

Many-Body Multifractality throughout Bosonic Superfluid and Mott Insulator Phases

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We demonstrate many-body multifractality of the Bose-Hubbard Hamiltonian's ground state in Fock space, for arbitrary values of the interparticle interaction. Generalized fractal dimensions unambiguously signal, even for small system sizes, the emergence of a Mott insulator that cannot, however, be naively identified with a localized phase in Fock space. We show that the scaling of the derivative of any generalized fractal dimension with respect to the interaction strength encodes the critical point of the superfluid to the Mott insulator transition, and provides an efficient way to accurately estimate its position. We further establish that the transition can be quantitatively characterized by one single wave function amplitude from the exponentially large Fock space.

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The properties of a quantum system are crucially determined by the statistical features of its Hamiltonian, as manifestly shown by the applicability of random matrix theory in a variety of scenarios. For instance, the system's dynamical behavior (e.g., the presence of localization, relaxation, or long-time equilibration [1,2]) depends decisively on the nature of the eigenenergies and eigenstates, which can exhibit high statistical complexity in the form of *multifractality* [3,4]. Multifractal wave functions appear in random matrix models [5–9], quantum maps [10–14], and most prominently at the disorder-induced metal-insulator transition [15–18], in the absence (see Refs. [19–21] for recent numerical studies) and in the presence of interactions [22–27]. The role of multifractality for this transition in involved geometries [28–32] as well as in the many-body localization context [33–37] is currently a subject of intense research. Interestingly, in the absence of any disorder, multifractality seems to be a generic property of the ground state of many-body spin Hamiltonians [38–42], in which different quantum phases can be identified by corrections to multifractal scaling [43,44].

In this work, we demonstrate that the statistical complexity of many-body states in “clean” (not disordered) bosonic systems can be described in terms of multifractality. Such characterization can not only provide an unambiguous identification of localized, extended, and ergodic wave functions, but also exposes how the presence of different macroscopic properties (phases) of the system is rooted in the Hilbert-space structure of quantum states. Here, we exemplify the potential of such analysis by showing that the multifractal properties of the Bose-Hubbard Hamiltonian (BHH) ground state in the Fock basis carry a distinctive signature of the transition from superfluid (SF) to Mott insulator (MI), as shown in Fig. 1. This novel approach reveals that the transition is fully encoded in the behavior of one single wave function amplitude in Fock space, and

it further provides an efficient way to locate the critical point.

Let us consider the expansion of a quantum state in an orthonormal basis of the underlying Hilbert space of size \mathcal{N} , $|\Psi\rangle = \sum_{j=1}^{\mathcal{N}} \psi_j |j\rangle$, and define the q moments of the distribution of intensities as $R_q = \sum_{j=1}^{\mathcal{N}} |\psi_j|^{2q}$, for $q \in \mathbb{R}^+$. The scaling of R_q with \mathcal{N} reveals the asymptotic statistics (for large \mathcal{N}) of the participation of the basis elements $|j\rangle$ in the state $|\Psi\rangle$. Such scaling is generically expected to be of the form $R_q \sim \mathcal{N}^{-(q-1)D_q}$, where $0 \leq D_q \leq 1$ are the *generalized fractal dimensions* (GFDs). An ergodic extended state in the considered basis, defined by $|\psi_j|^2 \sim \mathcal{N}^{-1}$ as $\mathcal{N} \rightarrow \infty$, has $D_q = 1$ for all q . On the other hand, if for any $q > 1$ saturation of R_q with \mathcal{N} is observed we speak

