Finite-size scaling of eigenstate thermalization

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According to the eigenstate thermalization hypothesis (ETH), even isolated quantum systems can thermalize because the eigenstate-to-eigenstate fluctuations of typical observables vanish in the limit of large systems. Of course, isolated systems are by nature finite, and the main way of computing such quantities is through numerical evaluation for finite-size systems. Therefore, the finite-size scaling of the fluctuations of eigenstate expectation values is a central aspect of the ETH. In this work, we present numerical evidence that for generic non-integrable systems these fluctuations scale with a universal power law $D^{-1/2}$ with the dimension $D$ of the Hilbert space. We provide heuristic arguments, in the same spirit as the ETH, to explain this universal result. Our results are based on the analysis of three families of models, and several observables for each model. Each family includes integrable members, and we show how the system size where the universal power law becomes visible is affected by the proximity to integrability.

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I. INTRODUCTION

In recent years, non-equilibrium unitary evolution of isolated quantum systems has emerged as a key topic in many-body physics. In this context, the issue of thermalization in isolated quantum systems has received fresh and growing attention. The eigenstate thermalization hypothesis (ETH) is widely thought to encapsulate the mechanism by which thermalization occurs in isolated non-integrable systems [1–3].

The basic statement of the ETH is that, for a large isolated system, the diagonal matrix elements of typical observables in the Hamiltonian eigenstate basis, known as the eigenstate expectation values (EEVs), depend smoothly on the corresponding energy eigenvalues. Despite intense recent research [3–20], understanding of several aspects of the ETH remains incomplete. For example, it is not fully known exactly which observables will or will not serve as “typical” observables. Another issue is the specification of “large” isolated systems — how large does the system have to be? Clearly, a proper understanding of this question requires a finite-size scaling study of the ETH. This is an important question for any actual experimental study of thermalization, because any isolated system is in practice finite. Size dependence is also vital for evaluating numerical studies, which are performed on finite systems. This is the subject of the present manuscript.

It is generally understood that the fluctuations ($\sigma_{\Delta A}$) of EEVs should decrease exponentially with system size [1, 8, 10, 20], so that the EEVs become very smooth as a function of energy for reasonably large isolated systems. For discrete systems with a finite Hilbert space, this means a power-law dependence of the fluctuations with the dimension $D$ of the Hilbert space. In this work, we identify the exponent of this power-law behavior as $-1/2$. Examining several non-integrable models, we provide strong numerical evidence for $D^{-1/2}$ behavior of EEV fluctuations. The $D^{-1/2}$ behavior generally becomes clear only at the largest sizes accessible through full numerical diagonalization. Our analysis therefore uses a comparison of several sizes, at varying distances from integrability. We use Hamiltonians designed to be tunable between two integrable limits, and thus examine how this finite-size dependence is affected by proximity to integrable points. As the integrable points are approached, larger sizes are required for the $D^{-1/2}$ behavior to set in, and for purely integrable systems the size dependence is no longer $D^{-1/2}$.

The exponent $-1/2$ suggests the central limit theorem, which would predict power-law dependences if $\sigma_{\Delta A}$ is the average of $O(D)$ random variables. We distinguish between two plausible mechanisms, and identify the correct explanation: The exponent arises from the averaging over effectively random coefficients of individual eigenstates, and not from an average over $O(D)$ eigenstates in the definition of $\sigma_{\Delta A}$. This explanation relies on assumptions of effective randomness which are difficult to prove rigorously, but are in the same spirit as the ETH itself. A particularly nontrivial aspect is that it is not immediately obvious why this argument should break down for integrable systems. While the concept of effective randomness provides useful insight, the unavoidably heuristic nature of such arguments means that our numerical analysis is essential for determining the finite-size scaling of EEV fluctuations.

We use several observables for each model Hamiltonian, to show the validity of the $D^{-1/2}$ law for a wide variety of observables. Unlike some of the previous studies of the ETH (e.g., [3]), we do not refer to particular quench protocols, which corresponds loosely to focusing on particular parts of the eigenspectrum. Instead, we examine the complete spectrum, and thus a broad class of quantum quenches. The robustness of our results for different observables, Hamiltonians, and quench protocols, provides compelling evidence for the universality of the $D^{-1/2}$ scaling.

The structure of this article is as follows. In Sec. II, we introduce our measure for the amplitude of EEV fluctuations. We define our models and observables in Sec. III. The $D^{-1/2}$ scaling of the EEV fluctuations is presented in Sec. IV, where we give both numerical results and a heuristic argument. The conclusion and discussion appears in Sec. V. The Appendices provide further details: App. A discusses issues related to our definition of the EEV fluctuations, App. B elaborates on the heuristic argument for $D^{-1/2}$ scaling, and App. C provides detail on the numerical methods.
II. FORMULATION; EEV FLUCTUATIONS

The ETH states that the diagonal matrix element of a typical operator $\hat{A}$ in the eigenstates $|\psi_\alpha\rangle$ of the Hamiltonian, i.e., the EEVs $A_{\alpha\alpha} = \langle \psi_\alpha | \hat{A} | \psi_\alpha \rangle$, vary smoothly with the corresponding energy eigenvalues $E_\alpha$. Thus, the EEVs may be considered as constant within an energy window $[E - \Delta E, E + \Delta E]$. In other words, the values of $A_{\alpha\alpha}$ approximately coincide with the microcanonical average $\langle \hat{A} \rangle_\mu(E_\alpha, \Delta E)$, defined as the average EEV within this window:

$$\langle \hat{A} \rangle_\mu(E_\alpha, \Delta E) = \frac{1}{N_{E,\Delta E}} \sum_{\alpha : E_\alpha \in [E - \Delta E, E + \Delta E]} A_{\alpha\alpha},$$

where $N_{E,\Delta E}$ is the number of states in this window. If the initial non-equilibrium state has weights constrained to such a "microcanonical" window, then the ETH guarantees that the long-time average will be equal to the canonical expectation value.

