in the MBL regime, both for soft- and hard-core bosons. Moreover, the full distribution of the densities of the physical particles provides a one-particle measure for the detection of the ergodic-MBL transition which could be directly accessed in experiments with ultra-cold gases.

I. INTRODUCTION

Closed quantum systems with an interplay of interactions and disorder represent a paradigmatic case of systems where thermalization is believed to fail [1–5]. The original concept of disorder-driven Anderson localization [6] and its generalization to systems of interacting electrons developed into the more generic framework of many-body localization (MBL) [7, 8] for closed quantum systems. The delocalization to many-body localization (or ergodic-MBL) transition is an unconventional phase transition at finite energy density, i.e., not related to symmetry and not seen in thermodynamics, and it can be interpreted as an eigenstate transition [2]. The MBL phase is a phase of matter with emergent local integrals of motion [9–12] where eigenstates exhibit area-law entanglement [13–15] and where slow logarithmic entanglement entropy growth can be observed in global quenches [9, 16, 17]. For an overview of this rapidly evolving field, we refer to recent reviews [1–5].

Insights from numerical investigations of MBL in spin-1/2 XXZ chains (or the equivalent model of spinless fermions) [4, 16–26] by means of exact diagonalization or by means of tensor-network methods greatly contributed to the current understanding of the MBL phase. Most of the numerical simulations investigated either the properties of the eigenspectrum and the eigenstates and the violation of the eigenstate thermalization hypothesis (ETH), e.g., the level statistics, the number variance, the entanglement entropy, and Fock-space localization, or the dynamics of initial states after a global quench, such as the entanglement growth or the imbalance decay of spatially inhomogeneous initial states. Recently, a controversial discussion emerged on whether the existence of MBL can be inferred from finite-size data from some of measures of the energy-level distributions [25–27].

Experimental progress was made with both ultracold atoms and trapped ions where various lattice models with disorder can be emulated. The observation of signatures of the MBL phase was achieved in the quasiperiodic Aubry-André Fermi-Hubbard model [28, 29], the disordered Ising model [30], the disordered Bose-Hubbard model (BHM) [31] and the quasiperiodic Aubry-André Bose-Hubbard model [32, 33]. The experiments measure the dynamics of the imbalance decay [28, 29, 31] or the dynamics of the entanglement entropy [32].

However, so far, only a few numerical studies considered the experimentally relevant disordered BHM [34–38] or the BHM with random interactions [39]. One reason, perhaps, for the lack of numerical studies are the numerical costs: full exact diagonalization is feasible only for small system sizes and the studies are thus limited to 1D [34, 35, 37]. For larger 1D or 2D systems, using approximative methods is unavoidable [36, 38]. Nevertheless, these numerical studies suggest that the ergodic-MBL transition in the disordered BHM most likely exists. The signatures of the transition were measured, for example, by the imbalance decay [34], the entanglement-entropy growth [37], the level statistics of many-body eigenspectra [34, 35, 37], the gap ratio and the fractal dimension statistics of the full low-energy quasiparticle spectra [38] or by the entanglement entropy [36, 37]. Furthermore, the existence of one [34, 36] or more many-body mobility edges [38] was proposed. However, the understanding of the ergodic-MBL transition in disordered BHM is still far from complete.

Motivated by all these considerations, we here follow an approach based on the one-particle density matrix (OPDM) to study the structure of real-space and Fock-space localization in the disordered BHM. By diagonalising the OPDM, we obtain the natural orbitals and their occupations which can be used to characterize the real-space localization and Fock-space localization, respectively [21]. The method was shown to detect the ergodic-MBL crossover in the model of spinless fermions from the emergence of a steplike discontinuity in the disorder-averaged occupations of the natural or-
Here, we extend these ideas to the bosonic case. We first consider the spin-1/2 Heisenberg model, which is equivalent to a model of hard-core bosons, and which is, at the same time, the standard model of MBL. We demonstrate that by diagonalization of the spin-correlation matrix we obtain the natural orbitals and their eigenvalues, which can be further used to characterize the real-space localization and Fock-space localization, respectively. The development of a steplike discontinuity in the disordered-averaged spin-projections and the disordered-averaged occupations of the natural orbital is observed, analogously to the fermionic case [21]. Furthermore, we define a Fock-space localization measure from the full distributions of the physical spin-projections and the occupations of natural orbitals. The system-size dependence of this measure is different in the ergodic and the MBL phase and the change in the finite-size dependence occurs close to transition point estimated from other measures [20].

