

## Quantum Ergodicity in the Many-Body Localization Problem

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We generalize Page’s result on the entanglement entropy of random pure states to the many-body eigenstates of realistic disordered many-body systems subject to long-range interactions. This extension leads to two principal conclusions: first, for increasing disorder the “shells” of constant energy supporting a system’s eigenstates fill only a fraction of its full Fock space and are subject to intrinsic correlations absent in synthetic high-dimensional random lattice systems. Second, in all regimes preceding the many-body localization transition individual eigenstates are thermally distributed over these shells. These results, corroborated by comparison to exact diagonalization for an SYK model, are at variance with the concept of “nonergodic extended states” in many-body systems discussed in the recent literature.

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**Introduction.**—Complex quantum systems exposed to external disorder may enter a phase of strong localization. About two decades after the prediction of many-body localization (MBL) [1–3], there is still no strong consensus about the stability of the MBL phase and/or the possible presence of an intermediate phase between MBL and the thermal phase. One class of models where these questions can be explored with more analytic control is confined many-body systems with long-range interactions. Under these conditions, the interaction operator couples all single-particle states, which facilitates the analysis. At the same time, the Hilbert space dimension is still exponentially large in the particle number, which leads to rich physics relevant to systems such as chaotic many-body quantum devices [4–7], small sized optical lattices [8–10], or qubit arrays [11,12].

In recent years, the complex structure of many-body quantum *states* in MBL has become a focus of intensive research. Unlike with single particle problems, where extended wave functions uniformly cover real space, increasing the disorder in a phase of extended many-body states  $|\psi\rangle$  leads to a diminished wave function support in Fock space. This phenomenon, which shows, e.g., in a suppression of wave function moments (WFM)  $|\langle n|\psi\rangle|^{2q}$  in an occupation number basis  $|n\rangle$ , has led to the proposal of a phase of “*nonergodic extended states*” [13–16] intermediate between the phases of absent and strong localization. An alternative scenario is that for each realization of the disorder only a subset of states  $\{|n\rangle\}$  have finite overlap with the eigenstates of energy  $E$ , and in this way define a quantum *energy shell* in Fock space. A uniform (thermal) distribution of the exact eigenstates on this shell would then be the defining criterion for maintained quantum *ergodicity* on the delocalized side of the MBL transition.

At this stage, there is mounting evidence in favor of the second scenario [17–20]. However, in order to firmly characterize the physics of a globally realized many-body ergodic quantum phase, two questions need to be addressed: How can the energy shell be described in quantitative terms? And what is the distribution of quantum states on that shell? As indicated above, wave function statistics can provide at least part of an answer to the first question. In this Letter, we focus on the equally important second part of the problem and demonstrate that the key to its solution lies in concepts of quantum information. Specifically, we will compute pure state entanglement entropies (EE) under a relatively mild set of assumptions. Within this framework we find that to zeroth order wave functions remain thermally distributed over the shell. This establishes a microcanonical distribution, in agreement with the second scenario—maintained ergodicity in all regimes prior to the transition. In addition, the EE contains subleading terms which reflect the characteristic way in which the energy shell is interlaced into Fock space. These contributions sharply distinguish the energy shells of genuine many-body systems from those of phenomenological high dimensional models such as the random energy model (REM) or sparse random states [21]. In this way the combined analysis of WFMs and EEs becomes a sensitive probe into the complex manifestation of wave function ergodicity in many particle systems.

**Pure state entanglement entropies.**—For a pure state  $\rho = |\psi\rangle\langle\psi|$ , the entanglement entropy relative to a partitioning  $\mathcal{F} = \mathcal{F}_A \otimes \mathcal{F}_B$  of Fock space is defined as the von Neumann entropy,  $S_A = -\text{tr}_A(\rho_A \ln \rho_A)$  of the reduced density matrix  $\rho_A = \text{tr}_B(|\psi\rangle\langle\psi|)$ . The entanglement entropies of pure maximally random states were calculated in the

classic Ref. [22]. More recent work [23] emphasizes the utility of the concept in the context of random matrix models serving as proxies of high-dimensional localizing systems [14]. In these systems, quantum interference shows in a contribution to the entanglement entropy proportional to the ratio of subsystem Fock-space dimensions. A main finding of the present work is that energy-shell correlations distinguishing microscopic systems from random matrix models open a second channel of quantum information and exponentially enhance the suppression of the entanglement below its thermal value. In this way, the entanglement sharply distinguishes between genuine many-body wave functions and wave functions on generic high-dimensional random lattices.

