

Complexity measure diagnostics of ergodic to many-body localization transition

Khen Cohen¹, Yaron Oz¹, and De-liang Zhong (钟德亮)²¹*School of Physics and Astronomy, Tel Aviv University, Ramat Aviv 69978, Israel*²*Blackett Laboratory, Imperial College London SW7 2AZ, United Kingdom*

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We introduce diagnostics of the transition between the ergodic and many-body localization phases, which are based on complexity measures defined via the probability distribution function of the Lanczos coefficients of the tridiagonalized Hamiltonian. We use these complexity measures to analyze the power-law random banded matrix model as a function of the correlation strength and show that the moments and the entropy of the distribution diagnose the ergodic to many-body transition, as well as the distinctive feature of the phases concerning the memory of the initial conditions.

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Introduction. The classification of phases of matter along with the identification of their diagnostics is a fundamental scientific challenge. Generically, isolated many-body quantum systems furnish two phases, the ergodic phase that exhibits late-time thermalization and the many-body localization (MBL) phase [1,2] that fails to reach thermal equilibrium and retains a memory of the initial conditions (for a review, see Refs. [3–5]). One diagnostic that distinguishes between the two phases is the entanglement entropy quantum information measure calculated by partitioning the system into two subsystems A and B and tracing out the degrees of freedom of one of them, say B . The ergodic phase exhibits a large entanglement spreading and the entanglement entropy scales as the volume of the subsystem A (volume law), while the MBL phase exhibits less spreading of the entanglement and the entanglement entropy scales as the area of the boundary of A (area law). Another diagnostic is a measure of the chaotic structure of the systems quantified by the level spacing eigenvalue statistics of the Hamiltonian or, alternatively, the r statistics [6–14], that follow a random matrix ensemble distribution in the ergodic phase and a Poisson ensemble distribution in the MBL phase.

A complexity analysis approach to study the dynamics of quantum systems [15–18] is rooted in the recursion method for solving the Schrödinger equation [19] and the tridiagonalization of the Hamiltonian of the physical system rather than its diagonalization. This has been successfully applied to diverse physical systems, including quantum systems with finitely many degrees of freedom, quantum field theories, and holographic theories [4,18,20–47].

Our aim in this Letter is to introduce diagnostics of the two phases and the transition between them, which are based on complexity measures defined via the probability distribution

function of the Lanczos coefficients that arise in the tridiagonalization of the Hamiltonian. We will argue that the moments and entropies of the distribution diagnose the ergodic-MBL transition and its distinctive feature concerning the *memory of the initial conditions*. We will study the power-law random banded matrix (PRBM) model [48], calculate the complexity measures, and showcase the ergodic-MBL transition.

The existence of different diagnostics of the ergodic to MBL transition indicates that there are several different properties that distinguish the two phases, corresponding to quantum information, quantum chaos, and the complexity of the dynamics.

The Letter is organized as follows. In Framework, we provide the framework for the analysis including a brief discussion of the Krylov basis, the Lanczos coefficients, and the PRBM model. In Complexity diagnostics, we introduce complexity measures based on the distribution of the normalized Lanczos coefficients and apply them to the analysis of the ergodic-MBL transition in the PRBM model. Discussion is devoted to conclusions and outlook. Details and additional numerical results are given in the Supplemental Material [49].

Framework: Krylov basis and lanczos coefficients. Consider a time-independent quantum Hamiltonian H realized as a Hermitian matrix in a Hilbert space $\mathcal{H}$. Starting from an initial state $|\psi_0\rangle \in \mathcal{H}$, one constructs a sequence of states by repeated actions of the Hamiltonian:

$$|\psi_1\rangle = H|\psi_0\rangle, \quad |\psi_2\rangle = H^2|\psi_0\rangle, \dots \quad (1)$$

The states $|\psi_\ell\rangle$ encode the evolution in time $|\psi(t)\rangle = e^{itH}|\psi_0\rangle$. When H is finite-dimensional, one keeps acting with H until we get a state that is a linear combination of the previous ones, and for a generic initial state, this process will terminate at the order of the dimension of $\mathcal{H}$.