In the second part, we focus our investigation on the disordered BHM. We focus on experimentally relevant parameters regimes. We first consider the entanglement entropy to show that the disordered BHM indeed exhibits the ergodic-MBL crossover. Then, following the mapping of spin-1/2 degrees of freedom to hard-core bosons which transforms the spin-correlation matrix to the OPDM for bosons, we diagonalise the bosonic OPDM to obtain the natural orbitals and their occupations to characterize the real-space localization and Fock-space localization. First, we observe that the natural orbitals are extended in the ergodic phase and real-space localized when one enters into the MBL phase. We show that the disorder-averaging of the occupations of the natural orbitals clouds the information about Fock-space localization. Instead, with our measure defined from the full distributions of the natural-orbital occupations, we are able to extract information about the Fock-space localization. Interestingly, the Fock-space localization is also evident in the distributions of physical densities, which we analyse in the same way as the distributions of the natural-orbital occupations. Finally, analogously to spins, the system-size dependence of our Fock-space localization measure is different in the ergodic and in the MBL phase.

The plan of the paper is the following. We start with the introduction of the one-particle measures both for the spin-1/2 case and for bosons in Sec. II. We apply the one-particle characterization to the 1D spin-1/2 Heisenberg model in the random magnetic field in Sec. III. Then, we apply the one-particle characterization to the disordered BHM in Sec. IV. We conclude our study in Sec. V.

II. MODEL AND METHODS

We investigate the 1D spin-1/2 Heisenberg model with

\[ H = \sum_{i=1}^{L} \left[ -\frac{J}{2} (\hat{S}_{i}^{+} \hat{S}_{i+1}^{-} + \text{H.c.}) + J \hat{S}_{i}^{z} \hat{S}_{i+1}^{z} + h_{i} \hat{S}_{i}^{z} \right]. \]

Here, \( \hat{S}_{i}^{+} (\hat{S}_{i}^{-}) \) is a raising (lowering) spin-1/2 operator at site \( i \), \( \hat{S}_{i}^{z} \) measures the z-component of the spin and \( h_{i} \) represents a random local magnetic field drawn from a box distribution \( h_{i} \in [-W,W] \). From now on, all energies are expressed in units of the nearest-neighbour spin-exchange constant \( J \).

We further investigate the 1D Bose-Hubbard model with

\[ H = \sum_{i=1}^{L} \left[ -\frac{J}{2} (\hat{a}_{i}^{\dagger} \hat{a}_{i+1} + \text{H.c.}) + U \hat{\mathcal{N}}_{i} (\hat{n}_{i} - 1) + \epsilon_{i} \hat{n}_{i} \right], \]

where \( \hat{a}_{i}^{\dagger} (\hat{a}_{i}) \) is a creation (annihilation) operator for a boson at site \( i \), \( \hat{\mathcal{N}}_{i} = \hat{a}_{i}^{\dagger} \hat{a}_{i} \) is the density operator at site \( i \), \( U \) accounts for on-site bosonic repulsion and \( \epsilon_{i} \) represents an on-site (diagonal) disorder drawn from a box distribution \( \epsilon_{i} \in [-W,W] \). Similarly to spins, from now on, all energies are expressed in units of the nearest-neighbour hopping constant \( J \).

The models introduced above are investigated on systems of finite sizes up to \( L = 18 \) (and \( 10^{3} \) disorder realizations) for the Heisenberg model and up to \( L = 12 \) (and \( 10^{3} \) disorder realizations) for the Bose-Hubbard model where periodic boundary conditions are imposed. For the spins, the overall magnetization is kept to be zero \( \sum_{i=1}^{L} \langle \hat{S}_{i}^{z} \rangle = 0 \) and for the bosons, we set the filling to \( \frac{N_{f}}{L} = \frac{1}{2} \sum_{i} \langle \hat{n}_{i} \rangle / L = 0.5 \). We define the target energy density via \( \epsilon = \frac{2(E-E_{\text{min}})}{E_{\text{max}}-E_{\text{min}}} \), where \( E \) is the many-body energy of a particular eigenstate and \( E_{\text{max}} \) and \( E_{\text{min}} \) are the maximum and minimum energy for each disorder realization, respectively. The energy density \( \epsilon = 1 \) corresponds to the middle of the many-body spectrum. The eigenenergies and the corresponding eigenstates closest to the target energy density can be found either by full exact diagonalization or by the shift-invert method [47]. We take the six eigenstates closest to \( \epsilon \) for each disorder realization.

