Basis dependence of eigenstate thermalization

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Eigenstate thermalization refers to the property that an energy eigenstate of a many-body system is indistinguishable from a thermal equilibrium ensemble at the same energy as far as expectation values of local observables are concerned. In systems with degeneracies, the choice of an energy eigenbasis is not unique and the fraction of basis states exhibiting eigenstate thermalization can vary. We present a simple example where this fraction vanishes in the thermodynamic limit for one basis choice, but remains nonzero for another choice. In other words, the weak eigenstate thermalization hypothesis is satisfied in the first, but violated in the second basis. We furthermore prove that degeneracies must abound whenever a system is simultaneously symmetric under spatial translations and reflection. Finally, we derive general bounds on how strongly eigenstate thermalization may depend on the choice of the basis, and we reveal some interesting implications regarding the temporal relaxation properties of such systems.

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I. INTRODUCTION

The eigenstate thermalization hypothesis (ETH) [1–3] postulates that the expectation values of a local observable A in the eigenstates of a generic many-body Hamiltonian H approach the thermal expectation values at the corresponding energy in the thermodynamic limit. Put differently, an eigenstate $|n\rangle$ of H with energy E_n exhibits eigenstate thermalization if $A_{nn} := \langle n|A|n\rangle \to A_{\mathrm{th}}$ as the degrees of freedom $L \to \infty$, and the ETH conjectures that this holds for all eigenstates $|n\rangle$ (not too close to the edges of the spectrum). Here A_{th} is the thermal expectation value at energy $E = E_n$, e.g.,

$$A_{\mathrm{th}} := \frac{1}{|S|}\sum_{m\in S} A_{mm} \tag{1}$$

in the microcanonical ensemble, where S collects all indices m whose energies lie in a macroscopically small energy window around E, and $|S|$ indicates the number of elements in S.

This postulate has been verified in numerous numerical examples (see, for instance, Refs. [3–7]) and is generally believed to explain why generic many-body quantum systems thermalize, meaning that the expectation values of local observables become indistinguishable from the thermal equilibrium values at late times. However, it still amounts to an unproven hypothesis and there are several examples of mechanisms that may lead to violations of this (strong) ETH, such as integrability [8,9], many-body localization [10,11], quantum many-body scars [12–14], and Hilbert space fragmentation [13,14].

A weaker formulation of the ETH only asserts that the variance

$$\Delta_A^2 := \frac{1}{|S|}\sum_{n\in S}(A_{nn} - A_{\mathrm{th}})^2 \tag{2}$$

of the diagonal matrix elements of a local observable A vanishes in the thermodynamic limit $L \to \infty$. This so-called weak ETH is provably true for a large class of systems exhibiting translational invariance [15–20]. Moreover, even though the weak ETH is insufficient for thermalization in general, it can be used to demonstrate return to equilibrium after local quenches under certain additional assumptions [21,22].

The weak ETH still leaves room for the existence of nonthermal eigenstates. However, their relative number is bound to vanish in the thermodynamic limit, i.e., the weak ETH enforces eigenstate thermalization at least for *most* eigenstates [15–20]. In turn, a violation of the weak ETH means [23] that a nonvanishing fraction of eigenstates must be nonthermal (at least under the usual tacit assumption that local observables are bounded operators).

We also remark that the above-mentioned proofs of the weak ETH [15–20] are valid independently of whether the considered system is integrable or not (even translationally invariant systems consisting of noninteracting subsystems are admitted). Furthermore, and in contrast to the conventional (strong) ETH, neither the edges of the spectrum nor additional conserved quantities play any special role.

More precisely speaking, the proofs of the weak ETH demonstrate that, for any translationally invariant Hamiltonian H with local interactions, *there exists* an energy eigenbasis $\{|n\rangle\}$ such that $\Delta_A^2 \to 0$ as $L \to \infty$ [15–20]. This eigenbasis is unique (up to trivial phase factors) if the spectrum of H is nondegenerate. If there are degeneracies, however, the variance Δ_A^2 in (2) generally becomes basis dependent.

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In this work, we address this basis dependence of the weak ETH. In particular, (i) we demonstrate that the spectrum of a translationally invariant Hamiltonian must exhibit a large number of degeneracies in the most commonly studied cases obeying a spatial reflection symmetry; (ii) we identify the specific energy eigenbases in which Δ_A^2 (and thus any potential ETH violation) are minimal and maximal, respectively; (iii) we provide an example of a system that satisfies the weak ETH in one basis, but violates it in another one; (iv) we discuss various interesting implications of these findings for equilibration, thermalization, and dynamical autocorrelation functions.

Since the property of whether or not a system thermalizes cannot depend on the energy eigenbasis used to evaluate the ETH, our findings pinpoint a subtle, but important problem with the interpretation of eigenstate thermalization as the mechanism behind thermalization in systems with degeneracies. Fundamentally speaking, this may be considered as the main message of this paper. From a practical point of view, our findings imply that numerical studies of the ETH which exploit symmetries in the presence of degeneracies may lead to physically wrong conclusions.

II. DEGENERACIES IN TRANSLATIONALLY INVARIANT SYSTEMS

For the sake of simplicity, we focus in this section on one-dimensional lattice systems (generalizations are straightforward), where every lattice site is associated with a copy of the local, D-dimensional Hilbert space $\mathcal{H}_{\mathrm{loc}}$ with a local orthonormal basis (ONB) $\{|\sigma\rangle\}_{\sigma=0}^{D-1}$. The total Hilbert space is $\mathcal{H} = \mathcal{H}_{\mathrm{loc}}^{\otimes L}$, and we denote the D^L states of the associated product ONB by

$$|\boldsymbol{\sigma}\rangle \equiv |\sigma_1 \dots \sigma_L\rangle := \bigotimes_{l=1}^{L} |\sigma_l\rangle. \tag{3}$$

The translation operator T is defined as usual via its action on the product states,

$$T\,|\sigma_1\sigma_2 \dots \sigma_{L-1}\sigma_L\rangle := |\sigma_L\sigma_1\sigma_2 \dots \sigma_{L-1}\rangle. \tag{4}$$

One readily infers that T is a unitary operator and that $T^L = \mathbb{1}$ (identity operator).

Let us now consider a Hamiltonian H that is translationally invariant, i.e., it commutes with T. Hence, there exists a common eigenbasis $\{|n\rangle\}$ of H and T, meaning that $H|n\rangle = E_n|n\rangle$ and $T|n\rangle = \lambda_n|n\rangle$ for all n. Furthermore, defining

$$\gamma_\nu := e^{2\pi i \nu/L} \tag{5}$$

for $\nu \in \{0, \dots, L-1\}$, and recalling that $T^L = \mathbb{1}$, it follows that $\lambda_n \in \{\gamma_0, \dots, \gamma_{L-1}\}$ for all n and thus $T^{L-1}|n\rangle = \lambda_n^*|n\rangle$.

The salient point is that nearly all commonly considered Hamiltonians H which are invariant under T are also invariant under the action of the parity (spatial reflection) operator P with $P|\sigma_1 \dots \sigma_L\rangle := |\sigma_L \dots \sigma_1\rangle$. Common examples are Heisenberg- or Ising-type models.

Assuming this additional symmetry $[H, P] = 0$, we define $|n\rangle' := P|n\rangle$ and observe that $H|n\rangle' = E_n|n\rangle'$. One readily verifies $TP|\boldsymbol{\sigma}\rangle = PT^{L-1}|\boldsymbol{\sigma}\rangle$ for all $|\boldsymbol{\sigma}\rangle$, which implies $TP = PT^{L-1}$ and thus $T|n\rangle' = TP|n\rangle = PT^{L-1}|n\rangle = \lambda_n^*|n\rangle'$. Therefore, $|n\rangle'$ must be linearly independent of $|n\rangle$ whenever $\lambda_n^* \neq \lambda_n$, resulting in a degeneracy of the energy eigenvalue E_n. Furthermore, assuming $\lambda_n^* = \lambda_n$ for all n would imply $\lambda_n^2 = 1$ and thus $T^2 = \mathbb{1}$, which is obviously violated if $L > 2$. Consequently, many-body Hamiltonians that simultaneously commute with T and P must exhibit at least one degeneracy.