In the rest of this Letter, we will compute the entanglement entropy of pure states prior to the onset of strong localization under a minimal set of assumptions. We will compare our results to the entropies obtained for phenomenological models and to numerical data obtained for a Majorana Sachdev-Ye-Kitaev (SYK) model.

*Energy shell.*—We begin with a qualitative discussion of the Fock space energy shell. Consider a many-body Hamiltonian  $\hat{H} = \hat{H}_2 + \hat{H}_4$ , where  $\hat{H}_4$  is an interaction operator and  $\hat{H}_2$  a one-body operator defined by a single particle spectrum  $\{m_i\}$ ,  $i = 1, \dots, N$  distributed over a range  $\delta$ . Working in the eigenbasis of  $\hat{H}_2$ , Fock space is spanned by the  $D \equiv 2^N$  occupation number states  $n = (n_1, \dots, n_N)$ ,  $n_i = 0, 1$  for spinless fermions. We interpret these states as sites of a hypercubic lattice, carrying local potentials  $v_n = \sum (2n_i - 1)m_i$  with rms value  $\Delta_2 \equiv N^{1/2}\delta$ . Individual states  $n$  are connected to a polynomially large number  $N^\alpha$  of “nearest neighbors”  $m$  by the interaction  $\hat{H}_4$ . For interaction matrix elements  $t_{nm} \sim gN^{-\beta/2}$ , the rms eigenvalue of  $\hat{H}_4$  scales as  $\Delta_4 \sim gN^{(\alpha-\beta)/2}$ , with  $g$  an  $N$ -independent coupling energy for the interaction. These interactions change only an order-one number of occupation numbers, so  $|v_n - v_m|$  is of order  $\delta$  and thus for large  $N$  much smaller than the “bandwidth”  $\Delta_2$  of  $\hat{H}_2$ .

In the competition of the operators  $\hat{H}_2$  and  $\hat{H}_4$ , states  $n$  may hybridize with states  $m$  via the coupling  $t_{nm}$ . When the eigenstates of  $\hat{H}$  are delocalized in Fock space, this hybridization gives the local spectral density

$$\nu_n(E) \equiv -\frac{1}{\pi} \text{Im} \langle n | (E^+ - \hat{H})^{-1} | n \rangle, \quad (1)$$

a linewidth  $\kappa = \kappa(v_n, \delta, g)$  which must be self-consistently determined [24]. The solution of Eq. (1) for a given realization of the disorder contains the essential information on the distribution of the energy shell in Fock space. Specifically, for generic values of the energy  $E$  (we set  $E = 0$  for concreteness), the strength of the disorder  $\delta$  defines four regimes of different shell structure:

Regime I:  $\delta \ll N^{-1/2}\Delta_4$ : the characteristic disorder band width  $\delta N^{1/2} = \Delta_2 \ll \Delta_4$  is perturbatively small. In this regime, the spectral density  $\nu_n \equiv \nu$  is approximately constant over energy scales  $\sim \Delta_2$ .

Regime II:  $N^{-1/2}\Delta_4 \ll \delta \ll \Delta_4$ : the bandwidth of  $\hat{H}_2$  exceeds that of the interaction  $\hat{H}_4$ , but nearest neighbors remain energetically close  $|v_n - v_m| \sim \delta \ll \Delta_4$ . In this regime,  $\kappa \sim \Delta_4$ , indicating that the full interaction Hamiltonian enters the hybridization of neighboring sites.

Regime III:  $\Delta_4 \ll \delta \ll \delta_c$ : only a fraction  $\sim (\Delta_4/\delta)^2$  of nearest neighbors remain in resonance, and the broadening is reduced to  $\kappa \sim \Delta_4^2/\delta$ .

Regime IV: The threshold to localization  $\delta_c$  is reached when less than one of the  $\sim N^\alpha$  neighbors of characteristic energy separation  $\delta$  falls into the broadened energy window. Up to corrections logarithmic in  $N$  (and neglecting potential modifications due to Fock space loop amplitudes) this leads to the estimate  $\delta_c \sim N^{\alpha/2}\Delta_4$  for the boundary to the strong localization regime.