For a Heisenberg spin chain in a given many-body state, \( |\psi_{n}\rangle \), we measure the expectation value of the the z-component of the spin at site \( i \) is defined as \( s_{i} = \langle \psi_{n} | \hat{S}_{i}^{z} | \psi_{n} \rangle \). The expectation values \( s_{i} \) will be used as a measure of the real-space and the Fock-space localization. Additionally, we construct the spin-correlation matrix

\[ \hat{S}_{ij}^{\pm} = \langle \psi_{n} | \hat{S}_{i}^{\pm} \hat{S}_{j}^{\mp} | \psi_{n} \rangle. \]

Please note that the spin-correlation matrix does not transform exactly to the OPDM for spinless fermions under the Jordan-Wigner transformation. Compared to the
fermionic OPDM, it acquires additional phases from the string operators. However, the spin-correlation matrix still provides similar information about the MBL as the OPDM in the case of fermions. Below we show that the spin-correlation matrix is actually connected to the bosonic OPDM which ultimately justifies its use. The spin-correlation matrix and the $z$-components are connected via $S^z_i = s_i - \frac{1}{2}$. The spin-correlation matrix is then brought to its diagonal form

$$S^\pm |\phi_\alpha\rangle = s_\alpha |\phi_\alpha\rangle,$$  \hspace{1cm} (4)

where $|\phi_\alpha\rangle$ are the natural orbitals with $s_\alpha$ being the respective OPDM eigenvalues, i.e., the occupations. The eigenvalues $s_\alpha$ will be used as a measure for the Fock-space localization whereas the natural orbitals $|\phi_\alpha\rangle$ will be used as a measure for real-space localization.

For a Bose-Hubbard chain in a given many-body state $|\psi_n\rangle$, we measure the set of real-space site occupations $\{n_i\}$ where the occupation of site $i$ is defined as $n_i = \langle \psi_n | \hat{n}_i | \psi_n \rangle$. The expectation values $n_i$ will be used as a measure of the real-space and the Fock-space localization. Additionally, we construct the one-particle density matrix (OPDM) $\rho_{ij}$ defined as

$$\rho_{ij} = \langle \psi_n | \hat{a}_i^\dagger \hat{a}_j | \psi_n \rangle.$$  \hspace{1cm} (5)

Note that the OPDM and the site occupancies are connected via $\rho_{ii} = n_i$. The natural orbitals $|\phi_\alpha\rangle$ and their occupations $s_\alpha$ are obtained by diagonalization of the OPDM

$$\rho |\phi_\alpha\rangle = s_\alpha |\phi_\alpha\rangle.$$  \hspace{1cm} (6)

The eigenvalues $s_\alpha$ will be used as a measure for the Fock-space localization whereas the natural orbitals $|\phi_\alpha\rangle$ will be used as a measure for real-space localization.

Note the connection between the spins and the bosons, i.e., the spins can be represented as hard-core bosons: $\hat{S}_i^+ = \hat{a}_i^\dagger$, $\hat{S}_i^- = \hat{a}_i$ and $\hat{S}_i^z = \hat{n}_i - 1/2$ [48]. The hard-core bosons fulfill the commutation relations

$$[\hat{a}_i^\dagger, \hat{a}_j] = [\hat{a}_i^\dagger, \hat{a}_j^\dagger] = [\hat{a}_i, \hat{a}_j] = 0 \hspace{0.5cm} (i \neq j),$$  \hspace{1cm} (7)

for different sites and the anti-commutation relations

$$\{\hat{a}_i^\dagger, \hat{a}_i\} = 1 \hspace{0.5cm} \{\hat{a}_i^\dagger, \hat{a}_j\} = \{\hat{a}_i, \hat{a}_j\} = 0$$  \hspace{1cm} (8)

for the same site [49]. Then, the spin-correlation matrix $S^{\tilde{\alpha}}_\alpha$ corresponds to the OPDM $\rho_{\alpha\beta}$ in the bosonic picture, i.e., $S^{\tilde{\alpha}}_\alpha = \rho_{\alpha\beta}$ and $S^{\tilde{\alpha}}_\alpha = n_i - 1/2$. This also justifies the use of the spin-correlation matrix.

Besides the one-particle measure we also compute the bipartite entanglement entropy. We split the system into subsystems A and B, both of size $L/2$, and we expand the eigenstate $|\psi_n\rangle$ as $|\psi_n\rangle = \sum_i a_i |\phi_i\rangle_A |\chi_i\rangle_B$ where the $a_i$ are positive Schmidt coefficients of the expansion and $\{|\phi_i\rangle_A \}$ and $\{|\chi_i\rangle_B \}$ are orthonormal basis sets in A and B. The von-Neumann entropy between the two partitions is then defined as the Shannon entropy of square of the Schmidt coefficients

$$S_{VN} = -\sum_i a_i^2 \ln a_i^2.$$  \hspace{1cm} (9)