We wish to study how this behavior is approached with increasing system size. Therefore we study the fluctuations around the microcanonical average as a function of size. For every $\alpha$, we define $\Delta A_\alpha = A_{\alpha\alpha} - \langle \hat{A} \rangle_\mu(E_\alpha, \Delta E)$. We then consider the statistical properties of $\Delta A_\alpha$ over a large part of the Hilbert space. In the following, we take averages over all states in the central 20% of the total energy range of the spectrum, which we denote by $\langle \cdot \cdot \rangle_c$. This average typically includes more than half of all eigenstates. The highest and lowest end of the spectrum are left out because the spectrum edges are likely to show atypical behavior, cf. Fig. 1. The EEV fluctuations $\sigma_{\Delta A}$ are defined as the standard deviation of $\Delta A$,

$$\sigma_{\Delta A}^2 \equiv \langle (\Delta A_\alpha)^2 \rangle_c \equiv \langle (A_{\alpha\alpha} - \langle \hat{A} \rangle_\mu(E_\alpha, \Delta E))^2 \rangle_c.$$  

(2)

We note that $\sigma_{\Delta A}$ cannot be interpreted as a standard deviation of the $A_{\alpha\alpha}$, because of the microcanonical average $\langle \cdot \cdot \rangle_c$ rather than the ordinary average $\langle \cdot \cdot \rangle$ on the right-hand side of Eq. (2). In the definition above we have assumed that the average of $\Delta A$ is negligible, i.e., that

$$\text{var}(\Delta A_\alpha) \equiv \langle (\Delta A_\alpha)^2 \rangle_c \approx \langle \Delta A_\alpha^2 \rangle_c.$$  

(3)

While the smallness of $\Delta A_\alpha$ is intuitively reasonable, the definition of $\Delta A_\alpha$ in terms of the microcanonical average does not guarantee a priori that

$$\langle \Delta A_\alpha^2 \rangle_c \ll \langle \Delta A_\alpha^2 \rangle_c$$  

(4)

is valid. Numerical evidence for the validity of this inequality is presented in App. A. Given that this condition holds, the interpretation of $\sigma_{\Delta A}$ defined in Eq. (2) as a standard deviation of $\Delta A$ is justified.

In Fig. 1, the energies are divided by the system size $L$. The reason is that the upper and lower parts of the energy spectrum scale as $L$, thus the spectrum appears in the same range of $E_\alpha/L$. The microcanonical average curves for the EEVs also look roughly similar for different sizes, when plotted against $E_\alpha/L$, as does the density of states.

The dependence of $\sigma_{\Delta A}$ on the width $\Delta E$ of the microcanonical window is weak, as long as the range $[E - \Delta E, E + \Delta E]$ contains sufficiently many states for good statistics while it remains sufficiently narrow so that the microcanonical average follows the EEVs well. As a good tradeoff for satisfying both these conditions, we have used the value $\Delta E = 0.025L$ for all following results. Justification for this value can be found in App. A. As with the horizontal axes in Fig. 1, we rescale the window width by keeping $\Delta E/L$ constant. This window thus contains approximately equal fractions of the total number of eigenstates for different values of $L$.

III. MODELS AND OBSERVABLES

A. Tunable model Hamiltonians

We will present results for three families of Hamiltonians. These are designed to be tunable toward or away from integrable limits, to have good thermodynamic limits, and to avoid symmetries that lead to degeneracies in the spectrum. We use systems with a Hamiltonian of the form $H = H_0 + \lambda H_1$, such that the model is integrable if the control parameter $\lambda$ is 0 or $\infty$. For $\lambda \in (0, \infty)$, the system is non-integrable.

The first two are based on the spin-$^{1/2}$ anisotropic Heisenberg (XXZ) chain, which is integrable via the Bethe ansatz [21]. These Hamiltonians commute with the total $z$-component of spin, so that the number $N_T$ of ‘up’ spins is conserved. We examine finite-size scaling by increasing $(L, N_T)$. To suppress unwanted symmetries, e.g., SU(2), we take the anisotropy $\Delta$ to be away from 0 or 1; results are presented for $\Delta = 0.8$.

The Heisenberg ladder consists of two coupled XXZ chains (see Fig. 1, inset). The Hamiltonian for the $L = (2p + 1)$-site

$$(L, N_T) = (11, 5) \quad (L, N_T) = (15, 7) \quad (L, N_T) = (19, 9)$$

$\lambda = 0 \quad \lambda = 1 \quad \lambda = 0.5$
model is given by $H_{\text{ladder}} = H_{\text{leg}} + \lambda H_{\text{rung}}$, where

$$H_{\text{leg}} = \sum_{i=1}^{p-1} h_{i,i+1} + \sum_{i=p+1}^{2p} h_{i,i+1} \quad \text{and} \quad H_{\text{rung}} = \sum_{i=1}^{p} h_{i,i+p},$$

are the intrachain and interchain (rung) couplings, respectively, given in terms of the Heisenberg XXZ coupling

$$h_{i,j} \equiv \frac{1}{2}(S_{i}^{+}S_{j}^{-} + S_{i}^{-}S_{j}^{+}) + \Delta S_{i}^{z}S_{j}^{z},$$

where $S_{i}^{\pm} = S_{i}^{x} \pm iS_{i}^{y}$ and $S_{i}^{z}$ are the spin operators on site $i$ ($\hbar = 1$). In order to suppress reflection symmetries, one leg has an extra site compared to the other. We will focus on the $S_{i}^{z}$ sector of filling factor $\lambda B_{i}$ respectively, given in terms of the Heisenberg XXZ coupling $\lambda B_{i}$.

