Chaos and ergodicity across the energy spectrum of interacting bosons

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We identify the chaotic phase of the Bose-Hubbard Hamiltonian by the energy-resolved correlation between spectral features and structural changes of the associated eigenstates as exposed by their generalized fractal dimensions. The eigenvectors are shown to become ergodic in the thermodynamic limit, in the configuration space Fock basis, in which random matrix theory offers a remarkable description of their typical structure. The convergence of the eigenvectors towards ergodicity, however, is ever more distinct from random matrix theory as the Hilbert space dimension grows.

Ergodicity, understood as the ability of a system to dynamically explore, irrespective of its initial state, all possible configurations at given energy, is, in general, an exceedingly difficult to prove and rather rare property, at the classical and quantum level [1–3]. On the quantum side, safe ground is established by (intrinsically ergodic [4]) random matrix theory (RMT), which describes systems with classically strictly chaotic (“K-systems” [1–3, 5]) dynamics [6]. RMT predictions for energy spectra and eigenstates [7, 8] define popular benchmarks to certify ergodicity [9, 10].

Ergodicity can, however, emerge on widely variable time scales, hinging on finer structures of phase space, and, at the quantum level, on the effective coarse graining thereof induced by the finite size of $\hbar$ [11]. Since the majority of dynamical systems features mixed rather than strictly chaotic dynamics [12–17], one therefore expects detectable deviations from RMT ergodicity [18, 19], in particular at the level of the eigenvectors’ structural properties— which reflect the underlying phase space structure [12–16, 20]. This holds on the level of single as well as of many-body quantum systems, with engineered ensembles of ultracold atoms [21–26] as a modern playground: Notably interacting bosons on a regular lattice provide a paradigmatic experimental setting to explore the questions above [27–31]; they feature chaos on the level of spectral [32–35] and eigenvector properties [32, 33, 36–39] as well as quenched dynamics [40–44].

Here we consider the Bose-Hubbard Hamiltonian (BHH) and combine state-of-the-art numerical simulations with analytical calculations to establish a so far missing integral picture of its chaotic phase, providing deeper insight into the concept of chaos and ergodicity in the quantum realm. We demonstrate that (i) the energy-resolved chaotic phase is signalled by a clear correlation between spectral features and eigenstate structural changes captured by generalized fractal dimensions (GFD) (cf. Fig. 1), whose fluctuations exhibit qualitatively a basis-independent behavior, (ii) eigenvectors within the chaotic phase become ergodic in the thermodynamic limit in the configuration space Fock basis, where RMT provides a remarkable description of the eigenstates’ typical (i.e., most probable) GFD, (iii) despite such agreement, BHH and RMT depart from each other in an unequivocal statistical sense with increasing size of Hilbert space. This implies that the fluctuations of the eigenstates’ structure along the path to ergodicity (even if it be arbitrarily close to RMT at a coarse-grained level) contain statistically robust fingerprints of the specific underlying Hamiltonian.

In terms of standard bosonic operators associated with $L$ Wannier spatial modes, the BHH [45–47] is the sum of a tunneling and a local interaction Hamiltonian with respective strengths $J$ and $U$,

$$H_{\text{tun}} = -J \sum_k b_k^\dagger b_{k+1} + b_{k+1}^\dagger b_k,$$

$$H_{\text{int}} = \frac{U}{2} \sum_k n_k (n_k - 1).$$

The BHH exhibits a $Z_2$ symmetry under the reflection operation ($\Pi$) about the center of the lattice. In the presence of periodic boundary conditions (PBC), the BHH additionally has translational symmetry, and Hilbert space can be decomposed into irreducible blocks distinguished by the center-of-mass quasimomentum $Q$. The $Q = 0$ block further disjoints into symmetric ($\pi = +1$) and antisymmetric ($\pi = -1$) subspaces. For hard-wall boundary conditions (HWBC), the latter $\pi$-division applies to the full Hilbert space.