The states $|\psi_\ell\rangle$ are neither normalized nor orthogonal. One performs a Gram-Schmidt procedure and gets an orthonormal set of states called the Krylov basis, denoted by $|\mathcal{K}_n\rangle$. The first state in the basis coincides with the initial state, $|\mathcal{K}_0\rangle = |\psi_0\rangle$. The Krylov basis is a basis of a subspace of $\mathcal{H}$ that depends both on $|\psi_0\rangle$ and on H .

The Hamiltonian on this basis has a tridiagonal form,

$$H = \begin{pmatrix} a_1 & b_1 & 0 & 0 & 0 & 0 \\ b_1 & a_2 & b_2 & 0 & 0 & 0 \\ 0 & b_2 & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & b_{N-1} \\ \cdots & \cdots & \cdots & \cdots & b_{N-1} & a_N \end{pmatrix}, \quad (2)$$

and the coefficients a_ℓ and b_ℓ are called Lanczos coefficients. The diagonal elements of the Hamiltonian a_ℓ vanish when it is invariant under the Z_2 transformation $H \rightarrow -H$. In practice, all b_ℓ coefficients can be taken to be positive by a redefinition of the basis $|\mathcal{K}_\ell\rangle \rightarrow -|\mathcal{K}_\ell\rangle$.

The Lanczos coefficients have the dimension of energy and they carry information on the complexity of the physical systems and their evolution in time. For instance, it has been proposed [15] that in the limit $\ell \gg 1$, the Lanczos coefficients distinguish between chaotic and integrable systems: For the chaotic system, $b_\ell \sim \ell$, while for the integrable system, $b_\ell \sim 1$ [50].

Power-law random banded matrix model. We will study the transition from the ergodic to the MBL phase in the power-law random banded matrix (PRBM) model employed in Refs. [48,51–61]. The Hamiltonian H is an element of the PRBM ensemble, represented by an $N \times N$ matrix whose (ij) element is given by

$$H_{ij} = \rho(|i - j|, \mu) \times a_{ij}. \quad (3)$$

Here, each a_{ij} is randomly sampled independently from a Gaussian distribution with a zero mean and a variance of one. The $\rho(r, \mu)$ is defined as follows:

$$\rho(r, \mu) := \begin{cases} 1 & \text{if } r < B \\ (1 + r^{2\mu})^{-1} & \text{if } r \geq B, \end{cases} \quad (4)$$

with $\mu \in \mathbb{R}_+$ being a free parameter that controls the strength of the correlation between the Hamiltonian matrix entries. The bandwidth parameter $B \in \mathbb{Z}_{>0}$ controls the interaction range of the model.

Analytics show that in the large $B \gg 1$ limit there is a phase transition at $\mu_c = 1$ [48,52,53]. For small B , there is no analytical result, but numerical observations indicate that for $B = 1$, this model undergoes a transition from ergodic to MBL phase in the vicinity of $\mu = 1$, as indicated by the r statistics of the eigenvalues level distribution and the entanglement entropy [51,61,62]. The special cases $\mu = 0$ and $\mu \rightarrow \infty$ correspond to chaotic and integrable Hamiltonians, and exhibit Gaussian orthogonal ensemble (GOE) and Poisson eigenvalue level spacing statistics, respectively.

In the following, we will introduce complexity measure diagnostics of the ergodic-MBL transition based on the Lanczos coefficients.

Complexity diagnostics: Lanczos coefficients distribution. We define the averaged Lanczos coefficients distribution (LCD) as follows. We choose a fixed initial state $|\psi_0\rangle$ and sample Hamiltonian matrices from the PRBM distribution (3), (4). For each sampled Hamiltonian, we construct the Krylov basis as described in the previous section and read out the Lanczos coefficients b_ℓ^μ from the Hamiltonian in that basis; see (2). We repeat the sampling several times and evaluate the dimensionless normalized ensemble

averages [63]:

$$\mathbf{b}_\ell^\mu \equiv \frac{\langle b_\ell^\mu \rangle}{\sum_{\ell=1}^{N-1} \langle b_\ell^\mu \rangle}, \quad \ell = 1, \dots, N-1. \quad (5)$$

According to the definition (5), they implicitly depend on the initial state. Also, b_ℓ decreases with μ and there is no clear indication of the transition, if we do not normalize as in (5); see Supplemental Material H for the raw data.

