Eigenstate Thermalization Hypothesis and Its Deviations from Random-Matrix Theory beyond the Thermalization Time

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The eigenstate thermalization hypothesis explains the emergence of the thermodynamic equilibrium in isolated quantum many-body systems by assuming a particular structure of the observable's matrix elements in the energy eigenbasis. Schematically, it postulates that off-diagonal matrix elements are random numbers and the observables can be described by random matrix theory (RMT). To what extent a RMT description applies, more precisely at which energy scale matrix elements of physical operators become truly uncorrelated, is, however, not fully understood. We study this issue by introducing a novel numerical approach to probe correlations between matrix elements for Hilbert-space dimensions beyond those accessible by exact diagonalization. Our analysis is based on the evaluation of higher moments of operator submatrices, defined within energy windows of varying width. Considering nonintegrable quantum spin chains, we observe that matrix elements remain correlated even for narrow energy windows corresponding to timescales of the order of thermalization time of the respective observables. We also demonstrate that such residual correlations between matrix elements are reflected in the dynamics of outof-time-ordered correlation functions.

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Introduction.-In the overwhelming majority of cases, isolated quantum many-body systems undergoing unitary time evolution are expected to reach thermal equilibrium at long times [1-5]. During the thermalization process, local memory of the initial nonequilibrium state is lost and observables reach a constant value that agrees with an appropriate thermodynamic ensemble average, as observed in some recent experiments, see, e.g., Refs. [6-13].

Motivated by seminal works on quantum chaos and random-matrix theory (RMT), see Refs. [14–19] for reviews, including intimate connections to transport in mesoscopic systems [20,21], the eigenstate thermalization hypothesis (ETH) explains eventual thermalization by postulating a particular structure of matrix elements of observable \mathcal{O} in the eigenbasis of a generic Hamiltonian \mathcal{H} [22–24],

$$\mathcal{O}_{mn} = O(\bar{E})\delta_{mn} + \Omega^{-1/2}(\bar{E})f(\bar{E},\omega)r_{mn},\qquad(1)$$

where $\omega = E_m - E_n$, $\bar{E} = (E_m + E_n)/2$, and $\mathcal{O}_{mn} = \langle m | \mathcal{O} | n \rangle$, with E_m and $|m\rangle$ denoting the eigenvalues and eigenstates of \mathcal{H} . Moreover, $\Omega(\bar{E})$ is the density of states, $O(\bar{E})$ and $f(\bar{E},\omega)$ are smooth functions, and the $r_{mn} = r_{nm}^*$ are usually assumed to be independent random Gaussian variables with zero mean and unit variance, see also Refs. [25–27] for early works on precursors of Eq. (1). While the general features of the ETH have been numerically confirmed for various nonintegrable models [28–38], recent works have proposed further generalizations [39–42], and scrutinized detailed aspects such as entanglement structure of highly excited eigenstates [43], or the presence of rare ETH-violating states [44].

The formulation of the ETH in Eq. (1) may essentially be regarded as an extension of the RMT applied to observables. It builds on earlier sophisticated models to describe physical systems by random matrices such as band matrices [45,46] and embedded ensembles [18,47–49], which take into account the locality of real systems. Numerical analyses have yielded a convincing agreement with the predictions of Eq. (1), for instance regarding the Gaussianity of the r_{mn} [35,50], the distribution of transition strengths $|\mathcal{O}_{mn}|^2$ [51–53], and the ratio of variances of diagonal and off-diagonal matrix elements [3,33,34,54]. Moreover, statistical properties of matrix elements have been analyzed semiclassically in few-body systems with a classically chaotic counterpart [55-57].

Physical Hamiltonians and observables clearly differ from genuinely random operators [18] (for instance, matrix elements $\langle m | \sigma_z | n \rangle$ of a Pauli operator must be correlated to yield the eigenvalues ± 1). In this context, the question whether and to what extent the r_{mn} in Eq. (1) can indeed be considered as *uncorrelated* random numbers has attracted increased attention recently [37,58,59]. In particular, it has been argued that correlations between matrix elements are necessary to explain the growth of out-of-time ordered correlation function (OTOC) [60–62], which is a central quantity to characterize scrambling in quantum systems [63]. Using full eigenvalue spectrum of operator submatrices as a sensitive indicator, correlations between matrix elements have been shown to persist to small energy scales, but appear to vanish at even lower ω [37]. The lack of correlations between r_{mn} at low ω is consistent with expected universality of the observable's dynamics at late times [64–67].