Both $H_{\text{tun}}$ and $H_{\text{int}}$ are integrable and analytically solvable in appropriate Fock bases. The eigenvectors of the interaction term are the Fock states of the on-site number operators, $|n⟩ \equiv |n_1, \ldots, n_L⟩$, with $|[n]| = N$, where $N$ is the number of bosons. The eigenvectors of $H_{\text{tun}}$ follow from the Fock states of number operators of spatially delocalized plane-wave or standing-wave modes, for PBC or HWBC, respectively.

The competition between tunneling and interaction makes the BHH non-integrable: For comparable $J$ and $U$, it exhibits spectral chaos [32–35], identified by short-range spectral measures in accord with the Gaussian orthogonal ensemble (GOE) of RMT. This may be traced back to the underlying classical Hamiltonian [16, 34, 48], whose dynamics are governed by the scaled energy $H/UN^2$ and the scaled tunneling strength $\eta \equiv J/UN$. In the quantum system, one therefore expects $\eta$ to control the emergence of chaos in sufficiently dense spectral regions.

We numerically analyze the BHH at unit filling ($N = L$): Eigenstates around chosen energy targets [49–51] as well as full spectra, scaled as $\epsilon \equiv (E - E_{\text{min}})/(E_{\text{max}} - E_{\text{min}}) \in [0, 1]$. 

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enabling the juxtaposition of results for different \(N\) and \(\eta\), are obtained by exact diagonalization. Since the form of \(H_{\text{fun}}\) and \(H_{\text{int}}\) reveals that \(E_{\text{max}} - E_{\text{min}} \sim UN^2\) for large \(N\), \(\epsilon\) effectively provides the classically scaled energy. Short-range statistical features of the spectrum are best captured by the level spacing ratios \([52, 53]\), \(r_n = \min(s_{n+1}/s_n, s_n/s_{n+1})\), where \(s_n = E_n+1 - E_n\) is the \(n\)-th level spacing. The distributions of \(r\) are known approximately analytically for Gaussian random matrix ensembles and accessible numerically without further unfolding procedures, e.g., \((r)_{\text{GOE}} \approx 0.5307\) [53].

The eigenstate structure of generic many-body Hamiltonians in Hilbert space exhibits multifractal complexity [54–64], and is conveniently described by finite-size generalized fractal dimensions (GFD) [62, 65],

\[
\tilde{D}_q \equiv \frac{1}{1-q} \log_N R_q, \quad \text{with} \quad R_q = \sum_\alpha |\psi_\alpha|^2 q^q, \quad q \in \mathbb{R}^+. \tag{3}
\]

for eigenvectors with amplitudes \(\psi_\alpha\) in a given orthonormal basis of size \(N\). The eigenvector moments are expected to scale asymptotically as \(R_q \sim N^{-(q-1)\tilde{D}_q}\), where the dimensions \(D_q \equiv \lim_{N \to \infty} \tilde{D}_q\) decide whether the state is localized (\(D_q = 0\) for \(q \geq 1\) [66]), multifractal (extended non-ergodic; \(q\)-dependent \(0 < D_q < 1\)), or ergodic (\(D_q = 1\) for all \(q\)), in the chosen expansion basis. Consequently, the support of ergodic eigenstates—e.g., the eigenvectors of the Wigner-Dyson RMT ensembles [68]—scales asymptotically as the full Hilbert space. Among all GFD, we focus on \(\tilde{D}_1\), governing the scaling of the Shannon entropy of \(|\psi_\alpha|^2\), \(\tilde{D}_2\), determining the scaling of the eigenstate’s inverse participation ratio, and \(\tilde{D}_{\infty} = -\log_N \max_\alpha |\psi_\alpha|^2\), unveiling the extreme statistics of the state’s intensities.