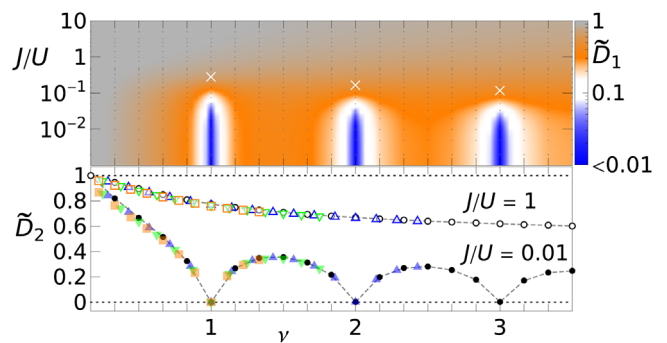


FIG. 1. Finite-size fractal dimensions of the BHH ground state versus J/U and filling factor ν (abscissa axis in both plots). Upper panel: Density plot of \tilde{D}_1 for $L = 6$ after linear interpolation of the numerically calculated points indicated by the black grid. White crosses indicate the position of the SF to MI transition [45,46]. Lower panel: \tilde{D}_2 for $J/U = 1$ (open symbols), $J/U = 10^{-2}$ (filled symbols) and $L = 6$ (black), 7 (blue), 8 (green), 9 (orange).

of localized states, for which, consequently, $D_{q>1} = 0$ [47]. If q -dependent values $0 < D_q < 1$ occur, the state is *multifractal* in the $|j\rangle$ basis [3,17,18]. The parameter q controls which wave function intensity (roughly, which value of $-\log_{\mathcal{N}}|\psi_j|^2$) dominates R_q for large \mathcal{N} . Thus, different dimensions D_q ensue if each set of points in the wave function with a certain intensity scales differently when enlarging the Hilbert space accessible to $|\Psi\rangle$, i.e., if the volume of each intensity set scales as a power law of \mathcal{N} with its own (in general noninteger) exponent. In such case, each intensity set is a fractal, and their superposition makes up the multifractal state.

In order to characterize multifractality, it is useful to define \mathcal{N} -dependent dimensions \tilde{D}_q ,

$$\tilde{D}_q \equiv \frac{1}{1-q} \log_{\mathcal{N}} R_q, \quad (1)$$

that for increasing \mathcal{N} converge to the GFDs, $D_q = \lim_{\mathcal{N} \rightarrow \infty} \tilde{D}_q$. Note that $\tilde{D}_q = S_q / \ln \mathcal{N}$, where S_q is the Shannon-Rényi entropy of degree q of the $|\psi_j|^2$ distribution. Among the GFDs, we single out the cases $q = 1, 2$, and ∞ . The exponent D_1 is known as the *information dimension* since it determines the scaling of the Shannon information entropy, $-\sum_j |\psi_j|^2 \ln |\psi_j|^2 \sim D_1 \ln \mathcal{N}$. The dimension D_2 controls the growth of the participation ratio, R_2^{-1} , which is regarded as a measure of the “volume” of the state: finite and \mathcal{N} independent for localized wave functions but unbounded for extended states. For a multifractal state $R_2^{-1} \sim \mathcal{N}^{D_2}$; i.e., its “volume” diverges with \mathcal{N} but it occupies a vanishing fraction of the total Hilbert space. Multifractal wave functions are therefore an example of nonergodic extended states. For $q = \infty$ the moments R_q are determined by the maximum value of the intensities, $p_{\max} \equiv \max_j |\psi_j|^2$, and $\tilde{D}_{\infty} = -\log_{\mathcal{N}} p_{\max}$. The GFDs as well as their finite-size counterparts are always monotonically decreasing functions of q [48]. Hence, the minimum GFD is D_{∞} (\tilde{D}_{∞} for fixed \mathcal{N}).

We apply this formalism to analyze the statistical properties of the ground state of the BHH in one dimension (1D) [49–51], which in terms of bosonic annihilation and creation operators, $b_k, b_k^{\dagger}, n_k \equiv b_k^{\dagger} b_k$, reads

$$H = -\eta \sum_k (b_k^{\dagger} b_{k+1} + b_{k+1}^{\dagger} b_k) + \frac{1}{2} \sum_k n_k (n_k - 1), \quad (2)$$

where $\eta \equiv J/U$ is the ratio of hopping to interaction strength ($U > 0$). Our system includes N bosons in L lattice sites with periodic boundary conditions (PBCs). In the thermodynamic limit ($N, L \rightarrow \infty$), at fixed integer filling factor $\nu \equiv N/L$, the ground state of H undergoes a Berezinskii-Kosterlitz-Thouless (BKT) phase transition as a function η , between a MI and a SF state [52–54]. In 1D,

the position of the critical point for $\nu = 1$ has been estimated to be $\eta_c \simeq 0.3$, both theoretically (see Refs. [51,55,56] and references therein) and experimentally [57].