The second Hamiltonian is the $XXZ$ chain in a harmonic magnetic trap, $H_{\text{trap}} = H_{\text{XXZ}} + \lambda H_{\text{magn}}$, with the open-XXZ-chain and magnetic-field terms,

$$H_{\text{XXZ}} = \sum_{i=1}^{L-1} h_{i,i+1} \quad \text{and} \quad H_{\text{magn}} = -\sum_{i=1}^{L} B_{i}S_{i}^{z},$$

respectively. Here, $\lambda B_{i}$ denotes the magnetic field at site $i$ where $\lambda$ parametrizes the strength of the trap, and $B_{i} = [2/(L - 1)^2]|i - i_{0}|^{2}$. Here the trap center is near the midpoint of the chain, $i_{0} = \frac{1}{2}(L + 1) - \Delta L$, with a shift $\Delta L$ that we choose to be irrational to avoid symmetries. The factor $2/(L - 1)^2$ ensures a meaningful thermodynamic limit. We use the sector of filling factor $\frac{1}{2}$ by defining $L = 3N_{f}$. A harmonic trap is a particularly important manner of breaking integrability, since the classic experiment exploring the role of integrability in time evolution [22] involved dynamics in a harmonic trap.

The third Hamiltonian is the Bose-Hubbard model on an open chain,

$$H_{\text{BH}} = -\sum_{i=1}^{L-1} (b_{i}^{\dagger}b_{i+1} + b_{i+1}^{\dagger}b_{i}) + \lambda \sum_{i=1}^{L} b_{i}^{\dagger}b_{i}b_{i}^{\dagger}b_{i},$$

where $b_{i}^{\dagger}$ and $b_{i}$ are the bosonic creation and annihilation operators at sites $i$ [23]. The model is integrable when only kinetic or only interaction terms are present, i.e., in the $\lambda = 0$ and $\lambda \rightarrow \infty$ limits. We avoid reflection symmetry by modifying the interaction at site 1 to be $1.1\lambda \lambda$ instead of $\lambda$. We present results for half filling, i.e., the number of bosons is $N_{b} = \frac{1}{2}L$.

B. Observables

An important issue in ETH studies is the question of which observables the ETH applies to. To show that our main result ($\sigma_{\Delta \lambda} \sim D^{-1/2}$ behavior) is valid for a wide range of observables, we use a number of different one-site and two-site observables. For the ladder model, we use the spin $z$-component $S_{i}^{z}$ at site $i$ and sums of these quantities with $i$ running over multiple sites, e.g., all sites of the bottom leg $S_{\text{bottom}}^{z}$. We also consider the two-site operators $C_{i,j} \equiv S_{i}^{z}S_{j}^{z}$, and sums of such operators over regions of the system. We similarly study a set of one- and two-site operators and their sums over regions of the system for the XXZ chain in a trap and for the Bose-Hubbard model: For the XXZ chain, we consider one-site (e.g., $S_{i}^{z}$) and two-site spin operators (e.g., $C_{i,j} = S_{i}^{z}S_{j}^{z}$ and $C_{i,j}^{xy} = S_{i}^{x}S_{j}^{x} + S_{i}^{y}S_{j}^{y}$) and their sums over the middle one-site terms ($S_{i}^{\text{middle}}$, $C_{i}^{\text{middle}}$, and $C_{i,j}^{\text{middle}}$). For the Bose-Hubbard model, we use on-site occupancies $n_{i} = b_{i}^{\dagger}b_{i}$, occupancies summed over the central sites $[n_{i}^{\text{middle}} = \sum_{i'=i+1}^{L-i'} n_{i'}/(L - 2i')]$ with $i' = [(L + 2)/4]$), and the operators for nearest neighbor two-point and four-point correlators ($b_{i}^{\dagger}b_{i+1} + b_{i+1}^{\dagger}b_{i}$ and $n_{i}n_{i+1}$).

IV. SCALING ANALYSIS OF EEV FLUCTUATIONS

A. Dependence on size and integrability

Figures 1 and 2 provide visual displays of some of the more dramatic aspects of the ETH.

In Figure 1, we use as observable $S_{i}^{z}$, the $z$ component of the spin at site $i = 2$. At the integrable point, the width of the distribution of EEVs can be seen to stay unchanged with system size (top row). For the non-integrable model, the EEV fluctuations clearly decrease with system size in the bulk of the spectrum. The top and the bottom of the spectrum do not show a similarly dramatic decrease with system size, demonstrating that the ETH should be considered relevant primarily to the bulk of the spectrum. The physical reason is that the edges of the spectrum tend to show emergent integrable (e.g., Luttinger liquid) behavior.

Figure 2 shows the typical dependence of EEV fluctuations on the parameter $\lambda$ for different system sizes. This plot corroborates the intuition that for increasing system size the fluctuations decay faster away from the integrable limits than close to them. For larger systems there is a pronounced minimum of $\sigma_{\Delta \lambda}$ at intermediate $\lambda$, where it is farthest from both integrable limits.

For the observable $\hat{A} \equiv S_{\text{bottom}}^{z}$ in the ladder system, Fig. 2(b), $\sigma_{\Delta \lambda}$ is smaller in the $\lambda \sim 1$ regime than it is in the integrable regions, even for the smallest system sizes. For the observable $\hat{A} \equiv C_{2,p+2}^{z} = S_{2,p+2}^{z}$, Fig. 2(a), some deviation is seen for very small systems, but the characteristic behavior...
sets in already at moderate sizes. This overall qualitative behavior is very typical, and is similar for all observables and all models we have investigated. The system size at which the crossover to large-system behavior (pronounced minimum in the non-integrable regime) takes place depends on the model and on the observable.