We first analyze the connection between spectral chaos and the eigenstates’ GFD. In Fig. 1, we show the evolution of \((r)\), \((\tilde{D}_1)\), and \(\text{var}(\tilde{D}_1)\), as functions of scaled energy \(\epsilon\) and scaled tunneling strength \(\eta\), for \(N = 12\) and PBC (subspace \(Q = 0, \pi = -1\)), evaluated in the eigenbasis of \(H_{\text{int}}\). The \(\epsilon\) spectrum is divided into 100 bins of equal width; mean values and variances are computed from eigenvalues and eigenvectors falling into each bin. Energy-resolved density plots expose the coarse-grained level dynamics of the system: Heavily degenerate manifolds of \(H_{\text{int}}\) fan out as \(\eta\) increases, overlap, and then form a bulk region massively populated by avoided crossings (observable upon finer inspection [69]), which eventually dissolves as the levels reorganize into the bands allowed by \(H_{\text{fun}}\), for \(\eta \gg 1\). We identify a slightly bent oval region of spectral chaos, centered around \(\eta \approx 0.1\) and extending over \(0.1 \leq \epsilon \leq 0.9\), where \((r)\) attains the GOE value. This region remains visible after averaging \(\epsilon\) over a large portion of the bulk spectrum, even without resolving the \(\Pi\)-symmetry [70]. The onset of spectral chaos correlates with a sudden increase in the eigenvectors’ GFD, which reach maximum values within the spectral chaos region, as demonstrated for \((\tilde{D}_1)\). Strictly simultaneously, the energy-resolved GFD variance undergoes a dramatic reduction by several orders of magnitude. This behavior is also revealed by \(D_2\) and \(D_{\infty}\), and qualitatively the same in any irreducible subspace, also for HWBC. The chaotic regime can therefore be identified by the unambiguous correlation between spectral features and structural changes of eigenstates, which, as revealed by the GFD, tend to homogenize their delocalization in Hilbert space, irrespective of their energy.

To elucidate the eigenstates’ structural dependence on Hilbert space’s size, Fig. 2 shows mean and variance of \(\tilde{D}_1\), for fixed \(\epsilon = 0.5\) (where the density of states is maximum once spectral chaos kicks in), versus \(\eta\), for increasing size (up to \(N = 2.6 \times 10^6\)) of the \(\pi = -1\) subspace with HWBC. \((\tilde{D}_1)\) registers a surge around \(\eta = 0.1\), and reaches a maximum that develops into a distinct plateau, extending towards larger \(\eta\) for increasing \(L\). (Also \((r)\) exhibits plateau broadening at \(\epsilon = 0.5\) [69].) This

![FIG. 1. Evolution of \((r)\) (left), \((\tilde{D}_1)\) (center) and \(\text{var}(\tilde{D}_1)\) (right), as functions of \(\eta\) and energy \(\epsilon = (E - E_{\text{min}})/(E_{\text{max}} - E_{\text{min}})\), for the irreducible Hilbert subspace of size \(N = 55,898\) spanned by the \(Q = 0\) and \(\pi = -1\) eigenstates of \(H_{\text{int}}\), for \(N = L = 12\) with PBC. The spectrum was obtained for 75 equally spaced values of \(\log_{10}(J/U) \in [-2.92, 3]\), and divided into 100 bins of equal width along the \(\epsilon\) axis. The value \((r)_{\text{GOE}}\) is highlighted over the left color bar. Blue dashed lines mark the value \(\epsilon = 0.5\) considered in Fig. 2.](image-url)
behavior is mirrored by the drastic (ever bigger, with increasing $L$) drop of $\text{var}(\tilde{D}_1)$, with plateaux at its minimum. Note that the plateau values of $\langle \hat{D}_1 \rangle$ and $\text{var}(\tilde{D}_1)$ agree well with those expected for GOE eigenvectors, indicated by dashed lines in Fig. 2. The same is qualitatively observed for $q = 2, \infty$, other irreducible subspaces, and PBC. The onset of the plateaux appears system size independent in terms of $\eta$ [70], confirming the relevance of the classically scaled tunneling strength.