A convenient basis of the Hilbert space of H , of size $\mathcal{N} = \binom{N+L-1}{N}$, is given by the Fock states of the on-site density operators, $|\mathbf{n}\rangle \equiv |n_1, n_2, \dots, n_L\rangle$, where $\|\mathbf{n}\|_1 = N$. Hence, the ground state of the system can be expanded as $|\Psi(\eta)\rangle = \sum_{\mathbf{n}} \psi_{\mathbf{n}}(\eta) |\mathbf{n}\rangle$. For integer ν and $\eta \rightarrow 0$, the ground state is given by one element of the Fock basis,

$$|\Psi(0)\rangle = |\nu, \nu, \dots, \nu\rangle \equiv |\nu\rangle. \quad (3)$$

Conversely, in the noninteracting limit ($\eta \rightarrow \infty$) the intensities of $|\Psi\rangle$ converge to

$$|\psi_{\mathbf{n}}(\infty)|^2 = \frac{N!}{L^N n_1! n_2! \dots n_L!}, \quad (4)$$

and the full Fock basis participates in the state. The extremely localized nature of the ground state for $\eta = 0$ leads to $\tilde{D}_{q>0} = D_{q>0} = 0$. For $\eta \rightarrow \infty$, the GFDs can also be analytically obtained, and have nontrivial q -dependent values, e.g., for $\nu = 1$, $D_1 = 0.941$, $D_2 = 0.907$, $D_{\infty} = (2 \ln 2)^{-1} = 0.721$; i.e., the ground state exhibits multifractality in the Fock basis [58,60].

How do the GFDs evolve with η between these two limits, and does this evolution expose the MI-SF transition? For such intermediate values of η , the multifractal analysis must be performed numerically: We combine exact diagonalization (for systems $L \leq 10$) with a recently proposed technique [43,61–63] based on quantum Monte Carlo (QMC) simulations to estimate the moments R_q for larger systems efficiently [64].

Remarkably, the analysis of the finite-size dimensions \tilde{D}_q for different η and varying filling factor reveals a distinct and unambiguous signal of the emergence of a MI state, as demonstrated in Fig. 1. Whereas for weak interaction the finite-size GFDs change monotonically with ν , they register a pronounced drop towards zero at integer densities in a range of η that clearly correlates with the MI phase. For integer density, all \tilde{D}_q vanish asymptotically as $\eta \rightarrow 0$. For noninteger filling, however, all \tilde{D}_q remain finite as $\eta \rightarrow 0$, signaling the persistence of a SF phase for any value of the interaction.

Let us further note that, for integer ν , according to Eqs. (3) and (4), the maximum intensity of $|\Psi(\eta)\rangle$ in the Fock basis occurs for the homogeneous state $|\nu\rangle$ in both limits $\eta = 0$ and $\eta = \infty$. The hopping and interaction terms of H minimize independently the energy by maximizing the amplitude on $|\nu\rangle$. This property persists for any value of η and L (when using PBCs) as illustrated in Fig. 2. This makes the dimension \tilde{D}_{∞} particularly accessible, since it will be entirely determined by the probability $|\langle \nu | \Psi(\eta) \rangle|^2$,

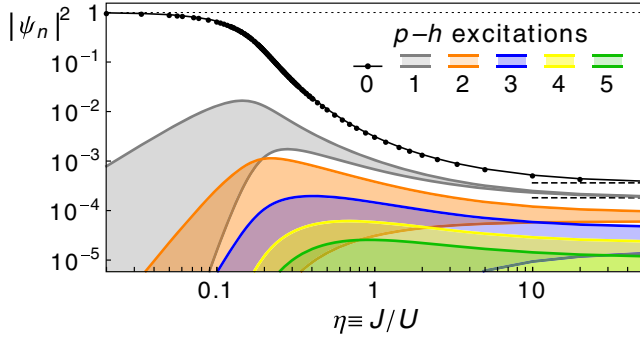


FIG. 2. Intensities $|\psi_n|^2$ in the Fock basis of the BHH ground state versus η for $L = 10$, $\nu = 1$. Solid lines highlight the maximum and minimum intensities on a Fock state with a certain number of particle-hole (p - h) excitations on top of the homogeneous state $|\nu\rangle$. The values of η considered are highlighted by symbols only for the maximum intensity. Dashed lines indicate the intensity value of the first two p - h manifolds for $\eta = \infty$ [see Eq. (4)].

which can be straightforwardly estimated using QMC simulations.