The natural next step is to show that there exist more than one degeneracy. To this end, we recall that all eigenvalues of T are of the form (5) for some $\nu \in \{0, ..., L-1\}$. Furthermore, for an arbitrary but fixed $\nu \in \{0, \dots, L-1\}$, we denote by $\mathcal{H}_\nu$ the eigenspace of T with eigenvalue γ_ν. Finally, we show in Appendix A that the dimension of each $\mathcal{H}_\nu$ can be lower bounded as

$$\mathrm{Dim}(\mathcal{H}_\nu) \geqslant \frac{D^L}{L}\left(1 - \frac{\ln L}{D^{L/2}\ln 2}\right) \tag{6}$$

for all $\nu \in \{0, \dots, L-1\}$. Observing that $\mathrm{Dim}(\mathcal{H}_\nu)$ equals $D^L - \sum_{\mu\neq\nu}\mathrm{Dim}(\mathcal{H}_\mu)$, and exploiting (6) for each summand $\mathrm{Dim}(\mathcal{H}_\mu)$ also yields an immediate upper bound for $\mathrm{Dim}(\mathcal{H}_\nu)$. For large L, those lower and upper bounds imply that the D^L simultaneous eigenvectors $|n\rangle$ of H and T are nearly equally distributed among the L different eigenspaces $\mathcal{H}_\nu$ of T (as one possibly might have intuitively expected). We also note that the derivation of this result in Appendix A is valid for any translationally invariant Hamiltonian H (independently of whether it commutes with P or not).

Equation (5) implies that $\gamma_\nu \neq \gamma_\nu^*$ unless $\nu \in \{0, L/2\}$ (the second option, $\nu = L/2$, is only possible for even L). It follows that there are at least $(L-2)$ eigenspaces $\mathcal{H}_\nu$ with the property $\gamma_\nu \neq \gamma_\nu^*$. All eigenvectors $|n\rangle$ contained in those eigenspaces thus fulfill the above-mentioned degeneracy criterion $\lambda_n^* \neq \lambda_n$. Exploiting Eq. (6), the total number N_{deg} of degenerate energy eigenvalues can thus be lower bounded as

$$N_{\mathrm{deg}} \geqslant D^L\left(1 - \frac{2}{L}\right)\left(1 - \frac{\ln L}{D^{L/2}\ln 2}\right). \tag{7}$$

In other words, among the D^L eigenvalues of a translational and reflection symmetric Hamiltonian, the fraction N_{deg}/D^L of degenerate eigenvalues approaches unity in the thermodynamic limit $L \to \infty$, while the fraction of *non*degenerate eigenvalues approaches zero. Note that all those degeneracies are predicted to be at least twofold, while no statement about possibly existing higher degeneracies is made.

This is the first main result of our paper: Commonly studied translationally invariant systems are usually at the same time also invariant under spatial reflection. If so, the vast majority of the energy eigenvalues must exhibit degeneracies.

III. MINIMALLY AND MAXIMALLY ETH-VIOLATING BASES

Let us now return to the general setup and consider a possibly degenerate Hamiltonian H. The nature of the Hamiltonian and the source of degeneracies (for instance symmetries) are irrelevant for the discussion in this section.

A. Main formal result

To begin with, we note that the ETH quantifier in Eq. (2) can be rewritten by means of Eq. (1) as

$$\Delta_A^2 = \left(\frac{1}{|S|}\sum_{n\in S} A_{nn}^2\right) - A_{\text{th}}^2 = \frac{1}{|S|}\sum_{n\in S}\left(A_{nn}^2 - A_{\text{th}}^2\right). \tag{8}$$

Next, we denote by W the set of all distinct energy eigenvalues in the microcanonical window S. Furthermore, we define g_E as the multiplicity of $E \in W$, i.e., the dimension of the eigenspace of energy E. Let $\{|E,\nu\rangle\}_{\nu=1}^{g_E}$ be an orthonormal basis of that eigenspace with energy E. For this basis, the ETH quantifier (8) can be decomposed as

$$\Delta_A^2 = \frac{1}{|S|}\sum_{E\in W} g_E\, \Delta_{A,E}^2, \tag{9}$$

$$\begin{aligned}\Delta_{A,E}^2 &:= \frac{1}{g_E}\sum_{\nu=1}^{g_E}\left(A_{E,\nu\nu}^2 - A_{\text{th}}^2\right)\\ &= \frac{1}{g_E}\left(\sum_{\nu=1}^{g_E} A_{E,\nu\nu}^2\right) - A_{\text{th}}^2\end{aligned} \tag{10}$$

with $A_{E,\mu\nu} := \langle E,\mu|A|E,\nu\rangle$. To find the minimal (maximal) possible value of Δ_A^2, it suffices to minimize (maximize) $\Delta_{A,E}^2$ for every E individually.

We first inspect the maximum. Denoting the projector onto the energy eigenspace of E by P_E, we observe that

$$\begin{aligned}\text{tr}[(P_E A)^2] &= \sum_{\mu,\nu=1}^{g_E} A_{E,\mu\nu}A_{E,\nu\mu}\\ &= g_E\left(\Delta_{A,E}^2 + A_{\text{th}}^2\right) + \sum_{\mu\neq\nu}|A_{E,\mu\nu}|^2,\end{aligned} \tag{11}$$

where the last sum runs over all $\mu,\nu \in \{1,\ldots,g_E\}$ with $\mu \neq \nu$. Next, we focus on a fixed subspace with energy $E \in W$ and $g_E > 1$, and introduce a second orthonormal basis $\{|E,\nu\rangle'\}_{\nu=1}^{g_E}$ with matrix elements $A'_{E,\mu\nu}$ of A and associated ETH quantifier $\Delta'^2_{A,E}$. Since the trace on the left-hand side of Eq. (11) is basis independent, the same expression on the right-hand side holds analogously for the second basis $\{|E,\nu\rangle'\}$, implying that

$$\Delta_{A,E}^2 + \frac{1}{g_E}\sum_{\mu\neq\nu}|A_{E,\mu\nu}|^2 = \Delta'^2_{A,E} + \frac{1}{g_E}\sum_{\mu\neq\nu}|A'_{E,\mu\nu}|^2. \tag{12}$$

If we now choose one of the bases, say $\{|E,\nu\rangle'\}$, such that $A'_{E,\mu\nu} = 0$ whenever $\mu \neq \nu$ (i.e., we diagonalize A within the eigenspace of energy E), then

$$\Delta_{A,E}^2 + \frac{1}{g_E}\sum_{\mu\neq\nu}|A_{E,\mu\nu}|^2 = \Delta'^2_{A,E} \tag{13}$$

and consequently

$$\Delta_{A,E}^2 \leqslant \Delta'^2_{A,E} = \frac{\text{tr}[(P_E A)^2]}{g_E} - A_{\text{th}}^2. \tag{14}$$

We thus arrive at the second main result of our paper: The energy eigenbasis where A is diagonal in every degenerate energy subspace maximizes the ETH quantifier (10) in every subspace and thus, via (9), also over the entire microcanonical energy window. In other words, this is the most "dangerous" basis with regard to violations of the weak ETH.

Aiming also for the opposite extreme of the basis that minimizes the ETH violation, we return to Eq. (10) and consider

$$\begin{aligned}\sum_{\nu=1}^{g_E} A_{E,\nu\nu}^2 &= \sum_{\nu=1}^{g_E}\left(A_{E,\nu\nu} - \frac{\text{tr}(P_E A)}{g_E}\right)^2 + \frac{[\text{tr}(P_E A)]^2}{g_E}\\ &\geqslant \frac{[\text{tr}(P_E A)]^2}{g_E}.\end{aligned} \tag{15}$$

Since the last term is basis independent, the relation (15) gives a lower bound for the sum of squared diagonal matrix elements in any basis. Substituted into Eq. (10), it yields

$$\Delta_{A,E}^2 \geqslant \frac{[\text{tr}(P_E A)]^2}{g_E} - A_{\text{th}}^2. \tag{16}$$

Furthermore, the bound is saturated if $A_{E,\nu\nu} = \text{tr}(P_E A)/g_E$ for all ν. The smallest ETH violation for a given observable A is thus obtained for the basis where all diagonal matrix elements of A assume the same value within degenerate energy subspaces (preserving the trace). Such a basis always exists because, as shown in Example 2.2.3 of Ref. [24], every complex matrix is unitarily similar to a matrix whose diagonal entries are equal.