The energy shell in the delocalized regimes II and III is an extended cluster of resonant sites embedded in Fock space. It owes its structure to the competition between the large number  $\mathcal{O}(N^\alpha)$  of nearest neighbor matrix elements and the detuning of statistically correlated nearest neighbor energies  $v_n, v_m$ . In regime II, only a polynomially (in  $N$ ) small fraction  $\kappa/\Delta_2 \sim \Delta_4/(\delta N^{1/2})$  of Fock space sites lie in the resonant window defining the energy shell, and in III this fraction is further reduced to  $\sim \Delta_4^2/(\delta^2 N^{1/2})$ , before the shell fragments at the boundary to regime IV.

We also note that if a site  $n$  lies on the shell, the probability that its neighboring sites of energy  $v_m = v_n \pm \mathcal{O}(\delta)$  are likewise on-shell is parametrically enhanced compared to that of generic sites with energy  $v_n \pm \mathcal{O}(\Delta_2)$ . It is this principle which gives the energy shell of many-body systems a high degree of internal correlations (absent in phenomenological lattice models with statistically independent on-site randomness) [26]. What physical quantities are sensitive to these correlations? And how do quantum states spread over the shell structure? As we are going to discuss next, the pure state entanglement entropy  $S_A$  contains the answer to these questions.

*Entanglement entropy.*—Consider a Fock space (outer product) partitioning defined by  $n = (l, m)$  where the  $N_A$ -bit vector  $l$  labels the states of subsystem  $A$  and  $m$  those of  $B$  with  $N_B = N - N_A \gg N_A$ . We are interested in the disorder averaged moments  $M_r \equiv \langle \text{tr}_A(\rho_A^r) \rangle$ , and the entanglement entropy  $S_A = -\partial_r M_r|_{r=1}$  of the reduced density matrix  $\rho_A = \text{tr}_B(|\psi\rangle\langle\psi|)$  defined by a realization-specific zero-energy eigenstate  $\hat{H}|\psi\rangle = 0$ . The bookkeeping of index configurations entering the moments  $\text{tr}_A(\rho_A^r) = \psi_{l^1 m^1} \bar{\psi}_{l^2 m^1} \psi_{l^2 m^2} \dots \psi_{l^r m^r} \bar{\psi}_{l^1 m^r}$  is conveniently done in a tensor network representation as in Fig. 1. Introducing a multi-index  $\mathcal{N} \equiv (n^1, \dots, n^r)$ , and analogously for  $\mathcal{N}_{A,B}$ , the figure indicates how the index-data

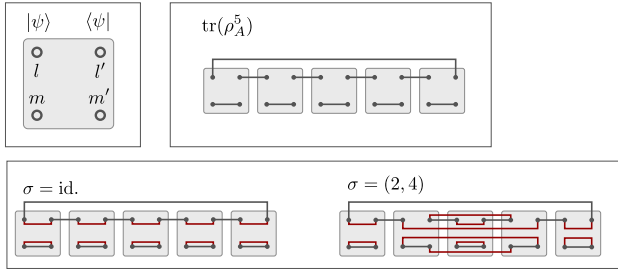


FIG. 1. Top left: graphic representation of the tensor amplitude  $\psi_{lm}\bar{\psi}_{l'm'}$ . Top right: contraction of indices defining  $\text{tr}(\rho_A^5)$ . Bottom: averaging enforces pairwise equality of indices  $n, n'$  in tensor products  $\langle \dots \psi_n \dots \bar{\psi}_{n'} \dots \rangle$ , as indicated by red lines. Left: identity pairing of indices within the five factors  $\langle \text{tr}_A(\rho_A \rho_A \rho_A \rho_A \rho_A) \rangle$ . Right: pairing of indices of the second and fourth factor.