An overview of the η dependence of \tilde{D}_q , for $q = 1, 2, \infty$, $\nu = 1$ and different L is shown in Fig. 3. The value of the finite-size GFDs is strongly suppressed for small η and rises quickly as the vicinity of the critical value η_c is approached. The SF phase thus correlates with higher values of \tilde{D}_q , indicating a faster growth of the ground state's volume in Fock space as $L \rightarrow \infty$. Although convergence towards the thermodynamic limit D_q is rather slow, the data strongly suggest that multifractality exists for any η . We emphasize that for $\eta \ll 1$ and $\eta \gg 1$ the GFDs for small L are very well described by perturbation theory [60], as shown in the inset of Fig. 3.

From the behavior observed in Fig. 3, it is rather appealing to think that \tilde{D}_q may vanish in the thermodynamic limit for

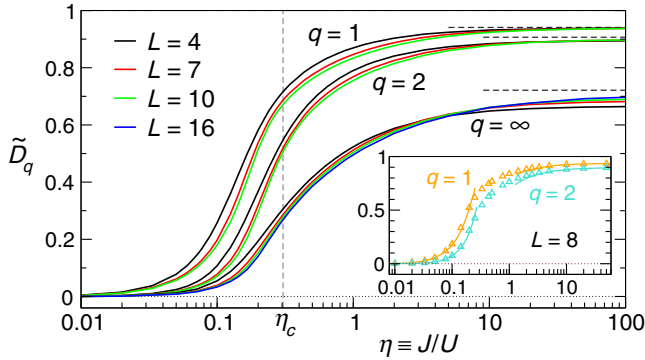


FIG. 3. Finite-size GFDs \tilde{D}_q ($q = 1, 2, \infty$) of the BHH ground state versus η for $\nu = 1$. Solid lines in main panel are numerical results ($L = 16$ only for $q = \infty$). Horizontal dashed lines mark the D_q values for $\eta = \infty$. The inset shows numerical (symbols) and analytical results from perturbation theory (solid lines) for $L = 8$.

$\eta \leq \eta_c$. In such a case, the MI phase would have a simple interpretation as a localized phase in Fock space—which can be viewed as an intricate lattice, whose nodes, i.e., the states $|\mathbf{n}\rangle$, have different energies and are connected by the hopping term of the Hamiltonian [Eq. (2)]. Nevertheless, as $\mathcal{N} \rightarrow \infty$, the coordination number of the Fock lattice diverges linearly with L , and therefore, naively, the existence of localization in the thermodynamic limit appears unlikely. In order to ascertain the presence or absence of localization in the MI phase, a proper $\mathcal{N} \rightarrow \infty$ extrapolation is required, for which knowledge of the expected finite-size corrections is essential. The analytical calculation of the GFDs in the noninteracting limit provides access to the leading finite- L corrections, whose form is essentially determined by the dependence of \mathcal{N} on L . Using insights from perturbation theory and the analysis of plausible asymptotic behaviors of R_q , we find that the dominant finite-size corrections in the scaling of the GFDs for any η are

$$\tilde{D}_q = D_q + \alpha \frac{\ln L}{L} + \beta \frac{1}{L} + \gamma \frac{\ln^2 L}{L^2} + \mathcal{O}(L^{-2} \ln L), \quad (5)$$

with η - and ν -dependent coefficients α, β, γ .

We analyzed the minimum dimension \tilde{D}_∞ for system sizes up to $L = 70$ at unit filling for $\eta = 1/7 < \eta_c$. The numerical data are perfectly described by the first four terms in Eq. (5), as shown in Fig. 4. Indeed, only if the four terms are present can a reliable fit be obtained. The resulting D_∞ is distinctively nonvanishing (consequently $D_q > 0$ for all q), and hence Fock-space localization in the MI phase is ruled out.