When $\mu = 0$ (GOE), there is no dependence on the initial state as all different initial states are related by $O(N)$ rotations that do not affect the distribution. The analytical expression for the ensemble average of b_ℓ (5) reads [64]

$$\langle b_\ell^{\mu=0} \rangle = \frac{\Gamma(\frac{N-\ell+1}{2})}{\sqrt{2}\Gamma(\frac{N-\ell}{2})}. \quad (6)$$

The limit $\mu \rightarrow \infty$ corresponds to the integrable ensemble with a Poisson distribution of the Hamiltonian's eigenvalues level spacing and vanishing Lanczos coefficients. However, the Lanczos coefficients averages (5) for a finite number M of sampled Hamiltonians (3) in the integrable regime $\mu \geq \sqrt{M}$ exhibit a uniform LCD, as explained and verified numerically in Supplemental Material D.

The distribution $\mathbf{b}_\ell^\mu$ has a compact support since $l \leq N$, which will be important for quantifying the differences between its various moments as diagnostics of the transition. Note that one can also take the continuum limit of the distribution as the infinite limit of l and N keeping $x = \frac{l}{N}$ fixed [65], but we will work with the discrete LCD.

Based on the distribution $\mathbf{b}_\ell^\mu$, we can study different observables that capture the complexity of the system as a function of μ , such as the (normalized) moments of the distribution,

$$\mathbb{E}_k^\mu := \sum_{\ell=1}^{N-1} \left(\frac{\ell}{N}\right)^k \mathbf{b}_\ell^\mu, \quad (7)$$

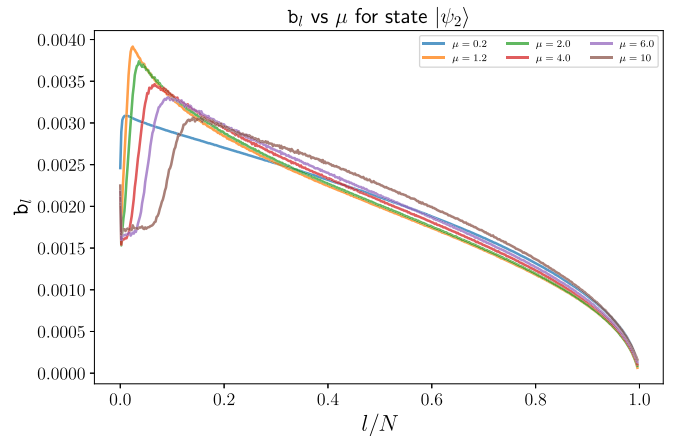


FIG. 1. The LCD $\mathbf{b}_\ell^\mu$ corresponding to the state $|\psi_2\rangle$ for various values of μ . Here the different colors represent different μ values rather than initial states. We see that the main difference is at low $\frac{l}{N}$. A detailed error analysis is shown in Supplemental Material E.