$\mathcal{N}$  and  $\mathcal{M}$  carried by  $\psi$  and  $\bar{\psi}$  is constrained by the summation as  $\mathcal{M}_B^i = \mathcal{N}_B^i$  and  $\mathcal{M}_A^i = \mathcal{N}_A^{\tau i}$ , where  $\tau i = (i+1) \bmod(r)$ . A further constraint, indicated by red lines in the bottom part of the figure, arises from the random phase cancellation under averaging, which in the present notation requires  $\mathcal{N}^i \equiv \mathcal{M}^{\sigma i}$ , for *some* permutation  $\sigma$ . [The figure illustrates this for the identity,  $\sigma = \text{id.}$ , and the transposition  $\sigma = (2,4)$ .] Combining the two constraints, we obtain the representation  $M_r = \sum_{\sigma} \sum_{\mathcal{N}} \prod_i \langle |\psi_{n_i}|^2 \rangle \delta_{\mathcal{N}_A, \sigma \circ \tau \mathcal{N}_A} \delta_{\mathcal{N}_B, \sigma \mathcal{N}_B}$ . This expression is universal in that it does not require assumptions other than the random phase cancellation. In a less innocent final step we establish contact to the previously discussed local density of states  $\nu_n$  and compare the two representations  $D\nu \equiv \sum_{\alpha} \delta(E - E_{\alpha}) = \sum_{n,\alpha} |\psi_{\alpha,n}|^2 \delta(E - E_{\alpha}) = \sum_n \nu_n$  to identify  $|\psi_n|^2 = \nu_n / D\nu$ . In other words, we identify the moduli  $|\psi_n|^2$  of a fixed eigenstate  $\psi = \psi_{\alpha}$  with the realization specific local density of states  $\nu_n$  at  $E = E_{\alpha}$ . For the legitimacy of this replacement for single particle random systems see Ref. [30], and for the SYK model the Supplemental Material [31] and Ref. [25]. With this substitution, we obtain the representation

$$M_r = \sum_{\sigma} \sum_{\mathcal{N}} \prod_{i=1}^r \lambda_{n_i} \delta_{\mathcal{N}_A, (\sigma \circ \tau) \mathcal{N}_A} \delta_{\mathcal{N}_B, \sigma \mathcal{N}_B}, \quad (2)$$

with  $\lambda_n \equiv \nu_n / D\nu$ . This expression describes two complementary perspectives of quantum states in Fock space: their support on a random energy shell defined by the coefficients  $\lambda_n \sim \nu_n$ , and random phase cancellations implicit in the combinatorial structure. In the following, we discuss the manifestations of these principles in the above regimes I–IV.

*Regime I, maximally random states.*—Here, wave functions are uniformly distributed,  $\nu_n = \nu$ , and the evaluation of Eq. (2) reduces to a combinatorial problem. The latter has been addressed in the string theory literature [37,38]

(where high-dimensional pure random states are considered as proxies for black hole micro states.) Inspection of the formula shows that increasing permutation complexity needs to be paid for in summation factors  $D_B$ . Keeping only the leading term,  $\sigma = \text{id.}$ , and the next leading single transpositions  $\sigma = (ij)$ , we obtain  $M_r \approx D_A^{1-r} + \binom{r}{2} D_A^{2-r} D_B^{-1}$ , and the subsequent differentiation in  $r$  yields Page’s result [22]

$$S_A - S_{\text{th}} = -\frac{D_A}{2D_B}, \quad S_{\text{th}} = \ln D_A. \quad (3)$$

Interestingly, higher order terms in the  $D_A/D_B$ -expansion vanish in the replica limit [22,37–40], and Eq. (3) is exact for arbitrary  $N_A \leq N_B$ , up to corrections small in  $1/D$ . (The case  $N_A \geq N_B$  follows from exchange  $A \leftrightarrow B$ .) The result states that to leading order the entropy of the subsystem is that of a maximally random (“thermal”) state,  $S_{\text{th}}$ . The residual term results from wave function interference across system boundaries. Reflecting a common signature of “interference contributions” to physical observables, it is suppressed by a factor proportional to the Hilbert space dimension.

*Regime II and III, energy shell entanglement.*—The energy shell now is structured and correlations in the local densities  $\{\nu_n\}$  lead to a much stronger correction to the thermal entropy. Since these contributions come from the identity permutation (do not involve wave function interference), we ignore for the moment  $\sigma \neq \text{id.}$ , reducing Eq. (2) to  $M_r \approx \sum_l \lambda_{A,l}^r$  with  $\lambda_A \equiv \text{tr}_B(\lambda)$ . This expression suggests an interpretation of the unit normalized density  $\{\lambda_n\}$  as a *spectral measure*  $\sum_n \lambda_n = 1$ ,  $\lambda_n \geq 0$  and of  $\lambda_A$  as the reduced density of system  $A$ . With this identification, the entropy

$$S_A \approx S_{\rho} \equiv -\text{tr}_A[\lambda_A \ln(\lambda_A)] \quad (4)$$

becomes the information entropy of that measure.