An important and less clear aspect is to connect the onset of RMT behavior, particularly the statistical independence of matrix elements, with the timescale of thermalization. Given a (one-dimensional) quantum many-body system of size L, the thermalization time au_{th} of an observable O is expected to scale as $\tau_{\rm th} \propto L^{\nu}$, where $\nu \geq 0$ depends on \mathcal{O} and details of the system, e.g., presence of conservation laws [68], or disorder [69]. Somewhat unexpectedly, it was analytically shown in [58] that in one dimensional systems, macroscopic thermalization dynamics prevents matrix elements of \mathcal{O} from becoming truly uncorrelated above a smaller energy scale $\Delta E_{\rm RMT} \propto 1/(\tau_{\rm th}L)$, and the system's dynamics is fully described by RMT only at much later times, $T_{\rm RMT} \propto 1/\Delta E_{\rm RMT} \propto \tau_{\rm th} L$. This has consequences, for instance, for the dynamics of certain initial states with a macroscopic spatial inhomogeneity of a conserved quantity, e.g., energy, which will display nontrivial dynamics even for $t > \tau_{\text{th}}$ and saturate into exponentially small fluctuations $\propto e^{-L}$ only at parametrically longer t [58].

We note that the time $T_{\rm RMT}$ explored here and in [58], which marks the absence of correlations between matrix elements, is different from the so-called "Thouless time" [70], see Ref. [71] for details, which has also been associated with the applicability of RMT to the energy spectrum, signaled by a ramp in the spectral form factor [67,73–76].

From a numerical point of view, a major complication to study matrix elements is given by the restriction of full exact diagonalization (ED) to small system sizes, such that the analysis of low-frequency or, correspondingly, longtime regimes is plagued by severe finite-size effects. In this Letter, we introduce a novel numerical approach based on quantum typicality (see Refs. [77,78] and references therein). We show that moments of operator submatrices, defined within energy windows of varying width, can be evaluated for system sizes beyond the range of ED, and provide a sensitive probe to study the presence of correlations between matrix elements. This allows us to shed new light on residual deviations of physical operators from genuine RMT ensembles, including the Gaussian orthogonal ensemble (GOE), which is expected to emerge for the models and operators with real and symmetric matrix representation considered here. For nonintegrable quantum spin chains, our analysis shows that matrix elements remain correlated even in narrow energy windows corresponding to timescales around the thermalization time of the respective observable. For shorter times, the residual correlations between matrix elements are manifest in the nontrivial dynamics of suitably defined OTOCs within such energy windows.

Setup.—We consider submatrices \mathcal{O}^T defined within energy windows of width $2\pi/T$ [37,54,58],

$$\mathcal{O}_{mn}^{T} = \langle m | P_T \mathcal{O} P_T | n \rangle = \begin{cases} \mathcal{O}_{mn}, & |E_{m,n} - E_0| \le \frac{\pi}{T}, \\ 0, & \text{otherwise,} \end{cases}$$
(2)

where $P_T = \sum_{|E_m - E_0| \le (\pi/T)} |m\rangle \langle m|$ is a projection on eigenstates of \mathcal{H} centered around E_0 . Parameter T controlling the size of the submatrix determines characteristic timescale (matrix elements at low ω contribute to dynamics at long times). We will compare the energy scale 1/T, where the \mathcal{O}_{mn}^T become uncorrelated, with the scale $1/\tau_{\text{th}}$ set by thermalization time of \mathcal{O} . Examples of \mathcal{H} , \mathcal{O} , and a definition of τ_{th} are given below.