In summary, the basis dependence of the ETH quantifier Δ_A^2 from (2) varies within the range

$$\frac{1}{|S|}\sum_{E\in W}[\text{tr}(P_E A)]^2 - A_{\text{th}}^2 \leqslant \Delta_A^2 \leqslant \frac{1}{|S|}\sum_{E\in W}\text{tr}[(P_E A)^2] - A_{\text{th}}^2. \tag{17}$$

The lower bound is assumed by choosing a basis with constant diagonal matrix elements for A in every degenerate energy subspace. The upper bound is assumed by choosing a basis such that A is diagonal in every such subspace. Note that generally those extremizing bases will depend on the observable A.

Since physical system properties cannot depend on the basis choice, conclusions about a system's behavior can only be drawn from the appropriate bound. In particular, a basis-independent weak ETH should instead be formulated as a vanishing upper bound in (17), i.e.,

$$\hat{\Delta}_A^2 := \frac{1}{|S|}\sum_{E\in W}\text{tr}[(P_E A)^2] - A_{\text{th}}^2 \to 0 \tag{18}$$

in the thermodynamic limit. We will come back to concrete physical implications of this in Sec. VI.

B. Generalization

The line of reasoning from the previous section can be readily generalized as follows: Consider an arbitrary "equilibrium ensemble" of the form

$$\rho_{\text{eq}} := f(H) \tag{19}$$

with any function f such that ρ_{eq} is a well-defined density operator, i.e., $\rho_{\text{eq}} \geqslant 0$ and $\text{tr}\{\rho_{\text{eq}}\} = 1$. By definition, for any given orthonormal eigenbasis $|n\rangle$ of H with corresponding

eigenvalues E_n, Eq. (19) thus assumes the form

$$\rho_{\mathrm{eq}} = \sum_n p_n |n\rangle\langle n| \tag{20}$$

with the "level populations" $p_n := f(E_n)$. It follows that ρ_{eq} commutes with H and therefore is a steady state (hence the name *equilibrium ensemble*). Moreover, it may be viewed as a so-called *diagonal ensemble*. Particularly important examples are the microcanonical and the canonical ensembles.

Similarly as in Eq. (1), the corresponding equilibrium value of an observable A is defined as

$$A_{\mathrm{eq}} := \mathrm{tr}\{\rho_{\mathrm{eq}} A\} = \sum_n p_n A_{nn}, \tag{21}$$

while the ETH quantifier (2) now assumes the form

$$\Delta^2_{A,\mathrm{eq}} := \sum_n p_n (A_{nn} - A_{\mathrm{eq}})^2. \tag{22}$$

By means of a straightforward modification of the arguments in the previous section, this quantity can again be shown to assume its maximal (minimal) value when choosing the basis $|n\rangle$ such that A is diagonal (has constant diagonal matrix elements) in every eigenspace of H. The basis-independent upper bound analogous to (18) is then given by

$$\hat{\Delta}^2_{A,\mathrm{eq}} := \sum_E f(E)\,\mathrm{tr}[(P_E A)^2] - A^2_{\mathrm{eq}}, \tag{23}$$

where the sum runs over all pairwise distinct eigenvalues of H.

IV. EXAMPLE FOR BASIS DEPENDENCE OF THE WEAK ETH

To illustrate the basis dependence of weak eigenstate thermalization, we consider the spin-1 Hamiltonian with periodic boundary conditions

$$H = -\sum_{l=1}^{L} [s^+_l (s^-_{l+1})^2 s^+_{l+2} + s^-_l (s^+_{l+1})^2 s^-_{l+2}], \tag{24}$$

where $s^\pm_l := s^x_l \pm \mathrm{i} s^y_l$, s^a_l $(a = x, y, z)$ are the standard spin-1 operators acting on site l, and $s^a_{l+L} := s^a_l$.

This model plays a prominent role in Ref. [25], where it has been shown to be magnetization- and dipole-moment-conserving (see also Appendix C), and, most importantly, to exhibit Hilbert space fragmentation. More precisely speaking, the main focus in Ref. [25] was on the correspondingly modified Hamiltonian (24) with open boundary conditions, while we will choose periodic boundary conditions in the following. This modification is essential since it ensures that the results from Refs. [15–20] are applicable, guaranteeing the existence of at least one energy eigenbasis in which the weak ETH holds, namely, any simultaneous eigenbasis of H and T.

We focus on the single-site magnetization $A = s^z_1$ and the ETH quantifier $\Delta^2_{A,\mathrm{eq}}$ from Eq. (22) for the canonical ensemble (Gibbs state)

$$p_n = Z^{-1} e^{-\beta E_n} \tag{25}$$

with $Z := \sum_n e^{-\beta E_n}$. Bearing in mind Sec. III B and the very generally established equivalence of the canonical and microcanonical ensembles in sufficiently large systems [19,20,26–28], it is expected that the canonical $\Delta^2_{A,\mathrm{eq}}$ from Eq. (22) and its microcanonical counterpart Δ^2_A from (2) show the same scaling behavior with the degrees of freedom L in a fixed basis. A more detailed justification will be provided in Sec. V B.

In Fig. 1, we show $\Delta^2_{A,\mathrm{eq}}$ as a function of $1/L$ for two different choices of the energy eigenbasis and system sizes $L = 7, 9, \ldots, 19$. Details on how $\Delta^2_{A,\mathrm{eq}}$ was evaluated numerically using dynamical typicality methods [29,30] are provided in Appendix C.

The first basis choice (blue squares in Fig. 1) consists of translationally invariant eigenstates $|n\rangle$. In this case, the results from Refs. [15–20] rigorously demonstrate the validity of the weak ETH. In combination with the above-mentioned equivalence of the ensembles, $\Delta^2_{A,\mathrm{eq}}$ is thus guaranteed to approach zero as $L \to \infty$ for any choice of the inverse temperature β. This is confirmed by our numerics upon extrapolating the finite-size results (blue lines): Fitting the numerical data to a linear function $\Delta^2_{A,\mathrm{eq}} = a + b/L$ yields values $|a| \leqslant 0.002$ (with uncertainties less than 0.002) for all β values shown in the figure.

The second basis choice (orange circles in Fig. 1) is the maximally ETH-violating basis identified in Sec. III, meaning that the observable $A = s^z_1$ is diagonal in every degenerate energy subspace. In this basis, we observe that the ETH quantifier $\Delta^2_{A,\mathrm{eq}}$ does *not* generally decay to zero as the system size is increased. Extrapolation to $L \to \infty$ (orange lines) instead yields a positive, β-dependent value as quoted in each of the figure panels. Only for asymptotically low temperatures (large β) $\Delta^2_{A,\mathrm{eq}}$ vanishes (and almost uniformly so in the system size L).

From a practical point of view, this amounts to the most important result of this paper: an explicit example where the weak ETH is violated in one basis, but satisfied in another one.

V. ANALYTICAL APPROACH

In the example from the previous section, we inspected the ETH quantifier $\Delta^2_{A,\mathrm{eq}}$ for the canonical ensemble (25). By tuning the inverse temperature β, we thus can effectively select an energy window around $E = \mathrm{tr}\{\rho_{\mathrm{eq}} H\}$, and by varying β we can scan the entire spectrum of the Hamiltonian for ETH violations. In this section, we provide a more rigorous treatment of this connection between energy windows in the canonical and microcanonical formalisms.