III. MBL IN 1D HEISENBERG MODEL

A. Disorder-averaged spin projections and OPDM eigenvalues

We start our discussion with the 1D Heisenberg model. In Fig. 1, we show the values of the all spin projections $s_i$ and $s_\alpha$ which are first re-ordered from the largest value to the smallest one for each eigenstate. The disorder-averaging is indicated by the bars. We can clearly observe the development of gaps between the values of $\overline{s_i}$ and $\overline{s_\alpha}$ for $i, \alpha = L/2$ and $i, \alpha = L/2 + 1$ as the disorder strength $W/J$ increases. These gaps are defined as $\Delta_i = \overline{s_i}_{L/2} - \overline{s_i}_{L/2+1}$ and $\Delta_\alpha = \overline{s_\alpha}_{L/2} - \overline{s_\alpha}_{L/2+1}$. Such gaps (or occupation discontinuities) were previously reported for spinless fermions [21, 40] and for $S = 1/2$ spins (or the hardcore bosons) [50]. The gaps reflect the fact that the sites and natural orbitals are either nearly occupied or nearly empty, i.e., the particles are more real-space localized and the eigenstates are more Fock-space...
localized. This may be considered as a consequence of emergent local integrals of motion [40, 50] in the MBL phase. It was also shown that the natural-orbital occupations give a better approximation to the quasiparticle occupations (i.e., the occupations of the local integral of motions) than the site-occupations or the occupations of Anderson orbitals [40]. In this respect, the creation operators of natural orbitals are the closest one to the creation operators of quasiparticles (local integrals of motions) globally [40].

In Fig. 2, we further show the values of the gaps as a function of disorder strength $W/J$ and the energy density $\epsilon$. The dependence of the gaps reflects the transition from the ergodic phase to the MBL phase. This was previously shown for $\Delta_\alpha$ in the model of spinless fermions [21, 42]. The crossover in the Heisenberg model and in the equivalent model of spinless fermions has been extensively studied and characterized by traditional measures such as the level statistics [18, 20], the entanglement entropy and its fluctuations and the participation entropy [20]. Based on such systematic studies, one can establish the phase diagram of the ergodic-MBL crossover (in finite-size systems). For the isotropic Heisenberg spin model, a careful numerical analysis by the exact-diagonalization method for chains of sizes $L = 14 - 22$ yields an estimate of the critical disorder strength of $W_c/J \approx 3 - 4$ [20]. However, numerical linked-cluster expansion simulations [51] or a study of the imbalance decay in the Heisenberg chains of $L = 100$ spins [24] find substantially larger values for the transition point of $W_c/J \approx 4.5 - 6$.

Looking at Fig. 2, the crossover can also be detected from the values of the gaps, sitting roughly in the range $W/J \approx 3 - 4$, in agreement with exact-diagonalization results [20]. The crossover is more visible for $\Delta_\alpha$ as the natural-orbital occupations are the optimal measure of the Fock-space localization [40]. Nevertheless, $\Delta_i$ can still be used to detect the MBL crossover as it is visible in Fig. 2. Moreover, $\Delta_i$ is the experimentally more accessible observable as it requires to measure only the diagonal part of the correlation matrix $S_{ii}^{\pm} = s_i - \frac{1}{2}$. This motivates our study of distributions of densities for the disordered BHM.

B. Full distributions of spin projections and OPDM eigenvalues

To better illustrate the behaviour of the one-particle observables, it is instructive to plot the full distributions of $s_i$ and $s_\alpha$ deep in the ergodic regime (see Fig. 3) and deep in the localized regime (see Fig. 4). At the same time, we also show the distributions of the von-Neumann entanglement entropy $S_{VN}$.

![FIG. 3. Spin-1/2 Heisenberg chain for $W/J = 1, \epsilon = 1$ in the ergodic phase: Full distributions of (a) von-Neumann entanglement entropy, (b) IPR, (c) spin projections and (d) OPDM occupations for $L = 10, 12, 14, 16$.](image-url)
The distribution of the spin projections $s_i$ develops a binary peak structure around the minimal $s_i = -0.5$ and maximal $s_i = 0.5$ possible values with increasing disorder strength $W/J$ [22, 52, 54]. For low disorder the distribution is size dependent, see Fig. 3(c), while for the larger disorder strength, the distribution is practically $L$-independent, see Fig. 4(c). The distribution of the occupations $s_α$ show a similar $L$-dependence, see Fig. 3(d) and Fig. 4(d). It develops two peaks when the disorder strength is increased and the peaks are located around the integer values $s_α = \{0, 1\}$ reflecting the Fock-space localization [21]. We also see that the OPDM occupations can exceed one. This is due to the bosonic character of the spin system, i.e., the spins can be mapped to hard-core bosons and the hard-core bosons do not obey the strict hard-core constraint in the basis of the natural orbitals. Such behaviour was reported before [50].