We study the presence of correlations between matrix elements by introducing the ratio Λ^T of moments of \mathcal{O}_c^T ,

$$\Lambda^T = \mathcal{M}_2^2 / \mathcal{M}_4, \qquad \mathcal{M}_k = \operatorname{Tr}[(\mathcal{O}_c^T)^k] / d, \qquad (3)$$

where $d = \text{Tr}[P_T] = \sum_{|E_m - E_0| \le \pi/T} 1$ and $\mathcal{O}_c^T = \mathcal{O}^T - \text{Tr}(\mathcal{O}^T)/d$. If \mathcal{O}^T were to be described by an ideal GOE, its eigenvalues would follow famous Wigner semicircle distribution, implying $\Lambda_{\text{GOE}}^T = 1/2$. Crucially, as we show in [79], $\Lambda^T \simeq 1/2$ can be derived also for weaker conditions on \mathcal{O}^T as long as the \mathcal{O}_{mn}^T are statistically independent. In particular, as discussed in [79] and demonstrated below, $\Lambda^T \to 1/2$ can serve as a sensitive indicator to locate the energy scale where \mathcal{O}_{mn}^T become uncorrelated and deviations from a strict GOE disappear.

Numerical approach.—To construct \mathcal{O}^T explicitly without using ED, it is crucial to rewrite P_T as $P_T = (1/T) \int_{-\infty}^{+\infty} \operatorname{sinc}(t/T) \exp[-i(\mathcal{H}-E_0)t] dt$ [58], where $\operatorname{sinc}(t) = \sin(\pi t)/\pi t$. In particular, by expanding the time evolution operator in terms of Chebyshev polynomials [81–83] and evaluating the integral analytically, one finds [79], $P_T = \sum_{k=0}^{\infty} C_k T_k [(\mathcal{H}-b)/a]$, where $T_k(x)$ are Chebyshev polynomials of the first kind, C_k are suitable coefficients [79], and $a = (E_{\max} - E_{\min})/2$, $b = (E_{\max} + E_{\min})/2$, where $E_{\max}(E_{\min})$ is the largest (smallest) eigenvalue of \mathcal{H} . Exploiting quantum typicality [77,78] (see also Ref. [79]) one can then calculate the second and the fourth central moments of \mathcal{O}^T as

$$\mathcal{M}_{2} \approx \frac{\langle \psi_{POP} | \psi_{POP} \rangle}{\langle \psi_{P} | \psi_{P} \rangle}, \qquad \mathcal{M}_{4} \approx \frac{\langle \psi_{(POP)^{2}} | \psi_{(POP)^{2}} \rangle}{\langle \psi_{P} | \psi_{P} \rangle}, \quad (4)$$

where $|\psi_P\rangle = P_T |\psi\rangle$, $|\psi_{POP}\rangle = P_T \mathcal{O}_c^T P_T |\psi\rangle$, $|\psi_{(POP)^2}\rangle =$ $(P_T \mathcal{O}_c^T P_T)^2 |\psi\rangle$, and $\mathcal{O}_c^T = \mathcal{O}^T - \langle \psi_P | \mathcal{O}^T | \psi_P \rangle / \langle \psi_P | \psi_P \rangle$. Here, $|\psi\rangle$ is a pure state drawn at random from the unitarily invariant Haar measure [84], i.e., in practice $|\psi\rangle$ is constructed in the computational basis with Gaussian distributed coefficients. The approximation of \mathcal{M}_k in Eq. (4) becomes very accurate for energy windows with sufficiently many eigenstates. For smaller windows with fewer eigenstates, the accuracy can be improved by averaging over multiple realizations of $|\psi\rangle$. The most demanding step of our approach is to restrict the random state to a narrow energy window, $P_T |\psi\rangle = \sum_{k=0}^{M} C_k T_k [(\mathcal{H} - b)/a] |\psi\rangle$, where P_T is approximated by a sum up to k = M, which has to be chosen large enough to yield accurate results [85]. Combined with efficient sparse-matrix techniques, \mathcal{M}_k and Λ^T can then be obtained for Hilbert-space dimensions far beyond the range of the ED. Note that other approaches exist to construct states in a specified energy window [86-89].