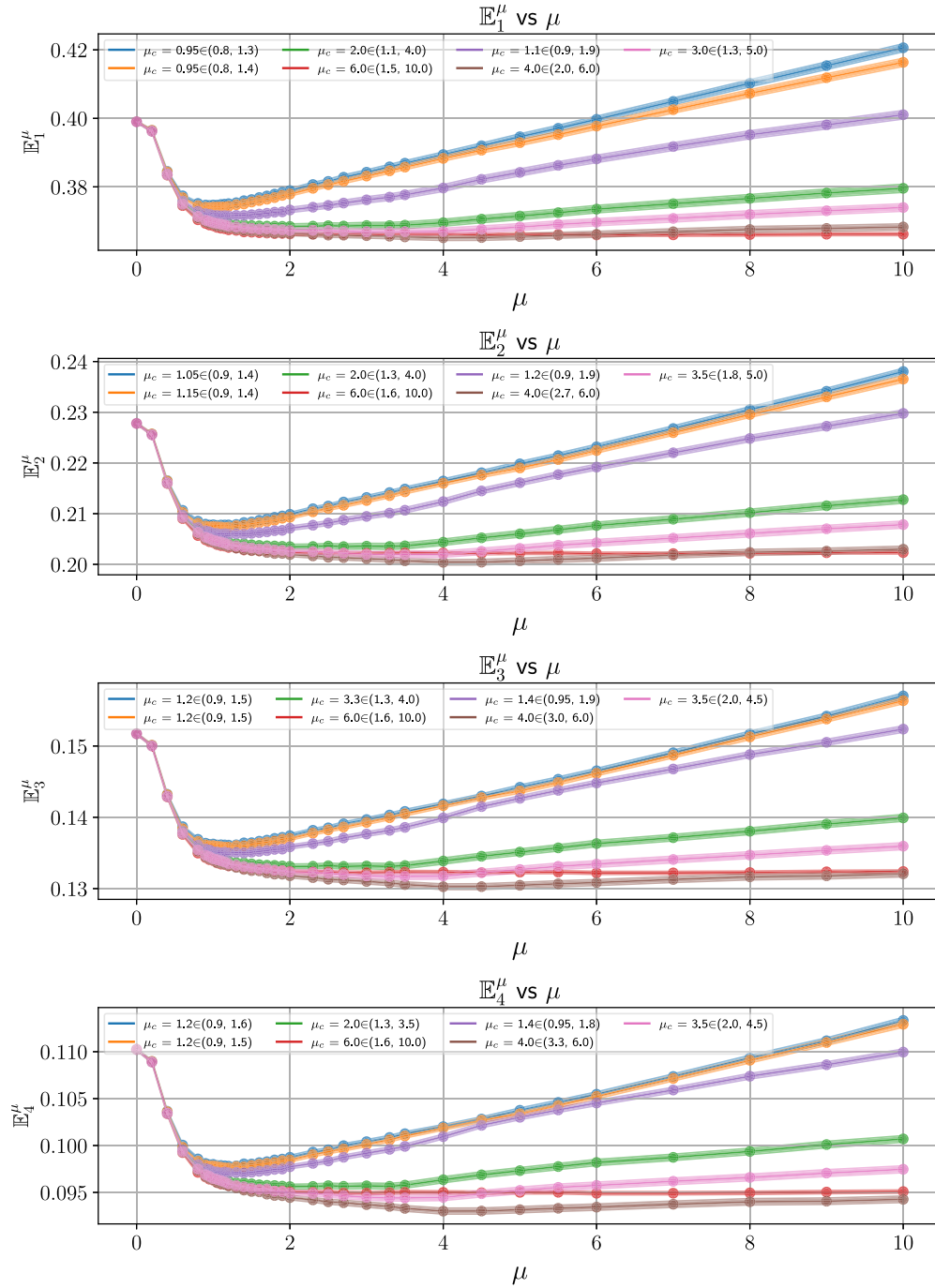


FIG. 2. The first four LCD moments across different μ values and initial states with error bars. We see the transition from the ergodic to MBL phase, as well as the memory of the initial state at the MBL phase and the memoryless ergodic phase.

and the Rényi entropy,

$$\mathbb{H}_\alpha^\mu := \frac{1}{1-\alpha} \log \sum_{\ell=1}^{N-1} [\mathbf{b}_\ell^\mu]^\alpha, \quad (8)$$

which in the $\alpha \rightarrow 1$ limit is the Shannon entropy:

$$\mathbb{H}^\mu := - \sum_{\ell=1}^{N-1} \mathbf{b}_\ell^\mu \log \mathbf{b}_\ell^\mu. \quad (9)$$

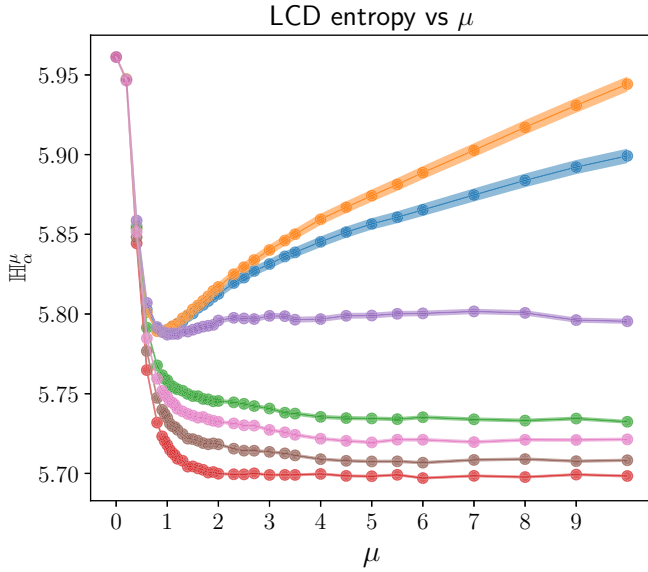


FIG. 3. The LCD Rényi entropy (8) evaluated at $\alpha = 10$ across different μ values and initial states. We see the transition and the initial state dependence of the MBL phase.