To shed further light on the GFD asymptotics within the chaotic region, the lower panels of Fig. 3 show $\langle \tilde{D}_q \rangle$ and $\text{var}(\tilde{D}_q)$ at $\epsilon = 0.5$ and $\eta = 0.25$, for increasing $N$ of four irreducible subspaces, evaluated in the corresponding eigenbases of $H_{\text{int}}$. The results are compared against the GOE values, which, using known distributions [73] and extreme statistics [74], can be estimated analytically [70]. We find, asymptotically,

$$\langle \tilde{D}_1 \rangle_{\text{GOE}} = 1 - \frac{1}{\ln N} \left[ 2 - \gamma - \ln 2 - \frac{1}{N} + O \left( N^{-2} \right) \right], \quad (4)$$

$$\langle \tilde{D}_\infty \rangle_{\text{GOE}} = 1 - \frac{\ln(2 \ln N)}{\ln N} + O \left( \ln \ln N / \ln^2 N \right), \quad (5)$$

where $\gamma$ is Euler’s constant, and

$$\text{var}(\tilde{D}_1)_{\text{GOE}} = \frac{1}{\ln^2 N} \left[ \frac{3\pi^2 - 28}{2N} + O \left( N^{-2} \right) \right], \quad (6)$$

$$\text{var}(\tilde{D}_\infty)_{\text{GOE}} \sim \ln^{-4} N. \quad (7)$$

For $q = 2$, we compare the results to the ensemble-averaged GFD, $\langle \tilde{D}_q^{(\text{ens})} \rangle_{\text{GOE}} = \log_2(GD)/[1 - (1 - q)]$, instead [19][70], with finite-size corrections found identical (up to coefficients) with those for $\tilde{D}_1$. As shown in Fig. 3, the GFD, as well as $\text{var}(\tilde{D}_q)$, in the eigenbasis of $H_{\text{int}}$ quickly approach GOE values, independently of subspace or boundary conditions (for the largest $N$ shown, $\langle \tilde{D}_1 \rangle_{\text{GOE}} - \langle \hat{D}_1 \rangle = 8 \times 10^{-4}$). The BHH data seem to exhibit the same dominant finite size correction as for GOE eigenvectors, and the GFD show clear evidence of converging to $1$ in the thermodynamic limit (as the corresponding variance vanishes). We therefore conclude that the BHH eigenvectors in the chaotic regime become ergodic in the eigenbasis of $H_{\text{int}}$ in the thermodynamic limit.

Hence, as $N \to \infty$, the plateau value of $\langle \hat{D}_1 \rangle$ in Fig. 2 approaches $1$, and, although the crossover into the chaotic region becomes more pronounced with larger $L$, we cannot definitely determine whether it turns into a sharp transition (i.e., a discontinuity of the derivative with respect to $\eta$) or remains smooth and differentiable. The integrability-chaos transition features a standard scaling behavior [59, 60, 63, 65] in terms of $c_1(N) \equiv (1 - \langle \hat{D}_1 \rangle) / N$: For increasing $L$, $c_1$ is unbounded in the non-ergodic phase (where $\langle \hat{D}_1 \rangle < 1$, i.e., the eigenstates are generically multifractal), and decreases to converge to a constant value in the chaotic phase if the dominant finite size correction is $\ln^{-1} N$. That is indeed the behavior observed numerically (inset of Fig. 2). Given the lack of analytical information, we refrain from detailed finite size scaling analyses on $c_1$. Nonetheless, close inspection of the tendency of the data locates the transition/crossover, at $\epsilon = 0.5$, in the thermodynamic limit within the region $\eta \in [0.15, 0.2]$ to a reasonable level of confidence. The plateaux’s right termination points show no hint of reaching a finite asymptotic value for increasing $L$, an absence less pronounced for PBC [70]. Although it is appealing to think that an infinitesimal interaction suffices to induce ergodicity in the thermodynamic limit (as discussed for fermions [75]), and hence that the chaotic phase might have no upper $\eta$ limit (the point $\eta = \infty$ then being a discontinuity), further investigation is necessary to verify such hypothesis.