Numerical analysis.—We consider the one-dimensional mixed-field Ising model, $\mathcal{H} = \sum_{\ell=1}^{L} \mathcal{H}^{\ell}$,

$$\mathcal{H}^{\ell} = J\sigma_z^{\ell}\sigma_z^{\ell+1} + \frac{h_x}{2}(\sigma_x^{\ell} + \sigma_x^{\ell+1}) + \frac{h_z}{2}(\sigma_z^{\ell} + \sigma_z^{\ell+1}), \quad (5)$$

where $\sigma_{x,z}^{\ell}$ are Pauli operators at lattice site ℓ , *L* is the length of the chain with periodic boundaries, and $J = h_x = 1.0$ and $h_z = 0.5$ in the following. Moreover, we add two defect terms $h_2\sigma_z^2$ and $h_5\sigma_z^5$ with $h_2 = 0.1665$ and $h_5 = -0.2415$ to lift translational and reflection symmetries, such that our simulations are performed in the full Hilbert space of dimension 2^L . We note that \mathcal{H} is nonintegrable, fulfills the ETH for these parameters [79], and exhibits diffusive energy transport [90]. We consider energy windows around $E_0 = 0$, corresponding to infinite temperature. We study Λ^T for two kinds of operators,

$$\mathcal{A} = \frac{1}{\sqrt{L}} \sum_{\ell=1}^{L} \cos\left(\frac{2\pi}{L}q\ell\right) \mathcal{H}^{\ell}, \qquad \mathcal{B} = \frac{1}{\sqrt{L}} \sum_{\ell=1}^{L} \sigma_x^{\ell}, \quad (6)$$

where \mathcal{B} exhibits no transport behavior and decays quickly. In contrast, dynamics of the density-wave operator \mathcal{A} depends on q, with a quick *L*-independent decay for q = L/2 and a slow hydrodynamic (diffusive) relaxation in the limit of small q [68]. For our numerical analysis, operators with short, *L*-independent, τ_{th} are beneficial as this allows us to reach regimes $T/\tau_{\text{th}} \gg 1$, which in contrast becomes very costly if $\tau_{\text{th}} \propto L^2$ scales diffusively.

A first glance of how Λ^T behaves upon varying the width of the energy window is given in Fig. 1, where we consider \mathcal{A} for a small system with L = 16 amenable to ED. ED values of Λ^T show convincing agreement with those obtained using the typicality approach for a wide range of T. Analyzing Λ^T behavior, we see that it deviates from



FIG. 1. Λ^T versus T/τ_{th} for \mathcal{A} with q = L/2 and L = 16. Results obtained by the typicality approach, averaged over 500 states, agree convincingly with ED data. As a comparison, Λ^T obtained from a sign-randomized operator [Eq. (7)] yields the GOE value $\Lambda^T = 1/2$. Insets show eigenvalue distributions $P(\lambda)$ of \mathcal{A}^T and $\tilde{\mathcal{A}}^T$ for different energy windows.

the GOE value for small *T* (i.e., large energy windows), but approaches it for larger *T*. As shown in the insets of Fig. 1, the full eigenvalue distribution $P(\lambda)$ of \mathcal{A}^T is approximately Gaussian for small *T* ($\Lambda^T = 1/3$ for strictly Gaussian distributions), while it takes an approximately semicircle shape for larger *T*, indicating a transition to GOE behavior [37]. Importantly, while Λ^T displays that strict GOE behavior only occurs at large *T*, other common randommatrix indicators, such as the mean ratio of adjacent level spacings $\langle r \rangle$ [91], turn out to be insensitive to the residual correlations between the \mathcal{O}_{mn}^T at small *T*, see Ref. [79]. In this context, it is also helpful to evaluate Λ^T for a signrandomized version of \mathcal{O}^T [37,92,93],

$$\tilde{\mathcal{O}}_{mn}^{T} = \begin{cases} \mathcal{O}_{mn}^{T}, & 50\% \text{ probability,} \\ (-1)\mathcal{O}_{mn}^{T}, & 50\% \text{ probability,} \end{cases}$$
(7)

where potential correlations between the \mathcal{O}_{mn}^{T} are thus manually destroyed. As shown in Fig. 1, $\tilde{\mathcal{A}}^{T}$ indeed yields $\Lambda^{T} \approx 0.5$ with semicircular $P(\lambda)$ for all *T*, which further confirms that $\Lambda^{T} \to 0.5$ is a good indicator for the absence of correlations between matrix elements.