C. Measure for the Fock-space localization

We have seen that the distributions develop peak structures around the values $s_i = \{-0.5, 0.5\}$ or the integers $s_α = \{0, 1\}$, respectively, which reflects the Fock-space localization, i.e., the proximity to Slater determinants. In order to quantify this fact we will device a measure applied to each element of the distributions. For the OPDM eigenvalues $s_α$, this is defined as

$$\delta s_α = |s_α - \lfloor s_α \rfloor|,$$

where $\lfloor s_α \rfloor$ is the closest integer to $s_α$. For the spin projections of physical particles, we alter the definition to

$$\delta s_i = \left| s_i - \frac{1}{2} - \left( s_i - \frac{1}{2} \right) \right|,$$

where $\lfloor s_i - 1/2 \rfloor$ is the closest integer to $s_i - 1/2$. We refer to these measures as distances to the closest integers (or more generally, distances to the eigenvalues of the corresponding density operators).

In Fig. 5, we illustrate the $L$-dependence of the gaps $\Delta_i$ and $\Delta_α$, as well as of the disorder-averaged distances $\delta s_i$ and $\delta s_α$ to the closest integers, all plotted as functions of the disorder strength $W/J$ for the energy density $\epsilon = 1$. We observe that both gaps $\Delta_i$ and $\Delta_α$ are increasing functions of the disorder strength and that the gap $\Delta_α$ increases faster than the gap $\Delta_i$ which reflects the fact that the basis of natural orbitals is the optimal measure for Fock-space localization. When plotted as a function of $1/L$ (not shown here), both gaps extrapolate to a finite value for $W \gtrsim 4J$, with $\Delta_α$ extrapolating to larger values than $\Delta_i$. The disorder-averaged distances $\delta s_i$ and $\delta s_α$ exhibit almost no $L$-dependence for $W/J > 4$ while for the lower disorder strengths, there is a clear $L$-dependence. At weak disorder, both $\delta s_i$ and $\delta s_α$ approach 0.5 as $L$ increases, as expected for this energy density and average density. Remarkably, the point separating these two different $L$-dependences is very close to the estimate of the ergodic-MBL transition estimated from other measures [20]. These results suggest that $\delta s_i$ and $\delta s_α$ are useful measures for the Fock-space localization (and better suited than $\Delta_i$ and $\Delta_α$) and motivate us to use the analogous measures to study the Fock-space localization in the disordered BHM.
IV. MBL IN THE 1D BOSE-HUBBARD MODEL

We now turn our discussion to the disordered BHM. Since we consider systems of finite size \( L \) with particle numbers \( N = L/2 \) and without any hard-core constraint, the local Fock space grows linearly \( n_{\text{loc}} = \{0, 1, 2, 3, \ldots, N = L/2\} \) with system size \( L \). We construct the Hamiltonian in the full many-body basis of size \( M \), i.e., without any truncations of the local site occupations in the basis states [55, 56]. In Fig. 6, we show a sketch of the typical eigenspectrum for a system in the low-interaction \((U/J = 1)\) regime, see Fig. 6(a), and in the high-interaction \((U/J = 25)\) regime, Fig. 6(b). The large-interaction regime is more relevant for the actual experiments [31].

For the low-interaction regime \((U/J = 1)\), the spectrum appears to be continuous. More interestingly, in the high-interaction limit \((U/J = 25)\) and for low disorder, the spectrum is divided into well separated sub-bands. The sub-bands are determined by the interaction energies of their eigenstates. Typically, the \( L \) highest eigenstates, see Fig. 6(b), correspond to configurations with \( N \) bosons occupying mostly one site. By going lower in energy in the many-body spectrum, the bosons are allowed to be delocalized. On the other hand, the configurations in the two lowest bands, i.e., the bands of yellow and turquoise colour in Fig. 6(b), can accommodate mostly 1 or 2 bosons per site, respectively.

For a system of finite size, the many-body spectrum has a maximum which is a function of the total boson number \( N \) and consequently, the BHM with a fixed filling has an unbounded energy per site in the thermodynamical limit. In the highest-energy states, all the bosons are located mostly at the same site and energies of such states are approximately given by \( E_{\text{max}} \approx U N(N-1)/2 \).

Then, considering the filling with \( N = L/2 \), the maximum energy can be written as \( E_{\text{max}} \approx U L (2L - 1)/8 \) and thus the maximum energy per site of such states is \( E_{\text{max}}/L \approx U (2L - 1)/8 \) is a linear function of the system size \( L \). This is different from the case of hard-core bosons where the maximum energy per site is bounded from above. One has to keep this in mind when considering the definition \( \epsilon = \frac{2(E - E_{\text{min}})}{E_{\text{max}} - E_{\text{min}}} \) from Sec. II where now \( \epsilon \) cannot be interpreted as the energy density.