We conclude that there is no fingerprint of the transition in the raw values of the GFDs: In the thermodynamic limit, the dependence of D_q with η will exhibit an overall behavior similar to that observed in Fig. 3 for finite Fock spaces. Yet the evolution of the GFDs might still encode the transition. The MI-SF crossover for finite L has recently been inspected from another perspective: In 2D via the η derivatives of the expectation value of simple

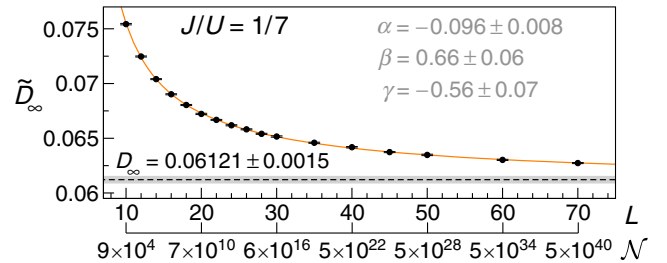


FIG. 4. Extrapolation of \tilde{D}_∞ as $L \rightarrow \infty$ for $\eta = 1/7$, $\nu = 1$. Symbols are numerical data. The solid line is the best fit to Eq. (5) (chi square $\simeq 10$ with 13 degrees of freedom). The horizontal dashed line and the shaded area mark, respectively, the D_∞ value and its 95% confidence interval. The secondary abscissa axis indicates the size of Fock space for each L .

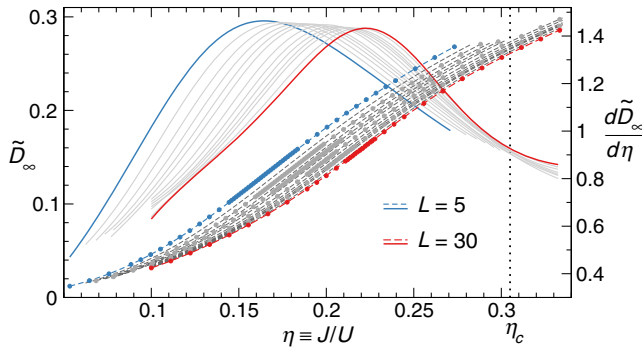


FIG. 5. Dimension \tilde{D}_∞ (left vertical axis) and its derivative (right vertical axis) versus η for the BHH ground state and $L = \{5-10, 12, 14, 16, 18, 20, 25, 30\}$, $\nu = 1$. Symbols indicate numerical data (errors within symbol size), dashed lines correspond to the best Padé fits and solid lines are their respective derivatives. For clarity, symbols are shown only for $L = \{5, 7, 9, 12, 18, 30\}$.

observables [67], and in 1D using the fidelity susceptibility [45,68,69]. The common underlying idea to these approaches is to use the η sensitivity of the ground state as a figure of merit. In our formalism, the η dependence of the dimensions \tilde{D}_q exposes manifestly the variation in the structure of the ground state in Fock space, and, consequently, we find that the rate of change of the GFDs with η reveals the critical point.

In Fig. 5, we show \tilde{D}_∞ as a function of η and its corresponding derivative $\tilde{D}'_\infty(\eta) \equiv d\tilde{D}_\infty/d\eta$ for $L \leq 30$. When approaching the transition from the MI side, the derivative develops a distinct single maximum at a certain value $\eta_*(L)$ that shifts towards η_c for increasing L . In order to locate reliably the position of the maximum, we first find the best fit of the numerical \tilde{D}_∞ data to a Padé approximant, which is then differentiated. The analysis of \tilde{D}_2 reveals the same behavior [70]. The scaling expected for the position of the maximum of the derivative follows from the assumption that at $\eta_*(L)$ the correlation length ξ [49] (ruling the spatial decay of the single-particle density matrix elements, $\langle b_k^\dagger b_{k+r} \rangle \sim e^{-r/\xi}$) is proportional to the system size. While ξ is finite and L independent in the MI phase, it diverges at the transition and within the SF phase [71]. We expect that the steepest change of each GFD with increasing η correlates with the region where $\xi \sim L$; i.e., it signals the crossover for a finite system. For $\eta < \eta_c$ the correlation length exhibits the exponential dependence $\xi \sim \exp(b/\sqrt{\eta_c - \eta})$ with $b > 0$. Hence, it ensues

$$\eta_*(L) = \eta_c - \frac{b^2}{\ln^2(L/|\ell_q|)}, \quad (6)$$

for suitable parameters η_c , b (which are q independent) and ℓ_q . Note that this same scaling holds for the position of