We now turn to the dependence of Λ^T on *T* for larger systems up to L = 26, using our novel typicality approach. First, we consider operator $\mathcal{O} = \mathcal{A}$ with q = L/2, for which the infinite-temperature autocorrelation function C(t) (also obtained by typicality [77–79,94]) exhibits a short *L*-independent τ_{th} [Fig. 2(a)], where

$$C(t) = \operatorname{Tr}[\mathcal{O}(t)\mathcal{O}]/2^{L}.$$
(8)

We here define τ_{th} as the time when $\tilde{C}(t) = [C(t) - C(t \to \infty)]/[C(0) - C(t \to \infty)]$ has decayed to $\tilde{C}(t) < 0.01$ and stays below this threshold afterward [95]. Note that by Fourier transforming $C(t), 2\pi/\tau_{\text{th}}$ sets the "Thouless



FIG. 2. Λ^T versus $T/\tau_{\rm th}$ for the density-wave operator \mathcal{A} with (a) q = L/2 and (b) q = 1. Data are obtained using the typicality approach up to L = 26, averaged over $500 \cdot 2^{16-L}$ random states [96]. The dashed line indicates the GOE value $\Lambda^T_{\rm GOE} = 0.5$. Insets show Λ^T versus $T/(\tau_{\rm th}L)$ and the rescaled correlation function $\tilde{C}(t)$. The dashed vertical line signals $\tau_{\rm th}$ according to our definition in the text. The data collapse of $\tilde{C}(t)$ and $\tilde{C}(t/L^2)$ indicates L independence of $\tau_{\rm th}$ for q = L/2 and diffusive behavior $\tau_{\rm th} \propto L^2$ for q = 1.

energy" below which $f(\bar{E}, \omega)$ in Eq. (1) becomes approximately constant [71,72]. Inspecting Λ^T at the energy scale which corresponds to thermalization, $T \approx \tau_{\text{th}}$, we find Λ^T is far from the GOE value but tends to approach it at larger values of *T*. The same behavior of Λ^T is also demonstrated by the second operator $\mathcal{O} = B$, see Fig. 3. Specifically, \mathcal{B} also has *L*-independent thermalization time τ_{th} and, especially for large *L*, Λ^T is still far from the GOE value even at long times $T \sim 20\tau_{\text{th}}$.

Next, we consider density-wave operator \mathcal{A} with the longest wavelength, q = 1. This is a diffusive operator and C(t) decays exponentially with $\tau_{\text{th}} \propto L^2$, as confirmed by



FIG. 3. Analogous data as in Fig. 2, but now for \mathcal{B} .

the collapse of $\tilde{C}(t/L^2)$ for different *L* [inset of Fig. 2(b)]. Similar to the previous case, we find that Λ^T is far from the GOE prediction at $T \approx \tau_{\text{th}}$, while it tends to approach it for larger *T*. Thus, in all cases shown in Figs. 2 and 3, we conclude that matrix elements of \mathcal{O}^T remain correlated around the energy scale defined by inverse thermalization time $1/\tau_{\text{th}}$, consistent with [58]. A *strict* description of \mathcal{O}^T by a random matrix drawn from a GOE may therefore apply only at much longer times $T_{\text{RMT}} \gg \tau_{\text{th}}$. This is the main result of this Letter.

It would be a natural step to quantify $T_{\rm RMT}/\tau_{\rm th}$ for different operators, and in particular its dependence on the system size L. In practice this requires extending numerical analysis to much larger T for which $\Lambda^T \approx 0.5$. which is a challenging task. Here, we particularly focus on the case of \mathcal{A} with q = L/2. Plotting Λ^T versus $T/(\tau_{th}L)$, see inset in Fig. 2(a), we observe a good data collapse extending over the entire range of T shown here. This tentatively suggests $T_{\rm RMT} \propto \tau_{\rm th} L$ for this particular operator, which is also consistent with [97]. Furthermore, in [79], we provide additional results for a nonintegrable XXZ chain with next-nearest neighbor interactions and a local operator exhibiting diffusive transport. Also in this case, the data are consistent with $T_{\rm RMT} \propto \tau_{\rm th} L$. Generally, however, the universality of this scaling remains unclear since such a collapse of Λ^T is absent in other cases [cf. Figs. 2(b) and 3(c)]. Nevertheless, at least for \mathcal{B} in Fig. 3, it appears that while $\tau_{\rm th} \approx {\rm const}, T_{\rm RMT}$ increases with L, which supports our main result that asymptotically $T_{\rm RMT} \gg \tau_{\rm th}$. While a potential confirmation of $T_{\rm RMT} \propto \tau_{\rm th} L$ would require a collapse in the immediate region of $T \approx T_{RMT}$, this is currently beyond our numerical capabilities and we here leave to future work to develop other indicators of $T_{\rm RMT}$ complementary to Λ^T .