B. Scaling with system size

In Fig. 3(a–c), we show the dependence of the EEV fluctuations on Hilbert-space size \(D\), for several values of the rung coupling parameter \(\lambda\) that tunes the system away from integrability. The data plotted in this figure involves vertical slices of the plots in Fig. 2 (size-dependence at constant \(\lambda\) values). The ETH fluctuations are commonly claimed to decrease exponentially with system size for non-integrable models, and hence should decrease as a power law with \(D\). We define an "exponent" \(e\) as the one that is obtained in a power-law fit, \(\sim D^{-e}\), to the data for \(\sigma_{\Delta A}\) for the available sizes. We make no a priori claims about the dependence being actually a power law, or the obtained values of \(e\) being the actual exponent in the large-size limit. In cases where the dependence is a power law, as expected in non-integrable systems, \(e\) is an estimator for the actual exponent. The exponent estimator \(e\) goes toward zero as one approaches the integrable points \(\lambda = 0\) or \(\lambda = \infty\). At the point \(\lambda = 0\) the dependence on \(D\) is presumably not even a power law.

Values of the exponent estimator \(e\) are plotted in Fig. 3(d,e) for the ladder system and in Fig. 4 for the XXZ-trap system and the Bose-Hubbard system. There is a clear and general trend for \(e\) to cluster around or approach 0.5 in all systems, when away from integrability. Taken together, we believe this provides compelling evidence of \(\sigma_{\Delta A} \sim D^{-1/2}\) dependence in generic non-integrable systems for generic few-body observables \(\hat{A}\). Figure 3(d) displays the general behavior for several different observables in the XXZ ladder: \(e \approx \frac{1}{2}\) for intermediate \(\lambda\) and vanishing \(e\) for \(\lambda\) approaching 0 or \(\infty\). Similar behavior is observed for the XXZ chain with a trap and for the Bose-Hubbard chain, see Figs. 4(a) and (c), respectively. For the three systems considered here, the results are qualitatively similar. The general trend is that for a fixed maximum system size \(L_{\text{max}}\), the exponent estimator \(e\) clusters around \(\frac{1}{2}\) for intermediate values of \(\lambda\), and has lower values close to the integrable limits. In Figs. 3(e), 4(b) and 4(d), we show more quantitative scaling behavior for the three tunable Hamiltonians, by plotting the exponent estimators \(e\) derived from power-law fits to the data of system sizes up to \(L_{\text{max}}\). We note a crossover from integrable-like to \(\sim D^{-1/2}\) behavior for non-integrable systems close to integrability [e.g., for the XXZ ladder at \(\lambda = 0.05\); see Figs. 3(b) and (e)], as the system size is increased. The trend with increasing \(L_{\text{max}}\) points to the large-system behavior of \(\sigma_{\Delta A}\) being \(\sim D^{-1/2}\) over the full range \(\lambda \in (0, \infty)\).

C. \(D^{-1/2}\) behavior from eigenstate size: A heuristic argument

The \(D^{-1/2}\) dependence of \(\sigma_{\Delta A}\) can be argued heuristically by considering projections of eigenstates onto the eigenbasis of the \(\hat{A}\) operator, and then invoking the central limit theorem. If \(\{\alpha_\gamma\}\) and \(\{|\phi_\gamma\}\) denote the eigenvalues and eigenvectors
of $\hat{A}$, and we expand the eigenvectors $|\psi_\alpha\rangle$ of $H$ as

$$|\psi_\alpha\rangle = \sum_\gamma c_\gamma^{(\alpha)}|\phi_\gamma\rangle$$  \hspace{1cm} (9)$$

then we can write the EEVs as

$$A_{\alpha\alpha} = \sum_{\gamma=1}^{D} |c_\gamma^{(\alpha)}|^2 a_\gamma.$$  \hspace{1cm} (10)$$

This is an average of $X_\gamma = D|c_\gamma^{(\alpha)}|^2 a_\gamma$. Under the hypothesis that the $X_\gamma$ can be regarded as random variables with $D$-independent variance, the central limit theorem guarantees that the fluctuations of $A_{\alpha\alpha}$ decrease as $D^{-1/2}$. (This argument is detailed further in App. B.) We are unable to prove the idea that $X_\gamma$ or $c_\gamma$ act as random variables. However, one can intuitively think of an eigenstate of a non-integrable system as being so complex that its projections onto the eigenbasis of a typical observable are effectively random. This is similar in spirit to the ETH itself (also difficult to prove rigorously), for which the argument is that when eigenfunctions are complex enough, EEVs of typical observables will contain no signature of the detailed structure of the wavefunction.

This argument relies on the assumption that the size (number of components) of the individual eigenvectors is $O(D)$. This is justified in Fig. 5(a,b) through the participation ratio (PR) in the computational (site) basis, defined for each eigenstate as

$$P_\alpha = \left[\sum_\gamma |c_\gamma^{(\alpha)}|^4\right]^{-1}.$$  \hspace{1cm} (11)$$

The PR measures the number of basis states contributing to the eigenstate. [For a single state, the commonly discussed inverse participation ratio (IPR) is $1/P_\alpha$.] Figure 5(b) shows that $P_\alpha$ is, on average, indeed proportional to $D$ in non-integrable cases. The $D^{-1/2}$ scaling of $\sigma_{\Delta A}$ and the $D$ scaling of the average $P_\alpha$ are, taken together, consistent with the expectation [17] that $\sigma_{\Delta A}^2$ should be proportional to the average inverse PR. The observations of Ref. [17], in terms of the average inverse PR in the momentum Fock basis, can also be cast as a heuristic argument for $D^{-1/2}$ scaling, roughly equivalent to the reasoning above.