To obtain a quantity which can be interpreted as an energy density we consider only the part of the spectrum where the local occupancy reaches at most some value. For example, if we consider only the states with local occupancy mostly up to 2 bosons per site the corresponding energy density \( \epsilon_2 \) is defined as \( \epsilon_2 = \frac{2(E - E_{\text{min}})}{E_{\text{max}} - E_{\text{min}}} \) where \( E_{\text{max}} \) is the maximal energy of the selected part of the spectrum, see Fig. 6(b) for an illustration. In practice, we first compute the size of the truncated basis \( M_{\text{red}} \) by selecting all basis state which have the local occupancy truncated to 2. We then construct and diagonalize the Hamiltonian in the full basis of size \( M \) and finally, we compute the energy density \( \epsilon_2 \) with respect to the lowest eigenenergies.

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**FIG. 6.** Sketch of the many-body eigenspectra of the disordered Bose-Hubbard model in the \( \epsilon - W \) plane for (a) \( U/J = 1 \) and (b) \( U/J = 25 \). The sketch corresponds to chains of size \( L = 8 \) where, for low disorder, the spectra develop five sub-bands in the high-interaction limit \( U/J = 25 \). The red dots indicate the parameter regimes for the results discussed in the main text in Sec. IV.

**FIG. 7.** Bose-Hubbard model: Full distributions of the entanglement entropy (a) in the ergodic phase and (b) in the MBL phase for \( L = 12 \). Parameters correspond to the circles in the sketch in Fig. 6 in the green \((U/J = 1 \text{ and } \epsilon = 1)\), turquoise \((U/J = 25, \text{ the } 2^{nd} \text{ sub-band})\) and yellow \((U/J = 25, \text{ the } 1^{st} \text{ sub-band})\) regions. For comparison, we also show results for 1D hard-core bosons without nearest-neighbour interactions, i.e., the spin-1/2 XX model, for \( L = 12, \epsilon = 1 \) (the orange colour).
The first quantity we look at is the bipartite entanglement entropy as a conventional measure of the ergodic-MBL transition. In Fig. 7, we show representative results for \( L = 12 \). For the low disorder \( W/J = 1 \), see Fig. 7(a), the entanglement-entropy distributions have a maximum at a finite value which is a typical shape of distribution in the ergodic system [52]. We also observe that in the strong-interaction regime at \( U/J = 25 \), the character of the entropy distributions for the states from the first and second lowest sub-bands is different, see the yellow and turquoise distributions in Fig. 7(a). The states of the first sub-band appear to be effectively as the states of the hard-core bosons (HCB) without nearest-neighbour interactions (equivalent to the spin-1/2 XX model) as there is no explicit interaction cost. Indeed, their entanglement-entropy distributions are similar, see the orange-coloured distribution in Fig. 7(a) for comparison. For the higher disorder, see Fig. 7(b), the distributions take the typical shapes in the MBL phase with the maximum close to zero and the resonant local maximum around \( S_{VN} = \ln(2) \) [22, 52].

In Fig. 8, we show the \( L \)-dependence of the entanglement entropy in the second lowest sub-band (for \( U/J = 25 \)). The second lowest sub-bands for \( L = 8, 10, 12 \) have similar energy density \( \epsilon_2 \), see Fig. 8(a). For low disorder \( W/J = 1 \), the distributions of the entanglement entropy exhibit a shift in their maxima towards higher values, see Fig. 8(b). This is the typical \( L \)-dependence in the ergodic regime [52]. On the other hand, at high disorder \( W/J = 10 \), the distribution is \( L \)-independent (not shown). In Fig. 8(c), we plot the dependence of the average fluctuation \( \langle S_{VN} \rangle \) of the entanglement entropy as a function of \( W/J \).

![Fig. 8. Bose-Hubbard model: (a) Typical sub-bands of the many-body eigenspectrum expressed in the energy density \( \epsilon_2 \) defined over the sector of eigenstates with maximally 2 bosons per site for system sizes of \( L = 8, 10, 12 \). The dotted lines denote the energy densities of the 2nd sub-bands used for the \( L \)-dependence analysis in (b) and (c). In (b), we plot the \( L \)-dependence of the full distributions of the von–Neumann entanglement entropy for the parameters corresponding to the dotted line in (a). In (c), we plot the \( L \)-dependence of the average fluctuation \( \langle S_{VN} \rangle \) of the entanglement entropy as a function of \( W/J \).](image1)

### A. Entanglement entropy

![Fig. 9. Bose-Hubbard model: Example of all natural orbitals of the OPDM computed from one representative eigenstate (a) in the ergodic \( (W/J = 1) \) and (b) in the MBL regime \( (W/J = 10) \) for the 1D disordered Bose-Hubbard model \( L = 12, \epsilon = 1, U/J = 1 \). The normalised potential landscape \( \frac{W}{|W|} \) is also displayed (the potential is shifted for clarity).](image2)