FIG. 2. Evolution of $\langle \hat{D}_1 \rangle$ (top) and $\text{var}(\tilde{D}_1)$ (bottom) at $\epsilon = 0.5$ versus $\eta$, for varying values of $L$ and size $N$ (as indicated by the legend) of the subspace spanned by the $n = -1$ eigenstates of $H_{\text{int}}$ with HWBC. Each data point results from the analysis of the 100 BHH eigenvectors closest to $\epsilon = 0.5$. Corresponding GOE values are indicated by dashed lines. The inset shows the behavior of $c_1(N) = (1 - \langle \hat{D}_1 \rangle) / N$ versus $\eta$ around the crossover region (solid lines are guides to the eye). The horizontal dotted line marks the GOE value of $c_1(N \to \infty)$.

FIG. 3. Average and variance of $\tilde{D}_1$, $\tilde{D}_2$, and $\tilde{D}_\infty$, at $\eta = 0.25$ and $\epsilon = 0.5$, versus size $N$ of four Hilbert subspaces (distinguished by symbols as indicated; each data point involves 100 eigenstates as in Fig. 2). Lower (upper) panels correspond to the analysis in the eigenbasis of $H_{\text{int}}$ ($H_{\text{subs}}$). Solid lines show GOE predictions. Whenever not shown, errors are contained within symbol size.
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this basis converge to the ergodic limit, too, this is a much slower process governed by stronger finite-size corrections. Such basis dependence reflects the different dynamics that excited eigenstates of $H_{\text{int}}$ or of $H_{\text{tot}}$ will exhibit under the BHH unitary evolution. While the first display indications of chaos already in relatively small systems [31, 41], the second may be substantially dominated by finite-size/finite-time effects.

We provided an integral view on the chaotic phase of the Bose-Hubbard Hamiltonian, established by an energy-resolved correlation between spectral features and eigenstate structural changes exposed by the typical values and fluctuations of generalized fractal dimensions. Our results suggest that GFD fluctuations may identify the chaotic phase in any non-trivial basis. In the eigenbasis of the Hamiltonian’s interaction part, the chaotic phase eigenvectors become ergodic in the thermodynamic limit, and are remarkably well described by RMT. Yet, their path towards ergodicity turns increasingly more distinguishable from RMT for larger Hilbert spaces, which suggests a statistical handle to discriminate bona fide BHH dynamics in the limit of numerically intractable Hilbert space dimensions. This relates our present results to the field of the certification of distinctive rather than universal features of complex quantum systems [78–81]. Whether this distinct GFD statistics of BHH with respect to RMT can be traced down to unambiguously unique features of the underlying Hamiltonian, or, alternatively, accommodated by more sophisticated random matrix ensembles [82–84], awaits further scrutiny.

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Given the demonstrated quality of RMT predictions, one may naively conclude that, at the level of simple eigenvector observables such as Hilbert space (de)localization captured by GFD, as $L$ grows the BHH unequivocally assumes universal RMT behavior within its chaotic phase. But a detailed inspection indicates otherwise: Analysis of the full GFD distributions in Fig. 4 reveals that, although the first and second moments approach the GOE values, the distributions become more distinguishable from GOE as $L$ increases. The distance between BHH and GOE distributions is quantified in Fig. 4(c) using the square root of the Kullback-Leibler divergence (relative entropy) [76, 77], $\sqrt{KL_q}$, and $\delta_q/\sqrt{\text{var}(\tilde{D}_q)}$, where $\delta_q \equiv \langle \tilde{D}_q \rangle_{\text{GOE}} - \langle \tilde{D}_q \rangle$. Both of these measures increase with $L$ for $q = 1, 2, \infty$, demonstrating that, even at the level of the GFD, the two models depart from each other in a statistically unambiguous way: For $N \geq 10^6$ ($L \geq 13, 15$, depending on boundary conditions) the typical $D_{1,2}$ lies more than 10\textsigma away from the most probable GOE value. Note that, for non-overlapping Gaussian distributions of similar width, $\sqrt{KL_q}$ is equivalent to $\delta_q/\sqrt{\text{var}(\tilde{D}_q)}$. Hence, comparison of these two quantities also provides the distributions’ deviation from Gaussianity, as manifestly visible for $q = \infty$.