We emphasize that the number $D_{\text{fluct}}$ of states included in the average $\langle \cdots \rangle_c$ does not account for the $D^{-1/2}$ dependence. The quantity $\sigma_{\Delta A}$ is the standard deviation of the distribution of the $D_{\alpha\alpha}$’s and it is independent of how many times one “probes” this distribution, i.e., the number of states that is used to compute $\sigma_{\Delta A}$. As shown in Fig. 5(c), the value of $\sigma_{\Delta A}$ is independent of $D_{\text{fluct}}$ as long as states at the edges of the spectrum are avoided. The slight dependence on $D_{\text{fluct}}$ is caused by the fact that at the edges of the spectrum, the fluctuations of $A_{\alpha\alpha}$ are different from those in the center of the spectrum. The edges of the spectrum, of course, are outside the purview of the ETH. This demonstrates that the $D^{-1/2}$ behavior arises not from the number of eigenstates averaged over, but from the complexity of the individual eigenstates themselves.

The fluctuations decrease more slowly with system size at the integrable points, as evidenced by the vanishing of the exponent estimator $\epsilon$ in the $\lambda \to 0$, $\infty$ limits in each of the models. This implies a difference in the structure of the individual eigenstates. One characterization of this difference is visible in Fig. 5(b) where the scaled average PR for the integrable model is seen to decrease with system size. A detailed study of eigenstates in integrable models from this perspective, to complement the studies of Refs. [18–20, 24–28], is interesting but is beyond the scope of the present work.

V. SUMMARY & DISCUSSION

For non-integrable systems, we have presented the size dependence of the deviation from ETH, as measured by the EEV fluctuations, $\sigma_{\Delta A}$, for lattice systems. It is well accepted that $\sigma_{\Delta A}$ decreases exponentially with the system size, $\sigma_{\Delta A} \sim \exp[-c_1 L]$, e.g., Ref. [20] has numerical data showing the exponential decay. In terms of the Hilbert-space size $D$, if $D \sim \alpha^{1/2}$ (see App. C 2), then

$$\sigma_{\Delta A} \sim D^{-\epsilon} \sim \exp[-e(\ln \alpha) L].$$  \hspace{1cm} (12)$$

Our work makes this relationship precise by determining the exponent to be $\epsilon = \frac{\alpha}{2}$, or equivalently, the coefficient to be $c_1 = \frac{1}{2} \ln \alpha$.

The $D^{-1/2}$ behavior is difficult to convincingly show from calculations for a fixed non-integrable Hamiltonian. We have therefore used a control parameter to move away from an integrable Hamiltonian; this makes clear the trend of $\epsilon$ approaching $\frac{1}{2}$ as one tunes away from integrability. In addition, the sizes at which the $D^{-1/2}$ behavior sets in are at the limit of sizes that can be comfortably addressed by full numerical diagonalization, which is the method used in current numerical studies of the ETH. Our use of sparse matrices with shift-and-invert algorithm (see App. C 1) has allowed us to reach larger sizes: we have used full diagonalization for sizes up to $D \sim 2 \times 10^4$, and sparse matrix methods for larger $D$, the largest being above $10^5$.

While the exponent $\epsilon = \frac{\alpha}{2}$ has not, to the best of our knowledge, appeared for the EEV fluctuations in the setting
of condensed-matter Hamiltonians, some similar or related results exist. The observations of Ref. [17] could be combined to construct an argument for $D^{-1/2}$ scaling, as discussed in IV C. In the literature on ‘typicality’ [29–33], there is the expectation that the deviation of random Hamiltonians from typicality (closely related to ETH) scales with system size such that measures of typicality behave as $\sim D^{-1/2}$. Ref. [30] shows this numerically for random Hamiltonians but finds other exponents for spin-chain Hamiltonians, for the sizes treated. Further work is needed for a full understanding of the connection between these results and ours.

Our work opens up several new questions. First, the $D^{-1/2}$ behavior does not set in at smaller sizes. It is obvious from Fig. 3(d,e) and Fig. 4 that larger sizes are necessary when integrability is weakly broken, since the $e$ values calculated from available sizes do not reach $\frac{1}{2}$ for $\lambda$ near the integrable points. This indicates a length scale associated with the degree of integrability breaking, a concept that might be possible to explore quantitatively. Second, our quantitative result $\sigma_{\Delta A} \sim D^{-1/2}$ requires a finite Hilbert-space dimension $D$. It is not obvious how to generalize this law to continuum systems. Finally, it would be interesting to ask how the finite-size behavior of EEVs is affected by proximity to (many-body) localization, which, like integrability, is expected to be detrimental for thermalization.

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Appendix A: EEV fluctuations: Definition issues

The width of the microcanonical window has been chosen to satisfy $\Delta E = 0.025 L$, as a good compromise between the conditions that it contain sufficiently many eigenstates for good statistics, and that the microcanonical average follows the EEVs well. To justify the choice of this value, we have plotted the fluctuation amplitudes $\sigma_{\Delta A}$ as a function of system size $D$ for several values of $\Delta E$ in Fig. 6(a). Here, we have chosen the observable $\hat{A} = S^z_{\text{middle}}$ for the trap system at $\lambda = 2$, which is characterised by a strongly nonlinear dependence of the microcanonical average $\langle A \rangle_{\mu}(E, \Delta E)$ on $E$. This situation is a worst-case scenario: We expect a relatively strong dependence of the resulting $\sigma_{\Delta A}$ on $\Delta E$, because for very large values, the microcanonical average does not follow the actual EEVs $A_{\alpha\alpha'}$ well. This mechanism is responsible for the fact that for very large values of $\Delta E$, the fluctuations are overestimated [see Fig. 6(a)]. In the case where $\langle A \rangle_{\mu}(E, \Delta E)$ would depend almost linearly on $\Delta E$, the dependence of $\sigma_{\Delta A}$ on $\Delta E$ would be weaker. Another feature that we find from Fig. 6(a) is that the fluctuations are underestimated if the number of states in the microcanonical average is very small, in the case of small $\Delta E$ and small system size. Finally, we may conclude from Fig. 6(a) that $\sigma_{\Delta A}$ is almost independent of $\Delta E$ for a large range of values around $\Delta E/L = 0.025$. Here, we emphasize that the values $\Delta E/L = 0.001$ and $\Delta E/L = 0.25$ present very extreme cases, where the microcanonical window encompasses only a few eigenstates (for the smaller system sizes) and almost the whole spectrum, respectively.