PRBM numerical simulations: Initial states. We have chosen seven typical normalized initial states to run the numerical simulations [66]. They include

$$\begin{aligned}
 |\psi_1\rangle &= (1, 0, 0, \dots, 0)^\top, \\
 |\psi_2\rangle &= \frac{1}{\sqrt{2}}(1, 0, 0, \dots, 0, 1)^\top, \\
 |\psi_3\rangle &= \frac{1}{\sqrt{N/4}} \underbrace{(1, 1, \dots, 1)}_{N/4 \text{ times}}, \underbrace{(0, \dots, 0)}_{3N/4 \text{ times}}^\top, \\
 |\psi_4\rangle &= \frac{1}{\sqrt{N/2}} \underbrace{(1, 1, \dots, 1)}_{N/2 \text{ times}}, \underbrace{(0, \dots, 0)}_{N/2 \text{ times}}^\top, \\
 |\psi_5\rangle &= \frac{1}{\sqrt{3N/5}} \underbrace{(1, 1, \dots, 1)}_{3N/5 \text{ times}}, \underbrace{(0, \dots, 0)}_{2N/5 \text{ times}}^\top, \\
 |\psi_6\rangle &= \frac{1}{\sqrt{3N/4}} \underbrace{(1, 1, \dots, 1)}_{3N/4 \text{ times}}, \underbrace{(0, \dots, 0)}_{N/4 \text{ times}}^\top, \\
 |\psi_7\rangle &= \frac{1}{\sqrt{N}}(1, 1, \dots, 1)^\top.
 \end{aligned} \tag{10}$$

These states have different structures of zero and one entries, which will be reflected in the LCD distribution of the MBL phase that keeps a memory of the initial state.

LCD. For any finite-dimensional Hilbert space, the iteration process (1) must terminate, so the LCD is a probability distribution with a compact support, $\ell/N \in [0, 1]$. In Fig. 1, we plot the LCD for $|\psi_2\rangle$ with six different values of μ (see also Figs. 9 and 10 in Supplemental Material B for the LCD of the other initial states). These values are selected to be before, match, and after the identified transition at $\mu_c \simeq 1.2$. We observe that the difference between the distributions at different μ comes mainly from the small ℓ/N range, while power-law tail region $\ell/N \sim 1$ is quite similar and state

independent. This structure of the LCD implies that while different moments can diagnose the transition, the low moments which are more sensitive to the small ℓ/N region have a memory of the initial state feature of the MBL phase; see Figs. 9 and 10 in Supplemental Material B for more details. In the literature, it is generally argued that the behavior of the large ℓ Lanczos coefficients b_ℓ quantifies the difference between integrable and chaotic systems. We see from the LCD distribution that, in fact, the small ℓ Lanczos coefficients are more effective diagnostics of this.

LCD moments and entropy. The first four moments of the LCD, along with the LCD entropy, are presented in Figs. 2 and 3, respectively. To enhance visual coherence, we have colored all initial states and ensured that the color of each initial state matched the color of the corresponding data points across all plots.

In both cases, the qualitative behavior exhibits notable similarities. For the case where $\mu < \mu_c \simeq 1.2$, the physical system exhibits a property of state independence: the LCD moments, as well as the LCD entropy, are identical for various initial states. The situation changes when $\mu > \mu_c$; here, the LCD moments and the LCD entropy begin to show a dependence on the initial states. This distinction can be understood in terms of the ergodicity of the physical system. Specifically, when the system is in the ergodic phase, which occurs before the transition at $\mu_c \simeq 1.2$, it remains unaffected by its initial state, as for the standard GOE ensemble case. However, after the transition, as μ exceeds μ_c , the system enters a nonergodic phase and the data starts to depend on the initial state. In this phase, the eigenstates' level spacing follows a semi-Poisson distribution. Consistent with the expectations for a gradual transition, the behavior of the moments post-transition varies depending on the chosen initial state.