We finally address the chaotic eigenstates’ features’ dependence on the expansion basis. Although the GFD are naturally basis dependent, the eigenstates’ ergodic character in the thermodynamic limit suggests some degree of invariance under rotations. An analysis performed in the eigenbasis of $H_{\text{int}}$, instead of $H_{\text{tot}}$, reveals the same qualitative behavior of the energy-resolved $\text{var}(\tilde{D}_q)$ [70]. Nonetheless, in the eigenbasis of $H_{\text{tot}}$, there is no clear identification of a $\langle \tilde{D}_q \rangle$ plateau in the chaotic region, and the typical GFD are distant from the GOE values, see the upper panels of Fig. 3. If the GFD in this basis converge to the ergodic limit, too, this is a much slower process governed by stronger finite-size corrections.

We provided an integral view on the chaotic phase of the Bose-Hubbard Hamiltonian, established by an energy-resolved correlation between spectral features and eigenstate structural changes exposed by the typical values and fluctuations of generalized fractal dimensions. Our results suggest that GFD fluctuations may identify the chaotic phase in any non-trivial basis. In the eigenbasis of the Hamiltonian’s interaction part, the chaotic phase eigenvectors become ergodic in the thermodynamic limit, and are remarkably well described by RMT. Yet, their path towards ergodicity turns increasingly more distinguishable from RMT for larger Hilbert spaces, which suggests a statistical handle to discriminate bona fide BHH dynamics in the limit of numerically intractable Hilbert space dimensions. This relates our present results to the field of the certification of distinctive rather than universal features of complex quantum systems [78–81]. Whether this distinct GFD statistics of BHH with respect to RMT can be traced down to unambiguously unique features of the underlying Hamiltonian, or, alternatively, accommodated by more sophisticated random matrix ensembles [82–84], awaits further scrutiny.

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Supplemental Material

Chaos and ergodicity across the energy spectrum of interacting bosons

![Graph](image)

**FIG. S1.** Average of \( r \) over the inner 70% of the eigenenergies as a function of \( \eta \) for varying values of \( L \) and size \( (N) \) (as indicated by the legend) of the reflection-antisymmetric subspace (top) as well as of the full Hilbert space with hard-wall boundary conditions. Expected results for GOE eigenvectors are indicated by dashed lines.

**FURTHER RESULTS ON SPECTRAL FEATURES AND EIGENSTATE STRUCTURE OF THE BHH**

Table I lists the sizes of the different irreducible Hilbert spaces considered in our numerical analysis. It is worth noting that while in the basis of \( H_{\text{int}} \), the number of non-zero elements per row in the Hamiltonian matrix grows linearly with \( L \), the sparsity is severely reduced in the basis of \( H_{\text{fun}} \), where the number of non-zeros scales as \( L^{5/4} \), which makes the numerical treatment far more demanding. The analysis in the tunneling eigenbasis is restricted to \( L \leq 12 \) (\( L \leq 14 \)) for hard-wall (periodic) boundary conditions.

The average over the energy axis of the level statistics, as usually considered in the literature [32–35], also reveals the existence of spectral chaos. Figure S1 shows the level spacing ratio averaged over the inner 70% of the eigenenergies as a function of \( \eta \equiv J/UN \) for varying system sizes with hard-wall boundary conditions. Agreement with the results expected for GOE eigenvectors is clearly observed within a range of the interaction strength which correlates with the behavior shown in Fig. 1. The region of spectral chaos is also visible even upon consideration of the full Hilbert space, i.e., without resolving the symmetric and antisymmetric subspaces induced by the reflection symmetry about the center of the chain.

As can be seen in Fig. 2 of the manuscript, the upper limit of the \( \langle \tilde{D}_1 \rangle \) plateau seems to keep increasing for larger \( L \). To quantify that behavior, we estimate the lower and upper limits of the plateaux as the positions where the difference between the typical GFD value and the corresponding GOE value is twice the minimum difference between these two, and show their evolution as functions of Hilbert space size for different boundary conditions in Fig. S2. While the lower limit, \( \eta_L \), converges to a value in the region [0.15, 0.2] for all the cases considered, the upper limit, \( \eta_U \), does not exhibit an asymptotic saturation (especially for HWBC) in the accessible range of \( N \).