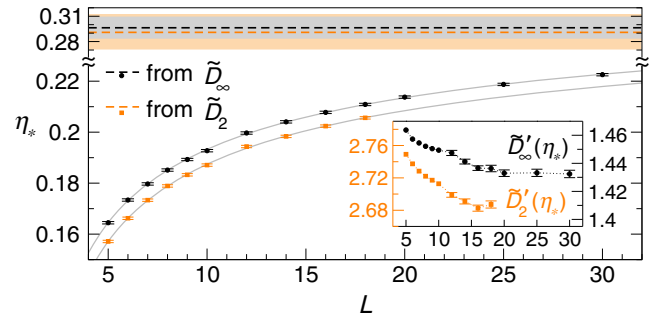


FIG. 6. Position $\eta_*(L)$ of the maximum of $\tilde{D}'_\infty(\eta)$ and $\tilde{D}'_2(\eta)$ for $\nu = 1$. Solid lines are best fits to Eq. (6), with $b = 1.92 \pm 0.18(1.85 \pm 0.27)$, $\ell_q = 0.025 \pm 0.009(0.032 \pm 0.018)$ for \tilde{D}_∞ (\tilde{D}_2) data. Dashed lines and shaded regions mark, respectively, the estimated η_c and its 95% confidence interval: $\eta_c \in [0.284, 0.308]$ from \tilde{D}_∞ , and $\eta_c \in [0.270, 0.312]$ from \tilde{D}_2 . The inset shows the maximum value of the derivatives versus L .

the maximum of the fidelity susceptibility at a BKT transition [72].

The scaling analysis of $\eta_*(L)$ is presented in Fig. 6 for \tilde{D}_∞ ($L \leq 30$) and for \tilde{D}_2 ($L \leq 18$). The data are described reliably by Eq. (6), which yields the following estimates for the critical point at unit filling: $\eta_c = 0.296 \pm 0.006$ from \tilde{D}_∞ and $\eta_c = 0.291 \pm 0.011$ from \tilde{D}_2 . Both values are compatible with each other and in perfect agreement with previous estimates. The maximum value of the derivatives seems to be finite for $L \rightarrow \infty$ (inset of Fig. 6), which has similarly been observed for the fidelity susceptibility at a BKT transition [72]. The scaling of the GFD derivatives provides a very good level of accuracy in the location of the critical point already from the analysis of modest system sizes. Furthermore, \tilde{D}_∞ is simply the value of the intensity $|\langle \nu | \Psi(\eta) \rangle|^2$ in log scale; hence, we have demonstrated that the MI-SF transition can be characterized by monitoring only one wave function amplitude in the exponentially large Fock space [73].

We have provided evidence of the significance of many-body multifractality in Fock space for bosonic systems. In particular, we have shown that the superfluid to Mott insulator transition in the Bose-Hubbard Hamiltonian (BHH) can be understood in terms of the rate of change of the generalized fractal dimensions (GFDs) with the interaction strength. Such novel perspective provides an efficient method to locate accurately the critical point using moderate system sizes. Remarkably, it furthermore reveals that the transition at integer densities can be analyzed from the examination of only one privileged (maximum) wave-function intensity. This observation opens a promising path for further theoretical and experimental studies of the BHH. We also note that the η dependence of the information entropy has been used to characterize the statistical nature of the BHH eigenstates [74] and to identify chaotic behavior [75]. Additionally, first results indicate that multifractality extends to the excited states, whose GFDs also

carry apparently a fingerprint of the transition. Whereas the rather expected absence of localization in Fock space has been confirmed, it remains to be seen whether (many-body) Fock-localized phases exist for the disordered BHH.

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