**FIG. 8.** **Bose-Hubbard model:** (a) Typical sub-bands of the many-body eigenspectrum expressed in the energy density \( \epsilon_2 \) defined over the sector of eigenstates with maximally 2 bosons per site for system sizes of \( L = 8, 10, 12 \). The dotted lines denote the energy densities of the 2nd sub-bands used for the \( L \)-dependence analysis in (b) and (c). In (b), we plot the \( L \)-dependence of the full distributions of the von–Neumann entanglement entropy for the parameters corresponding to the dotted line in (a). In (c), we plot the \( L \)-dependence of the average fluctuation \( \langle S_{VN} \rangle \) of the entanglement entropy as a function of \( W/J \).

**FIG. 9.** **Bose-Hubbard model:** Example of all natural orbitals of the OPDM computed from one representative eigenstate (a) in the ergodic \( (W/J = 1) \) and (b) in the MBL regime \( (W/J = 10) \) for the 1D disordered Bose-Hubbard model \( L = 12, \epsilon = 1, U/J = 1 \). The normalised potential landscape \( \frac{W}{|W|} \) is also displayed (the potential is shifted for clarity).

**B. Natural orbitals and IPR**

In the previous subsection, we have seen that the entanglement entropy gives signatures of the ergodic-MBL transition in the disordered BHM. In this subsection, we show that the ergodic-MBL transition is reflected also in properties of the natural orbitals. In Fig. 9(a), we plot all the natural orbitals for one typical eigenstate in the ergodic phase for a low disorder strength \( (W/J = 1) \), while in Fig. 9(b), we plot all the natural orbitals for one eigenstate in the MBL phase for a high disorder strength \( (W/J = 10) \). From the figures, a localization of the natural orbitals by disorder can be clearly observed, similarly to the localization of the natural orbitals for fermionic systems where it was originally discovered [21].

Similarly to the spin systems, we define the IPR for
bosons as

$$\text{IPR} = \frac{1}{N} \sum_{\alpha=1}^{L} n_{\alpha} \sum_{i=1}^{L} |\phi_{\alpha}(i)|^4$$

(13)

where \(N\) is the total number of bosons. The IPR measures the real-space localization of the natural orbitals \(\phi_{\alpha}(i)\). In Fig. 10, we show representative results of the full IPR distributions for the system size of \(L = 12\). For the low disorder \(W/J = 1\), see Fig. 10(a), the IPR distributions have a maxima for lower values of IPR with the high-IPR tails which means that the orbitals are mostly delocalized. On the other hand, in the high-disorder regime \(W/J = 10\), the maxima of IPR distributions shift towards the maximum value 1. The highest localization is observed for low interactions \(U/J = 1\). For the high interactions \(U/J = 25\), the IPR distributions for the states from the first and second lowest sub-bands are different, see the yellow and turquoise distributions in Fig. 10(b). The states of the first sub-band are more delocalized than the one of the second sub-band even though their entanglement entropy is lower, Fig. 7(b). This may be an artefact of the superfluid ground state of the clean BHM which is low-entangled but where the bosons are more real-space delocalized.

In Fig. 11, we show the \(L\)-dependence of the IPR in the second lowest sub-band (for \(U/J = 25\)) for the same parameters as in Fig. 8. For low disorder \(W/J = 1\) the distributions of the IPR exhibit a shift in their maxima towards lower values, see Fig. 10(a). For large disorder of \(W/J = 10\), the distribution is almost \(L\)-independent, see Fig. 10(b). This is consistent with the behaviour of the IPR distributions for fermionic systems [21].

**C. Occupations**

We have seen in the previous subsection that the natural orbitals contain information about real-space localization and that the OPDM accounts for the real-space (via the distribution of the IPR of \(|\phi_{\alpha}\rangle\)) and the Fock-space localization (via the distribution of \(n_{\alpha}\)). In this sub-section we further focus on how the occupations, both of the physical sites \(|i\rangle\) and of the natural orbitals \(|\phi_{\alpha}\rangle\) reveal the structure of Fock-space localization. Similarly to the spin model, we first consider the disorder-averaged occupations shown in Fig. 12. We observe that, opposite to the case of the hard-core bosons, the averaged occupations do not exhibit any discontinuity and they do not provide an obvious measure of the ergodic-MBL crossover.