Beyond the critical value $\mu_c \approx 1.2$, in the nonergodic regime, the system undergoes a nonsharp phase transition to the Poisson distribution and transitions into an

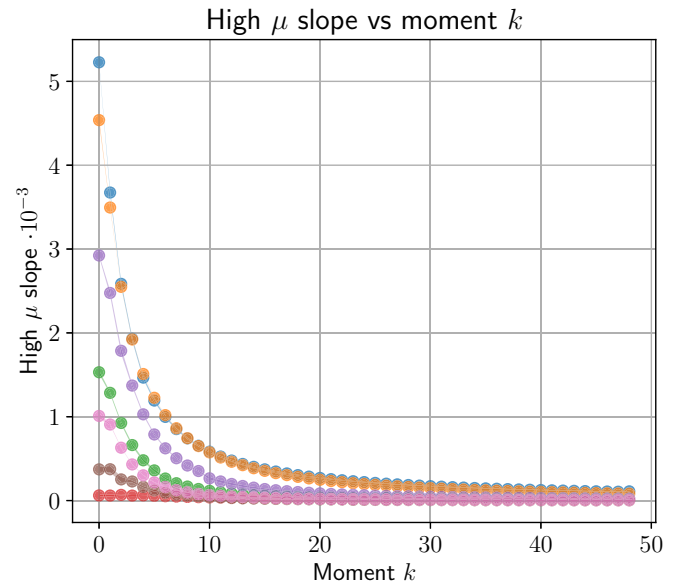


FIG. 4. The large μ slope function as the function of the k th moment. We see that the saturation values depend on the initial state.