In order for the interpretation of $\sigma_{\Delta A}$, as defined by Eq. (2), as standard deviation of the $A_{\alpha\alpha'}$ to be valid, we must test the condition that the average of $A_{\alpha\alpha'}$ is negligibly small, expressed by Eq. (4). In Fig. 6(b), we plot the ratio $\langle \Delta A_{\alpha\alpha'}^2 \rangle_{c}/\langle \Delta A_{\alpha\alpha'}^2 \rangle_{c}$ for the observable $\hat{A} = S^z_1$ in the ladder system, as a function of the Hilbert space $D$ and for several values of $\lambda$. We indeed observe that $\langle \Delta A_{\alpha\alpha'}^2 \rangle_{c}$ is negligibly small compared to $\langle \Delta A_{\alpha\alpha'}^2 \rangle_{c}$. The approximation $\text{var}(\Delta A_{\alpha\alpha'}) \equiv \langle \Delta A_{\alpha\alpha'}^2 \rangle_{c} - \langle \Delta A_{\alpha\alpha'} \rangle_{c}^2 \approx \langle \Delta A_{\alpha\alpha'}^2 \rangle_{c}$ generally improves for increasing system size. Thus, the interpretation of $\sigma_{\Delta A}$ as standard deviation of the $A_{\alpha\alpha'}$ is justified.

Appendix B: Mechanism for $D^{-1/2}$ decay of EEV fluctuations

In this section, we expand on the argument provided in Sec. IV C for the $D^{-1/2}$ decay of EEV fluctuations. The $D^{-1/2}$ behavior arises from the fact that the individual eigenstates have $D$ components, and not from the sum over $\mathcal{O}(D)$ different eigenstates in the definition of $\sigma_{\Delta A}$.

$D^{-1/2}$ from randomness of coefficients — Our argument is based on the expansion of the energy eigenstates $|\psi_\gamma\rangle$ in the basis of eigenvectors $|\phi_\alpha\rangle$ (with eigenvalues $a_\alpha$) of the operator $\hat{A}$, as given by Eq. (9). The EEVs are then realizations of a random variable which is the average of $D$ approximately random variables,

$$A_{\alpha\alpha'} = \sum_{\gamma=1}^{D}|\phi_{\gamma}\rangle^\dagger|\phi_{\alpha}\rangle a_\alpha = \frac{1}{D} \sum_{\gamma=1}^{D} X_\gamma,$$

where $X_\gamma = D|\phi_{\gamma}\rangle^\dagger|\phi_{\alpha}\rangle a_\alpha$. We will now regard $X_\gamma$ as random, quasi-independent, variables. There is no rigorous justification for this, but it can be argued in the same spirit as the arguments in favor of the ETH itself, namely, in a large non-integrable system the typical eigenstate is so complicated that
its components are effectively random in any reasonable basis. In principle, the randomness of \( |c^{(\alpha)}_\gamma|^2 \) and of \( X_\gamma \) may be different, due to the multiplication with the eigenvalues \( a_\gamma \). However, if these eigenvalues take only very few (\( \ll D \)) different values, then \( |c^{(\alpha)}_\gamma|^2 \) is random if and only \( X_\gamma \) is.

Assuming that the \( X_\gamma \) act as random variables, the central limit theorem implies that the EEVs have the standard deviation \( \sqrt{\text{var}(X_\gamma)/D} \). If the variance of \( X_\gamma \) is approximately \( D \)-independent (as argued below), the \( D^{-1/2} \) dependence of the fluctuations follows immediately.

We emphasize again that our reasoning is based on the assumption that the \( |c^{(\alpha)}_\gamma|^2 \) are “random enough” that the central limit theorem can be used. The extent or exact nature of this randomness is not understood in detail, to the best of our knowledge. At or near integrability, \( \sigma_{\Delta A} \) no longer scales as \( D^{-1/2} \), which suggests that the coefficients \( |c^{(\alpha)}_\gamma|^2 \) lose their randomness in such situations.

Even in the non-integrable case, the assumption is invalid for any conserved quantity \( A \). If \( \hat{A} \) commutes with \( \hat{H} \), one can choose a common eigenbasis, and consequently only one \( c^{(\alpha)}_\gamma \) is nonzero.

\[ \text{var}(X_\gamma) \text{ is independent of } D \] — We now argue that the variance of \( X_\gamma = D|c^{(\alpha)}_\gamma|^2a_\gamma \) is independent of \( D \). The eigenvalues \( a_\gamma \) of the operator \( \hat{A} \) are typically polynomial in system size, and hence at most logarithmic in \( D \). In addition, the average value of \( |c^{(\alpha)}_\gamma|^2 \) is \( 1/D \) by normalization. If the distribution of \( |c^{(\alpha)}_\gamma|^2 \) is not extremely pathological, this implies that the variance of \( |c^{(\alpha)}_\gamma|^2 \) scales as \( 1/D^2 \). With this observation, it follows that \( \text{var}(X_\gamma) \sim 1 \), i.e., constant in system size.

The variance of \( X_\gamma \) can be related to the participation ratio (PR) through

\[ P_{\alpha}/D = [1 + \text{var}(D|c^{(\alpha)}_\gamma|^2)]^{-1} \sim [1 + \text{var}(X_\gamma)]^{-1}, \tag{B2} \]

where the PR has been defined in Eq. (11). Thus, our previous statements are confirmed if the average scaled PR is constant as a function of system size. In addition to Fig. 5, we present a more detailed view of the PRs in Fig. 7. The average scaled PR decreases noticeably with size in the integrable case, while it remains constant for nonintegrable systems.