The reason why the averaged occupation spectra are not obvious indicators of the Fock-space localization can be understood by looking at full distributions of \(n_i\) and \(n_{\alpha}\), see the distributions in Fig. 13 in the green colour. The first to be noted is that the distributions in
the low-disorder regime, Figs. 13(a) and (b), are smooth functions with maxima close to the average density of 0.5 and with exponentially decaying tails. The occupations are distributed from 0 up to 4, while values above 4 are very rare for the eigenstates from the mid-spectrum. Oppositely, in the high-disorder regime, see Figs. 13(c) and (d), the occupation distributions develop a peak structure with peaks of different heights around the integers \( n_i = \{1, 2, 3, 4\} \) and \( n_\alpha = \{1, 2, 3, 4\} \). The heights of the peaks decay exponentially similarly to the exponential decays of particle occupations in the ergodic regime (the slope depends on the energy density). The development of the peak structure in the distributions reflects the ergodic-MBL transition. Thus, analogously to the distributions of \( s_i \) and \( s_\alpha \) in the spin system discussed above, the distributions of \( n_i \) and \( n_\alpha \) indeed reveal the structure of the Fock-space localization. However, such information in the distributions will be washed out if one averages \( n_i \) (or \( n_\alpha \)) for fixed \( i \) (or \( \alpha \)) over the eigenstates and disorder. In the localized regime, \( n_i \) (or \( n_\alpha \)) for fixed \( i \) (or \( \alpha \)) are distributed mostly close to the integers, however, the integers do not need to be always the same, e.g., for \( \alpha = 1 \) the value of \( n_\alpha \) can be 2, 3 or 4 but the average \( n_\alpha \) is between 2 and 3. This is different from the case of spin systems where \( s_\alpha \) can only be close to 0 or 1.

We next focus on the distributions in the high-interactions regime \( U/J = 25 \) in the first and second lowest energy sub-bands. The distributions are displayed in Fig. 13 in the yellow and turquoise colours and we can observe the development of the peak structure in the high-disorder regime. The peaks are located around the integer values \( \{0, 1\} \) and \( \{0, 1, 2\} \), respectively. Higher occupations in the eigenstates are strongly suppressed which is in agreement with the interaction energy contribution to the energy of the eigenstates in this particular sub-band. For example, the real-space occupations of bosons \( n_i \) in the first sub-band are mostly restricted to the interval \([0, 1]\) such that there is no interaction-energy cost \( U n (n - 1)/2 \) and the bosons in the first sub-band can be effectively considered as hard-core bosons (without any nearest-neighbour interactions). This is indeed true as can be seen in Fig. 13 when comparing the distributions of occupations for the bosonic states in the first sub-band (the yellow colour) and the states of true hard-core bosons (the orange colour). Despite the similarity, the bosonic states in the first sub-band can occasionally have contributions from the basis state with a site occupancy higher than one which is not possible for true hard-core bosons. This freedom of the bosonic states can lead
In Fig. 15, we show the $L$-dependences of $\bar{\delta n}_i$ and $\bar{\delta n}_\alpha$ as functions of disorder strength $W/J$ for the second lowest sub-band and $U/J = 25$, i.e., the same parameters as in Fig. 8. We observe that the values of $\bar{\delta n}_i$ and $\bar{\delta n}_\alpha$ are $L$-dependent for the disorder strength $W/J < 4$ while they are essentially $L$-independent for $W/J > 4$, suggesting that there is a transition from the ergodic to the MBL phase. Remarkably, the position of the crossover region $W/J \approx 4$ corresponds to the region where the fluctuations of entanglement entropy become also $L$-independent, see Fig. 8. We conclude that the $L$-dependences of average distances to the closest integer $\bar{\delta n}_i$ and $\bar{\delta n}_\alpha$ are useful measures for the Fock-space localization in the MBL phase.

V. CONCLUSIONS

We have shown that the one-particle density matrix, natural orbitals and their occupations can be used to reveal the structure of the real-space and the Fock-space localization in systems of interacting disordered bosons. The real-space localization is observed in the structure of the natural orbitals, in the system-size dependence of the inverse participation ratio and in the distribution of densities. The Fock-space localization is uncovered via studying distributions of occupations. Particularly, the distributions of the densities $n_i$ and the occupations of natural orbitals $n_\alpha$ are smooth functions in the ergodic regime whereas they develop into a peak structure in the MBL regime where the peaks are at the possible integer values. Based on this observation, we devised a measure of localization, the average distance to the closest integer of the occupation distributions, and we showed that its system-size dependence is strikingly different in the two phases. These findings further illustrate the conceptual picture that the many-body localization transition involves localization both in Fock space and in real space. The distributions of $n_i$ should be accessible in quantum-gas microscope experiments [28, 29, 31–33]. A measurement of the $n_i$’s at a certain density and disorder realization requires repeating projective measurements in the same disorder realization.

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