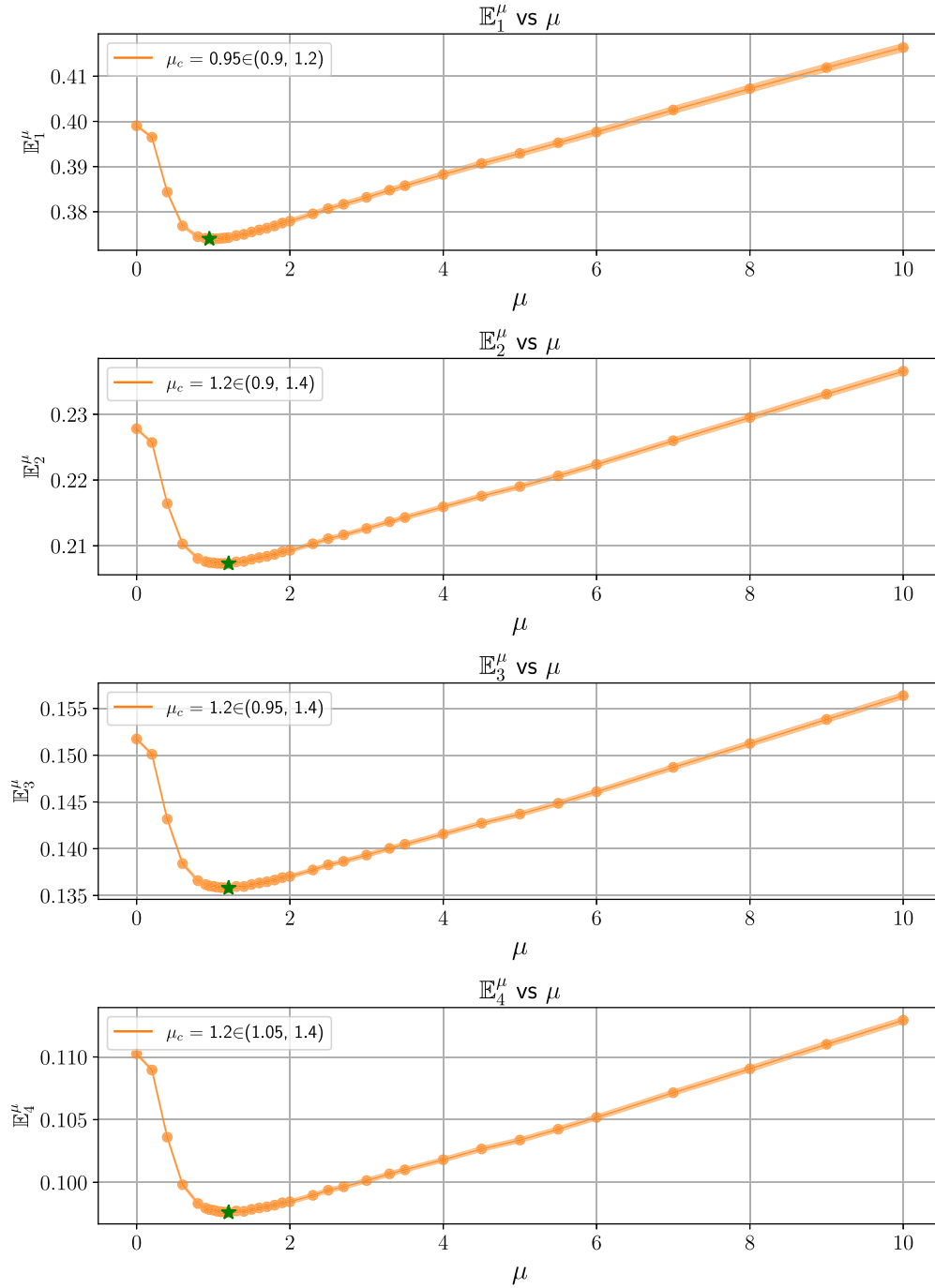


FIG. 5. The first four LCD moments as a function of μ for the state $|\psi_2\rangle$ defined in (10).

intermediate phase, as found in Refs. [67,68]. In this phase, the level-spacing statistics of the system follow a semi-Poisson distribution. Consistent with the expectations for such a nonsharp transition, the behavior of the moments' posttransition varies depending on the chosen initial state. For the initial states $|\psi_1\rangle$, $|\psi_2\rangle$ and $|\psi_3\rangle$, both the LCD moments and the LCD entropy begin to show linear growth. Conversely, for the other remaining initial states $|\psi_4\rangle$, $|\psi_5\rangle$, $\dots$, $|\psi_7\rangle$, both the LCD moments and the LCD entropy initially show a stable plateau before transitioning to linear growth. The width of the plateau and the slope of the initial growth depend on the initial state.

Initial state dependence. To study these dependencies on the initial states qualitatively, we need to relate the width and the slope to a physical observable that characterizes the initial states. A relevant physical observable that characterizes the spreading of a state is given by the inverse participation ratio (IPR), defined as

$$\text{IPR}(\psi) = \sum_{i=1}^N \|\psi_i\|^4, \quad (11)$$

where we have assumed that the normalized state $|\psi\rangle$ has N components, each denoted by ψ_i . By looking at the large

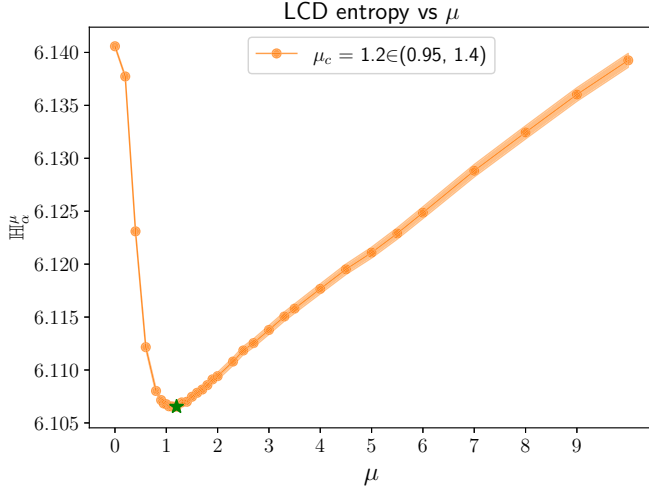


FIG. 6. The LCD Shannon entropy as a function of μ for state $|\psi_2\rangle$ defined in (10).

μ region, we conclude that the large μ asymptotic moments are proportional to the IPR of the corresponding initial state, where, for our chosen initial states (10), the IPR is given by the total number of nonvanishing components. The slope of the region is depicted in Fig. 4 and we see in the large k limit they all fit into the functional form $c_0/(k + c_1) + c_2$, where the constants c_j depend on the initial state.

For the LCD entropy, the dependence is more complicated and the endpoint values are not ordered by the IPR. The dominance of the $|\psi_2\rangle$, which is the only entangled state in all the candidate states, suggests that the entanglement structure of the state also plays a role. For the remaining product states, their endpoint values correlate proportionally with the IPR of the state, similarly to the moments. For results of the Rényi entropy for different α 's, refer to Supplemental Material F.