This is as far as the model-independent analysis goes. Further progress is contingent on two assumptions, which we believe should be satisfied for a wide class of systems in their regimes II and III: First, the exponentially large number of sites entering the computation of the spectral measure justifies a self-averaging assumption,

$$\begin{aligned} \sum_{n_x} F(v_{n_x}) &\approx D_X \langle F(v_X) \rangle_X \\ &\equiv \frac{D_X}{\sqrt{2\pi\Delta_X}} \int dv_X \exp\left(-\frac{v_X^2}{2\Delta_X^2}\right) F(v_X), \end{aligned} \quad (5)$$

where  $X = A, B, AB$  stands for the two subsystems, or the full space, respectively,  $D_X$  are the respective Hilbert space dimensions, and  $\Delta_X = \delta\sqrt{N_X}$ . In other words, we replace the sum over site energies by an average over a single variable whose Gaussian distribution follows from the



central limit theorem. Second, when integrated against the distribution of subsystem energies  $v_B$ , the local density of states at zero energy  $E \simeq 0$  acts as a smeared  $\delta$  function, setting the additive energy  $v = v_A + v_B \simeq 0$ , and effectively smoothing the distribution  $\lambda_{A,l}$ . Since  $\kappa \ll \Delta_2 \sim \Delta_B$ , the detailed value of the width of the shell  $\kappa$  is of no significance in this construction.

Under these assumptions, straightforward computations detailed in the Supplemental Material [31] yields, e.g., the density of states as  $D\nu = \sum_{AB} \nu_n \approx D \langle \delta_\kappa(v) \rangle_{AB} = D/(\sqrt{2\pi N}\delta)$ . Applied to the computation of the moments Eq. (2), the averaging procedure obtains the entanglement entropy as [31]

$$S_A - S_{\text{th}} = -\frac{1}{2} \ln\left(\frac{N}{N_B}\right) + \frac{1}{2} \frac{N_A}{N} - \sqrt{\frac{N}{2N_A} \frac{D_A}{2D_B}}. \quad (6)$$

A number of comments on Eq. (6) are needed: Provided the above assumptions on the spectral measure hold, the result has the same level of rigor as Page’s formula Eq. (3). The main difference is that (for small subsystems,  $N_A \ll N$ ) the information entropy  $S_A - S_{\text{th}} \approx -\frac{1}{4}(N_A/N)^2$  is exponentially enhanced compared to the correction in Eq. (3). Also note that there is no dependence on the disorder strength (see Supplemental Material [31] for more details).

*Comparison to phenomenological models.*—The entanglement entropy (6) is a universal signature of *correlations* (but not the volume) of the energy shell. Conversely, the WFMs  $|\psi_n|^{2q}$  describe the shrinking of the shell volume (but not its correlations). To see that these are independent pieces of information, it is instructive to compare to the random energy model [41], a phenomenological model replacing the one-body randomness by a set of statistically independent Fock state potentials  $\{v_n\}$ . For increasing  $\delta$ , the WFMs diminish as in microscopic models [42]. However, we have verified that the EE of REM states coincides with Page’s Eq. (3). The same result is obtained for sparse random states [21], as even more phenomenological proxies of many-body states. What is the origin of the difference to Eq. (6)? A genuine many-body model describes many “bodies,” representing the microscopic degrees of freedom. The Fock space is an outer product over the single body spaces, and the Hamiltonian contains only operators coupling  $\mathcal{O}(1)$  of these degrees of freedom. In this sense the REM is *not* a many-body model, since its nonlocal energy operator acts on the products of all (or most) degrees of freedom simultaneously. Specifically, it lacks the principle of energy subsystem additivity  $E = E_A + E_B$ , required by Eq. (6). In this way, the entanglement entropy becomes a sensitive indicator of whether quantum states are genuine many-body states or of different origin.