A. A simple special case

In this subsection, we restrict ourselves to Hamiltonians H and local observables A which satisfy several simplifying assumptions, and we show that these assumptions are sufficient to imply a violation of the weak ETH. An important example of this kind is the setup from Sec. IV above.

We consider a system of large but finite size L and our first assumption is that it exhibits a finite number N of energies $\{E_n\}_{n=1}^N$. Typical examples are spin-lattice models such as in Eq. (24), giving rise to an exponential growth of N with L. Second, we focus on cases where $A_{\mathrm{th}} = 0$ for any microcanonical energy window with concomitant subset $S \subset \{1, \ldots, N\}$

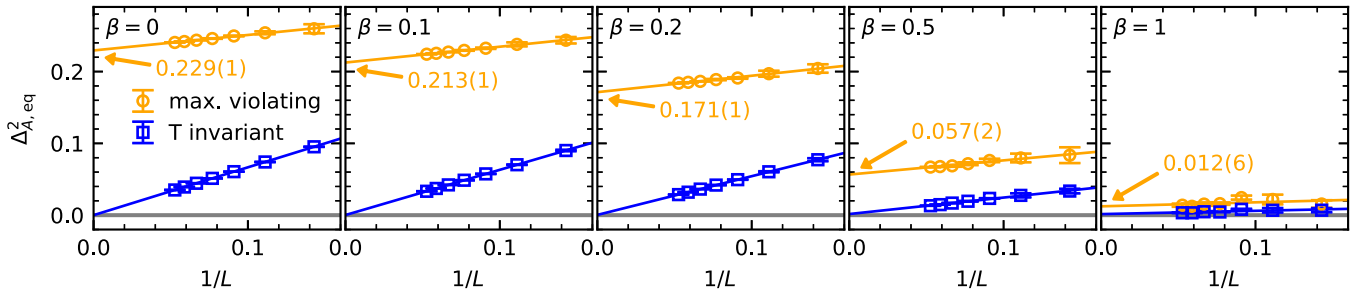


FIG. 1. ETH quantifier $\Delta^2_{A,\mathrm{eq}}$ from (22) vs L^{-1} for the canonical ensemble (25), Hamiltonian H from (24), and observable $A = s^z_1$, for two basis choices: one where A is diagonal in all energy eigenspaces (maximal ETH violation, orange) and a translationally invariant one (provably satisfying weak ETH, blue). Panels correspond to different values of the inverse temperature β. Symbols are numerical results obtained via dynamical typicality with error bars indicating the corresponding standard error (cf. Appendix C; most error bars are actually not discernible on the scale of these plots); lines are linear fits and orange numbers the resulting extrapolation of $\Delta^2_{A,\mathrm{eq}}$ to $L \to \infty$ (y-axis intercept, including, in parentheses, the uncertainty in the last digit).

in Eq. (1). Third, we assume that the local observable A exhibits a finite range of possible measurement outcomes (eigenvalues of A). More precisely speaking the operator norm $\|A\|_{\mathrm{op}}$ (largest eigenvalue in modulus of A) is assumed to remain bounded, say $\|A\|_{\mathrm{op}} < a$, for all L. It follows that

$$A^2_{nn} \leqslant a^2 \tag{26}$$

independently of n and L. Finally, we assume that the quantity

$$\Delta^2_{A,\mathrm{tot}} := \frac{1}{N}\sum_{n=1}^{N} A^2_{nn} \tag{27}$$

exhibits the property

$$\Delta^2_{A,\mathrm{tot}} \geqslant b > 0 \tag{28}$$

for all L. One thus can infer that $a^2 \geqslant b$.

We remark that while Eq. (2) (with $A_{\mathrm{th}} = 0$) may be viewed as an average over a relatively small microcanonical subset S, Eq. (27) represents the corresponding average over the full set $\{1, \ldots, N\}$. Hence, Eq. (28) amounts to yet another variety of ETH violation, slightly different from the previously discussed violation of the strong or weak ETH. Incidentally, $\Delta^2_{A,\mathrm{tot}}$ in Eq. (27) also happens to coincide with the ETH quantifier $\Delta^2_{A,\mathrm{eq}}$ from Eq. (22) for the canonical ensemble (25) with inverse temperature $\beta = 0$.

Let $S_1, \ldots, S_M$ be a finite partition of $\{1, \ldots, N\}$, i.e., $S_1 \cup \cdots \cup S_M = \{1, \ldots, N\}$ and $S_i \cap S_j = \emptyset$ if $i \neq j$. Furthermore, we denote by N_b the number of all indices $n \in \{1, \ldots, N\}$ with the property $A^2_{nn} \geqslant b/2$. Together with (26)–(28) it follows that

$$b \leqslant \frac{1}{N}\sum_{n=1}^{N} A^2_{nn} \leqslant \frac{1}{N}\left(N_b\, a^2 + (N - N_b)\frac{b}{2}\right) \tag{29}$$

and thus

$$\frac{N_b}{N} \geqslant \frac{b}{2a^2 - b} \geqslant \frac{b}{2a^2}, \tag{30}$$

where we exploited that $a^2 \geqslant b > 0$ in the last step [see in and below Eq. (28)]. Next, we denote by ν_m the number of all indices $n \in S_m$ with the property $A^2_{nn} \geqslant b/2$. It readily follows that $\nu_m/|S_m| \geqslant N_b/N$ for at least one $m \in \{1, \ldots, M\}$. Focusing on such a particular m value we thus obtain

$$\frac{1}{|S_m|}\sum_{n\in S_m} A^2_{nn} \geqslant \frac{\nu_m}{|S_m|}\frac{b}{2} \geqslant \frac{N_b}{N}\frac{b}{2} \geqslant \frac{b^2}{4a^2}. \tag{31}$$

Observing that the right-hand side is positive and independent of L, and assuming that the partition of $\{1, \ldots, N\}$ has been chosen such that each S_m corresponds to a microcanonical energy window as specified below Eq. (1), it follows that the variance in Eq. (2) is lower bounded by $b^2/4a^2 > 0$ for at least one microcanonical energy window, and thus the weak ETH is violated.

In summary, for setups satisfying the three assumptions from the beginning of this subsection, a nonzero value of $\Delta^2_{A,\mathrm{tot}}$ (tantamount to an ETH violation over the entire spectrum) implies a violation of the weak ETH in its standard formulation for microcanonical energy windows [15–20]. Notably, this applies to the example from the leftmost panel in Fig. 1 because $\Delta^2_{A,\mathrm{tot}}$ is equal to $\Delta^2_{A,\mathrm{eq}}$ for $\beta = 0$ [see below Eq. (28)].

B. More general treatment

As seen in Sec. I, the main focus in the context of the ETH, and of statistical physics in general, is on large system sizes L. It is therefore tacitly taken for granted that the considered Hamiltonians, states, and observables are such that the resulting properties of actual interest exhibit a well-defined thermodynamic limit $L \to \infty$. Most importantly, instead of energies E, one thus works with the corresponding energy densities

$$e := (E - \mathcal{E})/L, \tag{32}$$

where $\mathcal{E}$ is some physically reasonable (and generally L-dependent) reference energy, for instance the ground-state energy, or the average over all energy eigenvalues $\{E_n\}_{n=1}^N$ in cases where N is finite [see above Eq. (24)]. In particular, the counterparts of the energy eigenvalues E_n are given by

$$e_n := (E_n - \mathcal{E})/L. \tag{33}$$

Along these lines, the definitions in and around Eq. (1) are modified as follows: Given some energy density e, the set S consists of all indices m with the property that $e_m \in [e, e + \delta]$, where δ is macroscopically small and microscopically large,

meaning that it approaches zero for $L \to \infty$ in such a way that the number $|S|$ of elements in S tends to infinity. In other words, the corresponding quantity A_{th} in Eq. (1) is understood (and formally defined) analogously as when going over, e.g., from classical point particles to (local) particle densities, and it is taken for granted that such a "local density" of the A_{mm}'s in (1) is well defined and largely independent of any further details of how δ approaches zero for large L. In particular, $A_{\text{th}} = A_{\text{th}}(e)$ will be a practically L- and δ-independent function of e for sufficiently large L. Again in other words, this is the standard definition in statistical mechanics of the microcanonical expectation value of A for a system with energy density e, and as such can and will be considered as "well defined" from now on.