Transition region. Having understood the state dependence, we now undertake a more detailed examination of the LCD moments. For the sake of simplicity, throughout our analysis, we will focus on the initial state $|\psi_2\rangle$. In Figs. 5 and 6, we present the first four LCD moments and the Shannon entropy for $|\psi_2\rangle$, calculated with an enlarged ensemble size of $M = 190\,200$. We observe that an increase in the size of this order ensures the stabilization of numerical errors. Our findings indicate that, except for the first moment, the minima of all moments, as well as the Shannon entropy, are located at $\mu_c \approx 1.2$. The minimum of the first moment deviates from this value, but is still within the error bars of $\mu_c \approx 1.2$, as analyzed in Supplemental Material E. Thus, we cannot decide with certainty whether the ergodic-MBL transition takes place as a point or whether there is a transition region [61].

For $|\psi_2\rangle$, as there is no plateau region beyond the transition point, we can fit the scaling of the moments near the phase transition point $\mu_c \simeq 1.2$ as

$$\mathbb{E}_k^\mu = \mathbb{E}_k^{\mu=\mu_c} + \alpha_k(\mu - \mu_c)^2 + \mathcal{O}((\mu - \mu_c)^2), \quad (12)$$

and the result is presented in Fig. 7. We see that $\alpha_k \sim 1/k$ for $k \gg 1$. The error in Fig. 7 is smaller for higher moments,

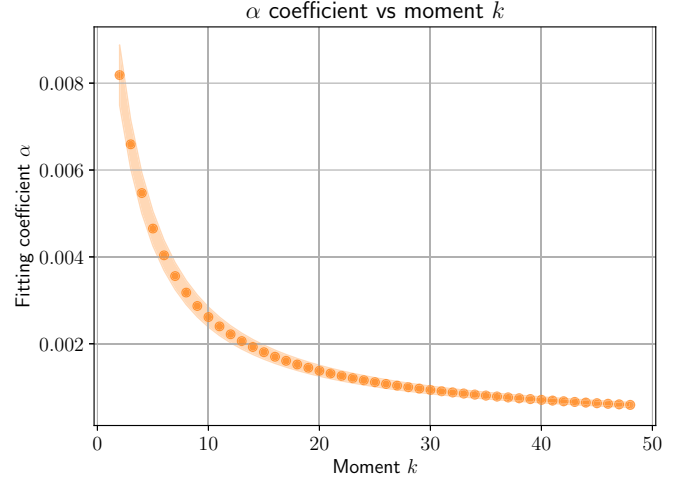


FIG. 7. The coefficient α_k (12) around the critical point $\mu_c \simeq 1.2$ versus different moments. Because of the different location of the minimal point, the first moment was not taken into account in the plot.

which is consistent with our observation that the tail region dominates the higher moments.

Discussion. The classification of phases of matter requires the introduction of effective diagnostics that distinguish between the different phases. In this Letter, we considered the transition between the ergodic and many-body localization phases and proposed diagnostics of the transition, which are based on complexity measures. We defined the probability distribution function of the Lanczos coefficients of the tridiagonalized Hamiltonian of the system and used these complexity measures to analyze the power-law random banded matrix model as a function of the correlation strength.

We showed that the moments and entropy of the distribution diagnose the ergodic to many-body transition as well as the distinctive feature of the phases concerning the memory of the initial conditions. The low moments, which are more sensitive to the small ℓ/N region, have a memory of the initial state feature of the MBL phase, and hence the small ℓ Lanczos coefficients are more effective diagnostics of this. We found that the LCD distribution has a power-law tail and a compact support, thus the higher moments localize in the same region of Lanczos coefficients and exhibit a similar structure. Our analysis allows within the error bars also the possibility that the ergodic-MBL transition does not happen at a sharp point $\mu = \mu_c$, but rather that there exists a transition region.

Our Letter opens up another avenue of using complexity measures in the study of different types of phase transitions at zero and nonzero temperatures, including quantum phase transitions, order-disorder transitions, and confinement-deconfinement phase transitions in quantum field theories and holography. It would also be interesting to compare our complexity diagnostics to other proposed criteria for quantum many-body integrability and chaos, see, e.g., Ref. [69].

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- Unless specified otherwise, the data points colored in blue, orange, purple, green, pink, brown, and red correspond to the initial states $|\psi_1\rangle, \dots, |\psi_7\rangle$, respectively, as defined in (10). The matrix size is $N = 500$ and the ensemble consists of $M = 9600$ samples.
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