The energy-resolved correlation between the spectral statistics and the eigenvector structure in the eigenbasis of \( H_{\text{fun}} \), as function of rescaled energy \( \epsilon \) and hopping strength \( \eta \), is presented for \( \langle \tilde{D}_1 \rangle \) in Fig. S3, and should be compared against Fig. 1 in the manuscript. Note that the overall evolution of the values of the GFD is inverted as compared to the analysis in the \( H_{\text{int}} \) basis, since the eigenvectors must be highly localized in the limit \( \eta \rightarrow \infty \). The evolution of var(\( \tilde{D}_q \)) in the \( H_{\text{fun}} \) eigenbasis shows a region of drastically suppressed GFD fluctuations that agrees with the corresponding area observed in Fig. 1. An inspection of \( \langle \tilde{D}_1 \rangle \) at \( \epsilon = 0.5 \) does not reveal the clear formation of a plateau, and the typical GFD values are rather far from the RMT prediction, as illustrated in Fig. 3 of the manuscript. Despite the basis dependence of the typical GFD, their fluctuations might be a basis-independent figure of merit to identify the emergence of a chaotic regime.

**GENERALIZED FRAC TAL DIMENSIONS FOR GOE EIGENVECTORS**

Since \( \tilde{D}_1 = -\langle \ln N \rangle^{-1} \sum_{\alpha} |\psi_{\alpha}|^2 \log_N |\psi_{\alpha}|^2 \), the calculation of its mean and variance can be carried out exactly from the known one- and two-intensity distributions of GOE eigenvectors [73]. For \( q = 2 \), the analytical calculations for the typical GFD are rather challenging, but the results for the ensemble-averaged GFD (obtained from the arithmetic average of the \( R_q \) moments, i.e., \( \langle \tilde{D}_q^\text{ens} \rangle = -\log_N \langle R_2 \rangle \)) provide excellent approximations...
$\log N$ \( (2^L $)

where $H$ (see Eq. 5.2.2 in Ref. [72]). We emphasize the importance of the variable mean and variance given above, as demonstrated in Fig. S4. After doing an appropriate change of variable and integrating by parts (neglecting one term that decreases exponentially with $N$), one can estimate the moments of $D_{\infty}$ from

$$
\langle \bar{D}_k \rangle = \frac{(-1)^k 12k}{\ln^k N} \int_{\sqrt{2}}^{\sqrt{N/2}} x Erf(\sqrt{2} / 2 \sqrt{N / x}) N^{N - 2} \ln^k (2x / N).
$$

(Fig. S3) Evolution of $\langle \bar{D}_1 \rangle$ (left) and $\text{var}(\bar{D}_1)$ (right) as functions of $\eta$ and rescaled energy $\epsilon = (E - E_{\min})/(E_{\max} - E_{\min})$, for the irreducible subspace of size $N = 55 898$ spanned by the $Q = 0$ and $\pi = -1$ eigenbasis of $H_{\text{int}}$ for $N = L = 12$ with PBC (cf. Fig. 1 in manuscript). The black dashed line in the right panel indicates the contour $\text{var}(\bar{D}_1) = 5 \times 10^{-5}$ for the analysis in the eigenbasis of $H_{\text{int}}$, shown in Fig. 1 of the manuscript.

\[ \langle \bar{D}_1 \rangle_{\text{GOE}} = \frac{H_{N/2} - 2 + \ln 4}{\ln N}, \quad (S1) \]

\[ \langle \bar{D}_2^{(\text{ens})} \rangle_{\text{GOE}} = \frac{\ln(N + 2) - \ln 3}{\ln N}, \quad (S2) \]

where $H_n = \sum_{k=1}^{n} \frac{1}{k}$ is the harmonic number, and

\[ \text{var}(\bar{D}_1) = \frac{(3 \pi^2 - 24)(N + 2) - 8}{2(N + 2)^2 \ln^2 N} - \psi\left(\frac{1}{2} + \frac{N}{2}\right), \quad (S3) \]