As a consequence, upon considering the auxiliary quantities $\tilde{A}_{nn} := A_{nn} - A_{\text{th}}(e_n)$ instead of A_{nn}, the second assumption above Eq. (26) takes the form $\tilde{A}_{\text{th}} = 0$, and is readily seen to be fulfilled for asymptotically large L. Likewise, one sees that the ETH quantifier for A_{nn} in Eq. (2) becomes asymptotically equal to the ETH quantifier for $\tilde{A}_{nn}$. Hence, the line of reasoning in Sec. V A can be adapted such that it remains valid even without the second assumption above Eq. (26). The final conclusion is that the weak ETH must be violated whenever

$$\frac{1}{N}\sum_{n=1}^{N}[A_{nn} - A_{\text{th}}(e_n)]^2 \geqslant b > 0 \tag{34}$$

for all sufficiently large L.

By means of analogous arguments as in our above considerations regarding $A_{\text{th}} = A_{\text{th}}(e)$, Eq. (2) can be rewritten as

$$\Delta_A^2(e) = \frac{1}{|S|}\sum_{n\in S}[A_{nn} - A_{\text{th}}(e_n)]^2, \tag{35}$$

and it is again taken for granted that this quantity exhibits a well-defined thermodynamic limit and thus will be a practically L- and δ-independent function of e for sufficiently large L. Accordingly, the weak ETH [see below Eq. (2)] now requires that $\Delta_A^2(e)$ approaches zero for large L. More precisely speaking, this must be the case for any given local observable A and any given energy density e. In turn, this implies that in order to show a violation of the weak ETH (and thus also of the strong ETH) it is sufficient that $\Delta_A^2(e)$ approaches a nonvanishing large-L limit for at least one (local) observable A and one energy density e.

Next we recall some elementary notions from the textbook treatment of many-body systems in terms of the microcanonical and the canonical formalism. As usual in this context, we thus implicitly take it for granted that these notions are well defined and that some of their basic qualitative properties (see below) are as commonly expected and indeed observed in many examples.

To begin with, the number of energy eigenvalues below any given upper limit E is denoted as $\Omega(E) := \sum_n \Theta(E - E_n)$, where $\Theta(x) := 1$ if $x \geqslant 0$ and $\Theta(x) := 0$ otherwise. More precisely speaking, the step of $\Theta(x)$ at $x = 0$ is considered to actually be slightly "washed out" such that $\Omega(E)$ becomes a reasonably smooth function of E with a well-defined derivative

$$\omega(E) := \Omega'(E) = \sum_n \delta(E - E_n), \tag{36}$$

where also $\delta(x) := \Theta'(x)$ now exhibits a slightly washed out δ peak at $x = 0$. Put differently, those washed out Θ and δ functions are understood to be chosen such that $\omega(E)$ can be considered as the (local) density of the energy levels E_n (analogously to the discussion in the second paragraph of this section). Once this somewhat subtle point of the standard microcanonical formalism is settled, the Boltzmann entropy can be defined in different (practically) equivalent ways, for instance as

$$\mathcal{S}_{\text{B}}(E) := k_{\text{B}} \ln \Omega(E) \tag{37}$$

with Boltzmann constant k_{B}. Finally, the temperature is defined as

$$T(E) := 1/\mathcal{S}_{\text{B}}'(E). \tag{38}$$

Next, we return to the canonical formalism as adopted already in Sec. IV. In particular, we focus again on the standard canonical level populations p_n from Eq. (25). Accordingly, the density operator ρ_{eq} in Eq. (20) can be identified with the canonical ensemble (Gibbs state)

$$\rho_{\text{eq}} = Z^{-1} e^{-\beta H}. \tag{39}$$

Likewise, A_{eq} in Eq. (21) amounts to the corresponding canonical expectation value of A, and is now implicitly understood to be a function of β. To make further progress, we exploit that generically the energy levels E_n become extremely (exponentially) dense for large L such that the level populations p_n in Eq. (25) are practically constant for a large number of closely adjacent E_n's. As far as the contributions to the sum in (21) are concerned, one thus can approximate the large number of corresponding A_{nn}'s by their local average $A_{\text{th}}(e_n)$ [see in and below Eq. (33)], yielding the asymptotically exact large-L approximation

$$A_{\text{eq}}(\beta) = \sum_n p_n A_{\text{th}}(e_n). \tag{40}$$

To make further progress, let us first consider, as a simple preliminary exercise, the partition function Z, which is defined [see also below (25)] for any given $\beta > 0$ as

$$Z := \sum_n e^{-\beta E_n}, \tag{41}$$

where we omitted the dependence of Z on β. Multiplying the right-hand side by $1 = \int dE\, \delta(E - E_n)$ and exploiting Eq. (36), one recovers the well-known relation

$$Z = \int dE\, \omega(E)\, e^{-\beta E}. \tag{42}$$

As usual, in case we are dealing with a model exhibiting a finite number N of energy levels [see above Eq. (24)], also $\beta \leqslant 0$ is admissible in Eqs. (41) and (42). Moreover, the case $\beta < 0$ can be readily reduced to the case $\beta > 0$ by considering the Hamiltonian $-H$ instead of H. Finally, the case $\beta = 0$ (infinite temperature) is covered by the considerations around Eq. (34). For simplicity, we therefore continue to focus on $\beta > 0$.

Returning to the actual quantity of interest in Eq. (40), we can rewrite it with the help of Eqs. (25) and (33) by means of

a similar line of reasoning as in the previous paragraph as

$$A_{\mathrm{eq}}(\beta) = \int dE A_{\mathrm{th}}((E-\mathcal{E})/L)\, Z^{-1} e^{-\beta E} \omega(E). \tag{43}$$

From Eqs. (36)–(38) one furthermore can infer that $\omega(E) = \Omega(E)/k_{\mathrm{B}}T(E)$ and thus

$$A_{\mathrm{eq}}(\beta) = \int dE\, A_{\mathrm{th}}((E-\mathcal{E})/L)\, Q(E), \tag{44}$$

$$Q(E) := [Z\, k_{\mathrm{B}} T(E)]^{-1} e^{q(E)}, \tag{45}$$

$$q(E) := k_{\mathrm{B}}^{-1} \mathcal{S}_{\mathrm{B}}(E) - \beta E, \tag{46}$$

where we omitted the dependence of $Q(E)$ and $q(E)$ on β. Going over from the integration variable E to $e := (E-\mathcal{E})/L$ [cf. Eq. (32)], and employing the correspondingly transformed quantities

$$\tilde{\mathcal{S}}_{\mathrm{B}}(e) := \mathcal{S}_{\mathrm{B}}(eL+\mathcal{E})/k_{\mathrm{B}}L, \tag{47}$$

$$\tilde{T}(e) := k_{\mathrm{B}} T(eL+\mathcal{E}), \tag{48}$$

$$\tilde{Q}(e) := L[Z\, \tilde{T}(e)]^{-1} e^{\tilde{q}(e)}, \tag{49}$$

$$\tilde{q}(e) := L[\tilde{\mathcal{S}}_{\mathrm{B}}(e) - \beta e] + \beta \mathcal{E}, \tag{50}$$

it follows that

$$A_{\mathrm{eq}}(\beta) = \int de\, A_{\mathrm{th}}(e)\, \tilde{Q}(e). \tag{51}$$

From Eqs. (38), (47), and (48), we furthermore can infer that $\tilde{\mathcal{S}}_{\mathrm{B}}'(e) = 1/\tilde{T}(e)$. Hence, the maximum of $\tilde{q}(e)$ is determined by $\tilde{q}'(e) = 0$, implying for the maximizing value of e, which we denote by $e(\beta)$, the implicit definition $\tilde{T}(e(\beta)) = 1/\beta$. Finally, one finds for the second derivative [and omitting all arguments $e(\beta)$] that $\tilde{q}'' = -L\tilde{T}'/\tilde{T}^2 = -L\beta^2\tilde{T}'$. Taking for granted the common assumption that the entropy density in Eq. (47) exhibits a well-defined thermodynamic limit (see also the first two paragraphs of this section), and that $\tilde{T}' > 0$ (positive heat capacity), it follows that $\tilde{q}(e)$ develops a very sharp maximum at $e(\beta)$ for large L. [Note that this argument would break down for $\beta = 0$.] Finally, choosing $A = \mathbb{1}$ in Eq. (51) implies $\int de\, \tilde{Q}(e) = 1$. Altogether, $\tilde{Q}(e)$ in Eq. (49) thus approaches a Dirac δ function for $L \to \infty$ and Eq. (51) yields the asymptotically exact large-L approximation

$$A_{\mathrm{eq}}(\beta) = A_{\mathrm{th}}(e(\beta)). \tag{52}$$

This finding is very closely related to the commonly assumed equivalence of the canonical and microcanonical ensembles [see also the discussion below Eq. (25)].