Normal distribution of \( A_{\alpha\alpha} \) — The central limit theorem does not only give a value for the variance, it also states that the distribution of the \( A_{\alpha\alpha} \) variables should be a normal distribution for large \( D \). In support of this statement, we present the distributions of the fluctuations \( \Delta A_\alpha \) in Fig. 8. The distributions show the fluctuations within one window of the microcanonical average centered at \( E/L = -0.1, 0 \), and 0.1. The results closely resemble normal distributions, indicated by the dashed curves. This provides indirect support to the conjecture that the coefficients \( |c^{(\alpha)}_\gamma|^2 \) are effectively random.

**Appendix C: Computational details: sparse-matrix methods and Hilbert-space sizes**

Hamiltonians in condensed matter physics generally lead to sparse matrices, so that it is often advantageous to use sparse matrix methods like the Lanczos algorithm, which accesses the lowest or highest parts of the eigenspectra. In studies of the ETH, however, we explicitly want to access parts of the spectrum away from the edges. In addition, we have taken the approach of looking at the entire bulk of the spectrum. Therefore, as conventional in computational research on the ETH, we have used full diagonalization of the Hamiltonian matrix, in order to treat Hilbert-space dimensions up to \( D \approx 20000 \). However, in this work, we have additionally gone beyond this size limit, by using sparse matrix methods that access non-extremal parts of the spectrum. This method is described in subsection C 1. In subsection C 2 we connect Hilbert-space sizes to system sizes, for our three model systems.

**1. Sparse-matrix methods**

In order to tackle larger systems than can be comfortably accessed with full diagonalization on present-day machines, we have used a divide-and-conquer technique to split the prob-
lem of diagonalization into smaller parts. We used the so-called shift-invert algorithm: for a matrix $H$ and a chosen value $\gamma$, one applies Lanczos diagonalization to the matrix $H - \gamma I$ , so that one effectively finds the eigenvalues of $H$ close to $\gamma$. In practice, one does not invert the matrix explicitly, since that would generate a non-sparse inverse matrix. Instead, the generation of the Krylov basis is performed by iteratively solving $(H - \gamma I)\psi_{i+1} = \psi_i$. There is thus an “inner” iteration necessary for generating the Krylov basis, in addition to the usual Lanczos iteration. Such methods are often known as “inner-outer” iterative methods.

While this method clearly takes significantly more run-time than bare Lanczos diagonalization, it has the advantage that any part of the spectrum can be accessed. For intermediate Hilbert-space sizes ($D \sim 10000$), we have performed several comparisons between the results of the sparse and the dense method, and we have found them to yield consistent results.

In order to find all eigenvalues and eigenstates of a large sparse matrix, we choose a set of initial energies $\{\gamma_i\}$, and compute in parallel typically 2000 eigenvalues close to each of these values together with the EEVs for a set of observables. Each application of the shift-invert method yields the eigenvalues within a certain (a priori unknown) energy interval. Afterwards, the results are “patched” together, i.e., for the energy regions where two or more such intervals overlap, the eigenvalues and EEVs are compared, and duplicates are removed such that each appears only once in the final result. Finally, the total number of eigenvalues is compared against the known dimension of the Hilbert space. If the result does not contain all the eigenstates, more shift-invert diagonalizations are performed until all eigenstates have been obtained. The largest system for which we have found the full eigenspectrum using this procedure is of Hilbert-space dimension $D = 116280$.

### 2. Hilbert-space dimensions and system sizes

Our results on the EEV fluctuations have been presented in terms of the Hilbert-space dimension $D$. In order to “translate” the results to system size $L$, one uses the relations

$$D = \left( \frac{L}{N_f} \right)^p$$

for an $L$-site XXZ model with $N_f$ spins up and for an $L$-site Bose-Hubbard model with $N_b$ bosons, respectively. In our numerical study, we approach the thermodynamic limit with systems with (almost) constant filling fraction $f \equiv v/u$ for integers $u$ and $v$. We perform our calculations for the sequences $(L, N_f) = (up + w, vp)$ and $(L, N_b) = (up + w, vp)$ ($p = 1, 2, \ldots$) for the XXZ and Bose-Hubbard models, respectively; $w$ is an additional constant integer. Table I provides an overview of the choices of the parameters and the resulting system and Hilbert-space sizes for the models discussed in this work.

With a constant filling fraction $v/u$, the Hilbert-space dimensions of Eq. (C1) can be approximated using Stirling’s formula, as

$$D \sim \frac{\sqrt{c_{u,v}}}{\sqrt{2\pi p}} (\beta_{u,v})^p,$$

where $c_{u,v}$ equals $u/v(u-v)$ for the XXZ models and $(u+v)/uv$ for the Bose-Hubbard model, and

$$\beta_{u,v} \equiv \begin{cases} 
  \frac{u^v}{v^u} (u-v)^{u-v} & \text{(XXZ)} \\
  \frac{(u+v)^{u+v}}{uv^{u+v}} & \text{(Bose-Hubbard)}
\end{cases}$$

defines the limiting ratio $\lim_{p \to \infty} D_{p+1}/D_p$ between the Hilbert-space dimensions of two subsequent realizations in the sequence of system sizes. In other words, the dimension of the Hilbert space is approximately exponential in the system size $L$, as $D \sim L^{\beta_{u,v}}$.

Assuming the power-law behavior $\sigma_{\Delta A} \propto D^{-\epsilon}$ of the EEV fluctuations (with $\epsilon = \frac{1}{2}$ for non-integrable models), we find that this quantity scales exponentially in the system size, as $\sigma_{\Delta A} \approx \text{const} \times (2\pi L)^{e/2} (\xi_f)^{-eL}$, where

$$\xi_f \equiv (\beta_{u,v})^{1/u} \begin{cases}
  \frac{1}{f} f(f-1)^{1-f} & \text{(XXZ)} \\
  (1+f)^{1+f} & \text{(Bose-Hubbard)}
\end{cases}$$

in terms of the filling fraction $f$.