\[ \text{var}(\bar{D}_2^{(\text{ens})}) = \frac{8(N - 1)}{3(N + 4)(N + 6) \ln^2 N}, \quad (S4) \]

where $\psi(1)$ denotes the first derivative of the digamma function (see Eq. 5.2.2 in Ref. [72]). We emphasize the importance of using the two-intensity distribution to calculate the variance of $\bar{D}_1$. The correlation among the intensities induced by the eigenstate normalization (such correlation does not seem to be crucial in this case). From the Porter-Thomas distribution $P(\langle \psi_{\alpha} |^2 \rangle)$ for the wavefunction intensities for large $N$ [73] the cumulative distribution function of $t$ thus reads

$$
F(t, N) = \int_{0}^{t} \int_{0}^{\infty} P(\langle \psi_{\alpha} |^2 \rangle) \, d\psi_{\alpha} = \left[ \text{Erf}(\sqrt{t N / 2}) \right] ^N,
$$

and consequently its PDF can be written as

$$
\rho(t, N) = \frac{N^{3/2}}{\sqrt{2 \pi t}} e^{-t N / 2} \left[ \text{Erf}(\sqrt{t N / 2}) \right] ^{N-1}. \quad (S5)
$$

The PDF for $\bar{D}_{\infty} = -\log N \, t$ is thus given by

$$
P(\bar{D}_{\infty}) = \rho(N^{-D_{\infty}}, N) N^{-D_{\infty}} \ln N, \quad (S6)
$$

which is in excellent agreement with the numerics, as we demonstrate in Fig. S4.

**TABLE I.** Size of the analyzed irreducible Hilbert spaces as function of $L$.

| $L$ | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 |
|-----|---|---|---|----|----|----|----|----|----|
| HWBC, $\pi = -1$ | 848 3200 | 12 120 | 46 126 | 176 232 | 675 808 | 2 599 688 |
| HWBC, $\pi = +1$ | 868 3235 | 12 190 | 46 252 | 176 484 | 676 270 | 2 600 612 |
| PBC ($Q = 0$), $\pi = -1$ | 1317 | 4500 | 15 907 | 55 898 | 199 550 | 714 714 | 2 583 586 |
| PBC ($Q = 0$), $\pi = +1$ | 1387 | 4752 | 16 159 | 56 822 | 200 474 | 718 146 | 2 587 018 |

**FIG. S4.** Comparison between analytical and numerical results for the GFD of GOE eigenvectors. Average and variance of $D_q$ as a function of the vector length $N$ are shown in the upper panels, while the lower plots display probability density functions of $D_q$ for $N = 2 599 688$. Solid lines follow from the evaluation of Eqs. (S1)-(S8); symbols and error crosses (indicating $\pm 1\sigma$) are obtained from the numerical sampling of GOE eigenvectors $[10^4$ for $\langle \bar{D}_q \rangle$, var($\bar{D}_q$), and $5 \times 10^4$ for the distributions].
After an adequate treatment of \([\text{Erf}(x)]^N\) for large \(N\), we find for \(k = 1\)

\[
\langle \tilde{D}_\infty \rangle_{\text{GOE}} = 1 - \frac{\ln(2\ln N)}{\ln N} + \frac{\ln(\ln^2(2)\pi \ln N)}{2 \ln^2 N} + O\left(\ln^2 N / \ln^3 N\right), \tag{S8}
\]

which provides a remarkable description of the numerical data, as shown in Fig. S4. It is worth noting that the leading correction for \(\tilde{D}_\infty\) exhibits the generic dependence expected for the extreme statistics of multifractal eigenvectors [71]. The calculation of the leading terms of the second moment, and thus of the variance, proves to be more involved, although analytical inspection suggests that \(\text{var}(\tilde{D}_\infty)_{\text{GOE}} \sim \ln^{-4} N\) as \(N \to \infty\). In any case, \(\langle \tilde{D}_2^2 \rangle\) can be estimated by evaluating numerically Eq. (S7).