Analogously, when choosing the canonical level populations (25), the ETH quantifier in Eq. (22) becomes a function of β and can be shown to satisfy the asymptotically exact large-L approximation

$$\Delta^2_{A,\mathrm{eq}}(\beta) = \Delta^2_A(e(\beta)), \tag{53}$$

where $\Delta^2_A(e)$ is defined in Eq. (35).

This is the main result of our present section: If the canonical ETH quantifier $\Delta^2_{A,\mathrm{eq}}(\beta)$ approaches a nonzero large-L limit for some $\beta > 0$, then the same applies to $\Delta^2_A(e(\beta))$ for the specific local observable A under consideration and for the specific energy density $e(\beta)$ (corresponding to the temperature $T = 1/k_{\mathrm{B}}\beta$). As explained below Eq. (35), this implies a violation of the weak ETH. Regarding the cases $\beta \leqslant 0$, we also recall the discussion below Eq. (42). All of these considerations apply again, in particular, to the example from Sec. IV.

VI. FURTHER IMPLICATIONS

A. Equilibration

Let us consider an arbitrary but fixed initial condition $\rho(0)$, which generally may be a pure or mixed state far from equilibrium, and which then evolves in time according to $\rho(t) = e^{-iHt}\rho(0)e^{iHt}$ (in units with $\hbar = 1$). The expectation value of an observable A at time t is thus given by $\langle A\rangle_t := \mathrm{tr}\{\rho(t)A\}$ and can be rewritten as

$$\langle A\rangle_t = \sum_{mn} \rho_{mn}(0)\, A_{nm} e^{i(E_n - E_m)t}, \tag{54}$$

where $\rho_{mn}(t) := \langle m|\rho(t)|n\rangle$ and $A_{nm} := \langle n|A|m\rangle$. Systems with many degrees of freedom are commonly said to exhibit equilibration if the expectation values (54) stay close to some constant value for the vast majority of all sufficiently late times t. (The excluded minority of times comprises the initial relaxation process as well as the very rare but unavoidable quantum recurrences.) This constant value can be identified with the long-time average of (54), which in turn can be rewritten as

$$\overline{\langle A\rangle_t} = \sum_{E_m = E_n} \rho_{mn}(0)\, A_{nm}, \tag{55}$$

where $\overline{f(t)}$ denotes the long-time average $\lim_{\tau\to\infty} \frac{1}{\tau}\int_0^\tau dt\, f(t)$ of an arbitrary function $f(t)$, and the sum runs over all indices m and n with the property $E_m = E_n$. In the absence of degeneracies, the basis is unique (up to trivial phase factors), and the condition $E_m = E_n$ in (55) is tantamount to $m = n$. However, when H exhibits degeneracies, there are many possible choices of the basis and things are more involved. Admitting general initial conditions $\rho(0)$ [without any further assumptions or restrictions concerning the matrix elements $\rho_{mn}(0)$ for $m \neq n$], it follows that the long-time average simplifies to

$$\overline{\langle A\rangle_t} = \sum_n \rho_{nn}(0)\, A_{nn} \tag{56}$$

if and only if the basis $|n\rangle$ is chosen so that A is diagonal in every eigenspace of H. Finally, the result in Eq. (56) may also be rewritten as $\mathrm{tr}\{\rho_{\mathrm{eq}}\, A\}$, where ρ_{eq} is the equilibrium or diagonal ensemble from (20) with $p_n := \rho_{nn}(0)$.

In conclusion, our main finding regarding the issue of equilibration is that, in order to represent the long-time average in terms of a diagonal ensemble, the pertinent eigenbasis of H must maximize the ETH quantifier from (2), meaning that its value is given by $\hat{\Delta}^2_A$ from (18). As an aside it follows that the corresponding basis $|n\rangle$ and thus the diagonal ensemble generally depend on the choice of the observable A.

B. Autocorrelation functions

Next, let us consider a system at equilibrium, described by some suitable equilibrium ensemble of the general form (20). Similarly as the corresponding equilibrium expectation values in Eq. (21), the so-called dynamical autocorrelation function is defined as

$$C_A(t) := \mathrm{tr}\{\rho_{\mathrm{eq}} A A(t)\} - A_{\mathrm{eq}}^2, \tag{57}$$

where $A(t) := e^{iHt} A e^{-iHt}$ is the observable at time t in the Heisenberg picture. Similarly as in Eqs. (54) and (55) it follows that

$$\overline{C_A(t)} := \sum_{E_m=E_n} p_n |A_{nm}|^2 - A_{\mathrm{eq}}^2, \tag{58}$$

and similarly as in Eq. (56) that

$$\overline{C_A(t)} = \sum_n p_n A_{nn}^2 - A_{\mathrm{eq}}^2 \tag{59}$$

if and only if the basis $|n\rangle$ is chosen such that A is diagonal in every eigenspace of H. For this choice, comparison with Eq. (22) and a straightforward calculation [similarly as in Eq. (8)] finally yield

$$\overline{C_A(t)} = \Delta_{A,\mathrm{eq}}^2 = \hat{\Delta}_{A,\mathrm{eq}}^2, \tag{60}$$

where we exploited (23) and $p_n = f(E_n)$ [see below Eq. (20)] in the second identity.

In conclusion, our maximized ETH quantifier is of immediate relevance for the long-time average of the dynamical autocorrelation function. Notably, this representation of $\hat{\Delta}_{A,\mathrm{eq}}^2$ can be used to calculate the basis-independent maximal violation numerically, which we exploited in Fig. 1 to evaluate said quantity via dynamical typicality methods (cf. Appendix C).

On the other hand, the time-averaged autocorrelation function $\overline{C_A(t)}$ can be bounded from below via Mazur inequalities [31–34] in terms of overlaps between the observable A and conserved quantities in the system. Through the relation (60), the Mazur bounds thus also yield lower bounds for the maximal ETH violation, providing a connection between the absence of eigenstate thermalization and the presence of conservation laws.

C. Rethermalization

We focus once more on the canonical ensemble from Eqs. (25) or (39), and on the concomitant time-averaged autocorrelation functions as discussed in Sec. VI B. Our goal is to show that these quantities exhibit an interesting connection to the issue of thermalization.

Let us therefore consider a modification (perturbation) of our original Hamiltonian H of the form

$$H_g := H - gA, \tag{61}$$

where A is a local operator (perturbation) and g a small parameter. (Later this perturbation A will again be identified with the observable of interest. Moreover, the coupling parameter g has nothing to do with the multiplicities g_E in Sec. III A.) Similarly as above Eq. (54), the system's initial condition is denoted as $\rho(0)$, and we assume that it is given by the canonical ensemble pertaining to the modified Hamiltonian (61), i.e.,

$$\rho(0) := Z_g^{-1} e^{-\beta H_g} \tag{62}$$

with $Z_g := \mathrm{tr}\{e^{-\beta H_g}\}$. Physically, the system may be viewed to be in thermal equilibrium with respect to the Hamiltonian H_g for all times $t < 0$, to experience a sudden change of the Hamiltonian at $t = 0$ (quantum quench), and to be governed by H for $t > 0$. Since A in Eq. (61) is a local operator, we are moreover dealing with a so-called local quench. Generally, $\rho(0)$ is thus a nonequilibrium initial state with respect to the Hamiltonian H of our actual system of interest, and its time evolution is expected to exhibit some nontrivial equilibration process as discussed in the first part of Sec. VI A.