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[1] J. M. Deutsch, Phys. Rev. A 43, 2046 (1991).
[2] M. Srednicki, Phys. Rev. E 50, 888 (1994).

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### Table I. Overview of the system sizes $L$ and Hilbert-space dimensions $D$ of the models used. The cases with bold-faced values have been investigated with the sparse diagonalization algorithm; in all other cases, full diagonalization has been used.

| Model                  | $u$ | $v$ | $w$ |
|------------------------|-----|-----|-----|
| XXZ ladder, $u = 2$, $v = 1$, $w = 1$: |
| $L$ | 9   | 11  | 13  | 15  |
| $N_f$ | 4   | 6   | 7   | 9   |
| $D$ | 126 462 1716 6435 |
| XXZ trap, $u = 3$, $v = 1$, $w = 0$: |
| $L$ | 9   | 12  | 15  |
| $N_f$ | 3   | 4   | 5   | 6   |
| $D$ | 84 495 3003 18564 116280 |
| Bose-Hubbard, $u = 2$, $v = 1$, $w = 0$: |
| $L$ | 6   | 8   | 10  |
| $N_f$ | 3   | 4   | 5   | 6   |
| $D$ | 56 330 2002 12376 77520 |
[3] M. Rigol, V. Dunjko, and M. Olshanii, Nature **452**, 854 (2008).
[4] A. Polkovnikov, K. Sengupta, A. Silva, and M. Vengalattore, Rev. Mod. Phys. **83**, 863 (2011).
[5] C. Kollath, G. Roux, G. Biroli, and A. M. Läuchli, J. Stat. Mech. **2010**, P08011 (2010).
[6] G. Roux, Phys. Rev. A **81**, 053604 (2010).
[7] A. Motohashi, Phys. Rev. A **84**, 053604 (2011).
[8] T. N. Ikeda, Y. Watanabe, and M. Ueda, Phys. Rev. E **84**, 021130 (2011).
[9] S. Genway, A. F. Ho, and D. K. K. Lee, Phys. Rev. A **86**, 023609 (2012).
[10] M. Rigol and M. Srednicki, Phys. Rev. Lett. **108**, 110601 (2012).
[11] E. Khatami, M. Rigol, A. Relaño, and A. M. García-García, Phys. Rev. E **85**, 050102 (2012).
[12] G. P. Brandino, A. De Luca, R. M. Konik, and G. Mussardo, Phys. Rev. B **85**, 214435 (2012).
[13] M. Rigol, Phys. Rev. A **80**, 053607 (2009).
[14] M. Rigol, Phys. Rev. Lett. **103**, 100403 (2009).
[15] L. F. Santos and M. Rigol, Phys. Rev. E **82**, 031130 (2010).
[16] V. A. Yurovsky and M. Olshanii, Phys. Rev. Lett. **106**, 025303 (2011).
[17] C. Neuenhahn and F. Marquardt, Phys. Rev. E **85**, 060101 (2012).
[18] A. C. Cassidy, C. W. Clark, and M. Rigol, Phys. Rev. Lett. **106**, 140405 (2011).
[19] T. N. Ikeda, Y. Watanabe, and M. Ueda, Phys. Rev. E **87**, 012125 (2013).
[20] R. Steinigeweg, J. Herbrych, and P. Prelovšek, Phys. Rev. E **87**, 012118 (2013).
[21] E. Fradkin, *Field Theories of Condensed Matter Systems*, Advanced Books Classics Series (Perseus Books, 1997); P. Kasteleijn, Physica **18**, 104 (1952); H. Bethe, Z. Phys. **71**, 205 (1931); M. Takahashi and M. Suzuki, Progress of Theoretical Physics **48**, 2187 (1972).
[22] T. Kinoshita, T. Wenger, and D. S. Weiss, Nature **440**, 900 (2006).
[23] M. P. A. Fisher, P. B. Weichman, G. Grinstein, and D. S. Fisher, Phys. Rev. B **40**, 546 (1989); D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, Phys. Rev. Lett. **81**, 3108 (1998); D. Jaksch and P. Zoller, Annals of Physics **315**, 52 (2005); M. Lewenstein, A. Sanpera, and V. Ahufinger, *Ultracold Atoms in Optical Lattices: Simulating quantum many-body systems* (Oxford University Press, 2012).
[24] M. Rigol and M. Fitzpatrick, Phys. Rev. A **84**, 033640 (2011).
[25] K. He and M. Rigol, Phys. Rev. A **85**, 063609 (2012).
[26] C. Gramsch and M. Rigol, Phys. Rev. A **86**, 053615 (2012).
[27] M. Kollar, F. A. Wolf, and M. Eckstein, Phys. Rev. B **84**, 054304 (2011).
[28] K. He, L. F. Santos, T. M. Wright, and M. Rigol, Phys. Rev. A **87**, 063637 (2013).
[29] J. Gemmer, M. Michel, and G. Mahler, *Quantum Thermodynamics* (Springer Berlin Heidelberg, 2009).
[30] S. Dubey, L. Silvestri, J. Finn, S. Vinjanampathy, and K. Jacobs, Phys. Rev. E **85**, 011141 (2012).
[31] J. Gemmer and M. Michel, Eur. Phys. J. B **53**, 517 (2006).
[32] P. Reimann, Phys. Rev. Lett. **99**, 160404 (2007).
[33] S. Goldstein, J. L. Lebowitz, R. Tumulka, and N. Zanghì, Phys. Rev. Lett. **96**, 050403 (2006).