*Regime boundaries.*—Upon approaching the boundary to the trivially ergodic regime I, the second condition gets

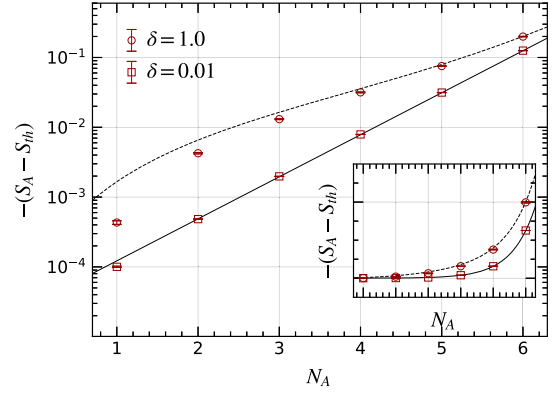


FIG. 2. Numerical entanglement entropies (symbols) vs analytical (lines) for a system of size  $N = 15$  in regime I,  $\delta = 0.01$  (solid) and III,  $\delta = 1$  (dashed). Inset: linear scale representation of the same data.

compromised, i.e., the width  $\kappa$  of individual states ceases to be small compared to the statistical fluctuations  $\sim \Delta_B$ . Leaving a detailed analysis of the crossover region to future work, our numerics below shows a collapse of Eq. (6) to Eq. (3) upon crossing the regime boundary. In the opposite MBL regime IV, eigenstates are concentrated on a small number  $\mathcal{O}(1)$  of isolated Fock states, and the concept of an energy shell becomes meaningless: to exponential accuracy in  $N$ , remote Fock states, even if they are close in energy, have no common matrix elements with individual eigenstates.

The entanglement entropy then scales as  $S_A \sim s(\delta/\delta_c)N_A/N$ , where  $s$  is related to the entropy of the distribution of the localized eigenstate in Fock space. For  $1 \ll N_A \ll N$ ,  $S_A \ll 1$  stays small down to  $\delta \sim \delta_c$ , where it jumps to  $S_A \sim N_A$  at the localization transition to regime III.

*Numerical analysis.*—Figure 2 shows a comparison of the analytical predictions of Eqs. (3) and (6) with numerical results obtained for the SYK Hamiltonian [31]. In that case,  $\hat{H}_4 = (1/4!) \sum_{i,j,k,l=1}^{2N} J_{ijkl} \hat{\chi}_i \hat{\chi}_j \hat{\chi}_k \hat{\chi}_l$ , where  $\{\hat{\chi}_l\}$  are Majorana operators [43,44]. The competing one-body operator reads  $\hat{H}_2 = \sum_{i=1}^N m_i (2c_i^\dagger c_i - 1)$ , where  $c_i = \frac{1}{2}(\hat{\chi}_{2i-1} + i\hat{\chi}_{2i})$  are complex fermion operators defined by the Majoranas [45,46]. Referring to the Supplemental Material [31] for details, the agreement is very good, and it becomes better with increasing  $N_A$ . (We have no certain explanation for the deviations at the smallest values of  $N_A$ .)

*Discussion.*—In this Letter, we applied a combined analysis of the statistics and the entanglement properties of pure quantum states to explore the delocalized phase of disordered many-body systems subject to long-range correlations. Our analysis supports the view that the appealing concept of “nonergodic extended states”—adopted including in publications of the present authors [25,42]—should be abandoned in favor of a qualified interpretation of many-body quantum ergodicity. Its key element is the support set

$\{n\}$  of states of a given energy, the quantum analog of an energy shell. We have shown how the entanglement properties of pure quantum states reveal ergodicity and in addition characteristic correlations distinguishing the energy shells of genuine many-body systems from those of phenomenological proxies.

What is the scope of the above findings? Referring to the Supplemental Material [31] for a more detailed discussion, the freedom to adjust the exponents  $\alpha$ ,  $\beta$  entering the definition of the model Hamiltonian, implies that our result applies to a wide class of *effectively* long-range interacting systems, among them realizations whose interaction operators are short range in a microscopic (“real space”) basis but long range in the eigenbasis of  $\hat{H}_2$ . It is tempting to speculate on generalizations to yet wider system classes. To this end, we note that the derivation of Eq. (6) relies on a number of necessary conditions: subsystem additivity  $E \simeq E_A + E_B$  (requiring that the coupling energy between the subsystems is negligibly small in the limit of large system sizes), statistically independent distribution of the energies  $E_{A,B}$ , and dependence of the spectral density (measure) on no more than the single conserved quantity, energy. Whether these criteria are not only required but actually sufficient to stabilize the result is an interesting question left for forthcoming research [47]. However, regardless of the scope of Eq. (6), we reason that the combination of wave function statistics and pure state entanglement defines the suitable diagnostic to characterize the ergodic phase of many-body quantum chaotic systems.

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