Next we restrict ourselves to the situation that we consider the same local observable A that also plays the role of the perturbation operator in (61). In this case it becomes possible to utilize the generalization of Onsager's regression hypothesis from Ref. [35], consisting in the analytical approximation

$$\langle A\rangle_t - A_{\mathrm{eq}} = g\beta \sum_{k=0}^{\infty} \frac{(i\beta)^k}{(k+1)!} \frac{d^k}{dt^k} C_A(t). \tag{63}$$

Basically, its relative error can be shown to become arbitrarily small for sufficiently small values of $g\beta\|A\|_{\mathrm{op}}$, where $\|A\|_{\mathrm{op}}$ is the operator norm of A (largest eigenvalue in modulus). A more detailed and rigorous discussion of this error bound can be found in Refs. [35,36].

Of particular interest in our present context is the long-time average [see in and around Eq. (55)]. Under very weak assumptions regarding the long-time behavior of $C_A(t)$, which we tacitly take for granted, the long-time average of $d^k C_A(t)/d^k t$ vanishes for all $k \geqslant 1$, and we can conclude from Eq. (63) that

$$\overline{\langle A\rangle_t} - A_{\mathrm{eq}} = g\beta\, \overline{C_A(t)}. \tag{64}$$

The difference on the left-hand side quantifies how well the expectation values $\langle A\rangle_t$ approach the canonical equilibrium value A_{eq} in the long run [see also the discussion below Eqs. (39) and (54)]. In particular, if this difference turns out to remain finite in the thermodynamic limit, we can conclude that the system does not exhibit thermalization [37]. According to Eq. (60) and the results from Sec. IV, it follows that this is indeed the case for the particular Hamiltonian from Eq. (24). In the same way, absence of thermalization can be deduced in full generality whenever the considered model violates the weak ETH in some basis.

In conclusion, the existence of a basis in which the weak ETH is satisfied, as demonstrated in Refs. [15–20] for translationally invariant systems, does not guarantee rethermalization after a local quench for systems with degeneracies, even though it is sufficient for systems without degeneracies [21,22,38]. Rethermalization can only be established if the basis-independent upper bound $\hat{\Delta}_{A,\mathrm{eq}}^2$ from (23) vanishes in the thermodynamic limit. The physically relevant generalization of the weak ETH should thus be formulated in terms of $\hat{\Delta}_{A,\mathrm{eq}}^2$ or $\hat{\Delta}_A^2$ from (18). Unfortunately, we are not aware of any proofs of such $\hat{\Delta}_A^2 \to 0$ statements for general classes of systems.

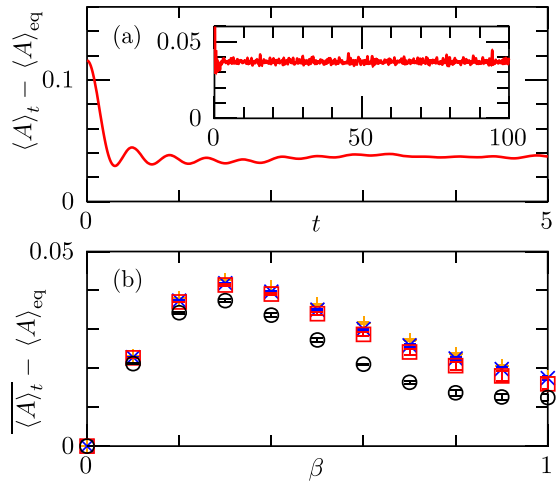


FIG. 2. (a) Numerically obtained time-dependent expectation values $\langle A\rangle_t - A_{\rm eq}$ for the observable $A = s_1^z$, the Hamiltonian (24), the initial condition (62), and the canonical ensemble (39) with parameter values $L = 15$, $g = 1$, and $\beta = 0.2$, see also Eqs. (21), (54), and (61). Main plot: Initial relaxation behavior for $t \in [0, 5]$. Inset: Long-time behavior for $t \in [0, 100]$. (b) Long-time average of the same expectation values as in (a) versus β. Orange crosses, blue crosses, and red squares correspond to $L = 11$, 13, and 15, respectively. Black circles with error bars: Extrapolations for $L \to \infty$. For further details regarding the numerical methods and the extrapolations we refer to Fig. 1 and its discussion in the main text.

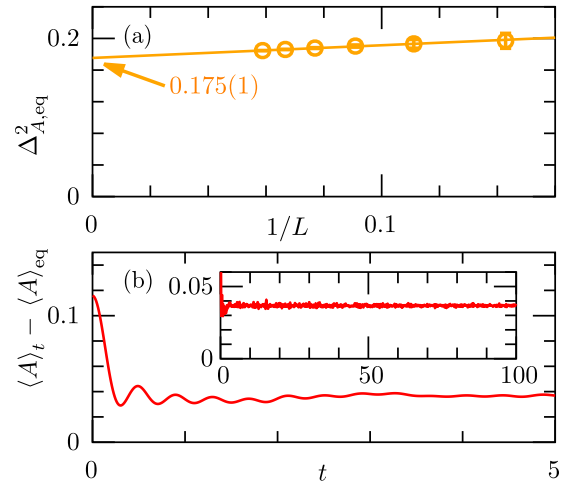


FIG. 3. (a) Same as the middle panel ($\beta = 0.2$) of Fig. 1, but now for the perturbed, nondegenerate Hamiltonian H' from Eq. (65). (b) Same as Fig. 2(a), but now again for the perturbed system H'.

A numerical illustration of these general analytical predictions is provided in Fig. 2 for the same model system as in Fig. 1. Figure 2(a) depicts the initial temporal relaxation process and the approach of an approximately steady long-time value which is clearly different from the thermal equilibrium value. The remnant small fluctuations (inset) are a well-known finite-size effect. Figure 2(b) shows the corresponding long-time averages for various different β and L values. Once again this exemplifies the analytically predicted absence of rethermalization after a local quench (except for the trivial case $\beta = 0$). Moreover, upon comparison with the results from Fig. 1 one could also confirm that the analytical approximation (64) [see also Eq. (60)] is indeed quite well satisfied. We omit here such a quantitative comparison since it goes beyond the actual main themes of this work.

D. Degeneracies and numerical ETH studies

The basis dependence of eigenstate thermalization observed here can only occur in many-body systems with degeneracies, which typically have their origin in some symmetries (or corresponding conserved quantities). As usual in the context of symmetry considerations, their implications are generally regarded as very interesting and useful in spite of the fact that these symmetries may only be approximately satisfied in realistic systems. This means that degeneracies are also only approximate, yet they can still have significant, macroscopically observable effects on the system. For example, if a system with exact symmetries fails to thermalize, a nearby, approximately symmetric cousin could still fail to thermalize, or it could exhibit extremely slow relaxation and fail to thermalize on any practically relevant timescale [39–46].

The critical question in our present case is whether the ETH quantifiers (2) and (22) in a weakly perturbed system without degeneracies approach zero or a nonzero value in the thermodynamic limit. In the former case, choosing the translationally invariant basis in the idealized (unperturbed) system would still yield the right conclusions for the more realistic (slightly perturbed) systems without degeneracies. In the latter case, however, any conclusions drawn from the ETH quantifiers in the translationally invariant eigenbasis would be wrong not only in the idealized (translationally invariant) system itself, but also in the weakly perturbed modifications without degeneracies.