Dynamics of OTOCs.—Correlations between \mathcal{O}_{mn}^T also manifest themselves in dynamical properties [59]. In particular, we consider an out-of-time-ordered correlation function, defined within the energy window $|E_m - E_0| \leq (\pi/T)$,

$$F_T(t) = \operatorname{Tr}[\mathcal{O}_c^T(t)\mathcal{O}_c^T\mathcal{O}_c^T(t)\mathcal{O}_c^T].$$
(9)

Assuming that off-diagonal matrix elements of \mathcal{O}_c^T are uncorrelated and that diagonal elements satisfy ETH [79],



FIG. 4. $F_T(t)$ [Eq. (9)] and $2\bar{C}_T(t)$ [Eq. (10)] for \mathcal{A} with q = L/2 and L = 16, for (a) $T = \tau_{\text{th}}$ and (b) $T = 25\tau_{\text{th}}$.

 $F_T(t)$ should reduce to $F_T(t) \simeq 2\bar{C}_T(t)$, where $\bar{C}_T(t)$ is the eigenstate-averaged two-point function,

$$\bar{C}_T(t) \equiv \sum_{m=1}^d \Re \langle m | \mathcal{O}_c^T(t) \mathcal{O}_c^T | m \rangle^2.$$
(10)

In Fig. 4, $F_T(t)$ and $\bar{C}_T(t)$ are shown for the densitywave operator \mathcal{A} with q = L/2. We consider L = 16 and two different energy windows, $T = \tau_{\text{th}}$ [Fig. 4(a)] and $T = 25\tau_{\text{th}}$ [Fig. 4(b)]. In the former case, we find $F_T(t) \neq 2\bar{C}_T(t)$, which is consistent with our earlier observation that $\Lambda^T \neq 0.5$ at $T = \tau_{\text{th}}$ [Fig. 2(a)] and supports our conclusion that higher-order correlations exist between the \mathcal{O}_{mn}^T . In contrast, in the latter case, $F_T(t) \approx 2\bar{C}_T(t)$, consistent with $\Lambda^T \to 0.5$ and signaling that correlations between the \mathcal{O}_{mn}^T vanish and strict GOE behavior emerges for such narrow energy windows.

Conclusion and outlook.-We have studied the presence of correlations between matrix elements of observables written in the energy eigenbasis of chaotic quantum manybody systems. We introduced a novel numerical method to evaluate higher moments of operator submatrices for system sizes beyond those accessible by ED. As a main result, we have shown that even for narrow energy windows, corresponding to timescales of the order of thermalization time for the given observable, matrix elements remain correlated. Consistent with the results of [37,58], our findings suggest that even though usual indicators of the ETH might be completely fulfilled [79], ETH has to be refined to properly describe all dynamical aspects of thermalization. Specifically, in addition to the usual thermalization or Thouless time controlling RMT behavior of energy levels, there exists another relevant time $T_{\rm RMT} \gg \tau_{\rm th}$, which marks the end of macroscopic thermalization dynamics (see also Ref. [58]) and the scale where \mathcal{O}_{mn}^T become uncorrelated. We demonstrated this fact by studying suitably defined OTOCs, which visualized the presence of correlations between \mathcal{O}_{mn}^T well beyond the thermalization time of the two-point function.

A natural next step is to systematically study L dependence of $T_{\rm RMT}/\tau_{\rm th}$ for various operators and to clarify the role of conservation laws giving rise to hydrodynamic behavior at late times. While we expect that our findings can be generalized to other systems, it would be interesting to study $T_{\rm RMT}$ in a wider class of models, including time-dependent Floquet models without energy conservation, as well as disordered systems which may exhibit subdiffusive transport or localization depending on the disorder strength [98]. Finally, another direction is to consider few-body systems with a classically chaotic counterpart and to explore $T_{\rm RMT}$ and its deviations from the Thouless time from a semiclassical point of view.

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