To test this, we perturb the Hamiltonian (24) by adding local magnetic fields in the z direction with amplitudes h_l drawn from a normal distribution with vanishing mean and standard deviation 0.1:

$$H' = -\sum_{l=1}^{L} \left[s_l^+ (s_{l+1}^-)^2 s_{l+2}^+ + s_l^- (s_{l+1}^+)^2 s_{l+2}^- + h_l\, s_l^z \right]. \quad (65)$$

The additional fields break the translation and spatial reflection symmetries, and we have verified numerically that this system indeed exhibits no degeneracies.

The results in Fig. 3(a) demonstrate that the violation of the weak ETH persists in the nondegenerate regime since the quantity $\Delta^2_{A,\rm eq}$ from (22), now being unique, approaches 0.175 as $L \to \infty$. Consequently, the system cannot be expected to rethermalize after a local quench, and Fig. 3(b) indeed confirms this absence of thermalization explicitly for a similar quench setup as in Fig. 2.

The crucial consequence of these results is that exploiting symmetries to evaluate the weak ETH numerically in a system with degeneracies can lead to physically wrong conclusions: Using translationally invariant eigenstates to calculate $\Delta^2_{A,\rm eq}$ from (22) in the system from (24) would suggest that the weak ETH is satisfied, and one could be tempted to conclude that this system rethermalizes after local quenches. This

conclusion would be wrong for both the symmetric, idealized case with degeneracies and the close-by, weakly perturbed versions without degeneracies from (65).

In principle, analogous problems may arise also for the strong (or any other) version of the ETH and numerical studies thereof. For example, if one evaluates the diagonal matrix elements of some observable by exploiting translational invariance in a system that is also reflection symmetric (and thus exhibits energy degeneracies, cf. Sec. II), there is no guarantee that a so-observed agreement with the strong ETH is inherited by the physically relevant basis in which the observable is diagonal in degenerate subspaces. Likewise, there is no guarantee that physically realistic, weakly perturbed, nondegenerate variations of such a system resemble the unperturbed behavior observed in the translation-symmetric basis.

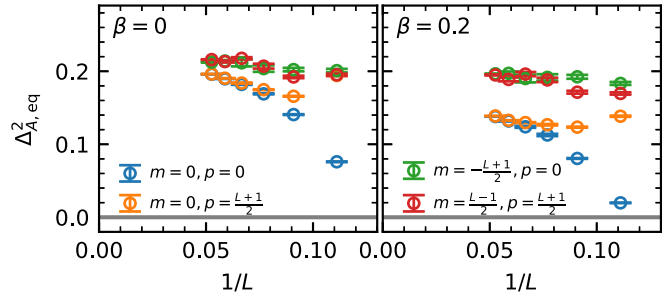


FIG. 4. Same as in Fig. 1 but now employing the maximally ETH-violating basis within various magnetization (m) and dipole-moment (p) subsectors (see also Appendix C).

E. Conserved quantities and symmetry sectors

It is widely taken for granted that information about conserved quantities represented by local extensive observables (sums of local operators) needs to be included to describe a system's long-term properties. The thermal state for a system conserving the total magnetization or the number of particles, for example, accounts for this either via appropriate restrictions to a macroscopically small window of states with similar expectation values of the conserved quantities (microcanonical approach), or via additional Lagrange multipliers besides the inverse temperature (grand-canonical approach) [47]. Likewise, equilibrium properties of integrable systems are described by generalized Gibbs ensembles (GGEs) that include their extensive number of conserved quantities [9,48,49].

Remarkably, previous results in the context of weak eigenstate thermalization (e.g., the proofs from Refs. [15–20] for translationally invariant eigenbases) do *not* need to include information about conserved quantities. However, tests of the strong ETH should usually be restricted to symmetry sectors of local conserved quantities [18,50,51]. On the other hand, it is widely believed that conserved quantities represented by nonlocal and/or many-body operators usually do not need to be considered when assessing the diagonal ETH [18,50–52]. This distinction is crucial because any quantum system exhibits as many conserved quantities as energy levels (take the projectors onto energy eigenspaces), so without a criterion for what constitutes physically relevant and irrelevant conserved quantities, a statement like the ETH would become void.

Our example system from Sec. IV conserves the energy and the (nonlocal) quasimomentum and spatial parity. It also exhibits two additional local conserved quantities: the magnetization and the dipole moment in the z direction [see also below Eq. (24) and Appendix C]. These were not taken into account in Fig. 1. For completeness, we show in Fig. 4 that the restriction to simultaneous magnetization and dipole-moment subsectors does not remove the ETH violation in the most dangerous basis in this model. On the other hand, it is impossible to restrict to a simultaneous subsector of definite magnetization, dipole moment, and quasimomentum because the latter two quantities do not commute.

A series of recent works have suggested extensions of thermal states [53–55] and the ETH [56–58] in the presence of noncommuting conserved quantities (see also the review [59]), which gives rise to degeneracies among other subtleties (cf. Sec. II). However, the mechanisms identified there, and the fixes suggested, do not apply to our present problem of basis-dependent ETH quantifiers. In all of these works, it is implicitly or explicitly assumed that the underlying symmetries are continuous and that the resulting conserved quantities are extensive operators. In particular, the equilibrium value $\langle A\rangle_{\mathrm{eq}}$ used in the examples from Figs. 2 and 3 coincides with the value that would be obtained from a non-Abelian thermal state (NATS) [56–58] constructed with the (nonlocal) conserved quasimomentum taken into account. The reason is that the expectation value of this operator vanishes in the initial state (62), hence, the associated Lagrange multiplier is zero in the NATS, and thus it coincides with the equilibrium state from (20) and (25). In other words, the NATS concept does not help to recover the correct long-term limit of the dynamics in Figs. 2 and 3.

Specifically in the context of non-Abelian ETH generalizations, the focus has mostly been on SU(2) symmetry in spin-$\frac{1}{2}$ models. For such a Heisenberg-type model, it was numerically observed in Ref. [57] that the generalized ETH for noncommuting charges can be evaluated across translational-symmetry sectors, just like in the traditional ETH framework.

For the possibility of basis-dependent ETH quantifiers, the key observation of this paper, the origin of the degeneracies does not matter. As we demonstrated in Sec. II, excessive degeneracies can already result solely from the interplay of symmetries with nonlocal conserved quantities (quasimomentum and spatial parity), which previous studies usually disregarded as irrelevant for (diagonal) ETH explorations [18,50–52,57].

In principle, one still might hope that this theoretically possible basis dependence of eigenstate thermalization is irrelevant in practice because the scaling of quantities like Δ^2_A from (2) and $\Delta^2_{A,\mathrm{eq}}$ from (22) with the system size could be identical for all basis choices. We demonstrate that this hope is in vain with our example in Fig. 1, and that this has practical implications as expounded in the previous subsections and Figs. 2 and 3 in particular.

In summary, while our present explorations are to some extent related to previously reported examples and reasons for ETH violations, our main point is actually a different one: The very question of whether a system satisfies or violates

the ETH is generally ambiguous and thus physically ill posed in systems with degeneracies.

VII. SUMMARY AND CONCLUSIONS

Various versions of the ETH have been proposed, and some of them are widely considered to explain why many-body quantum systems generically thermalize. Essentially, they consist in predictions regarding the diagonal matrix elements of local observables in the eigenbasis of the system's Hamiltonian. In general, the choice of the eigenbasis, and hence the properties of these diagonal matrix elements, are not unique, while physical system properties cannot depend on that choice. Given thermalization is such a property, and that some version of the ETH is supposed to explain it, also the answer to the question of whether the ETH is fulfilled or violated must be basis independent.

The upshot of our paper is that whether or not a given many-body Hamiltonian satisfies some form of ETH may in general depend on the choice of the energy eigenbasis. Specifically, we presented an explicit example where the weak ETH is satisfied in one basis and violated in another basis. Put differently (see Sec. I), eigenstate thermalization is violated by a nonzero fraction of all eigenstates in one basis and by a vanishingly small fraction in the other basis. These findings explicitly demonstrate that suitable, basis-independent generalizations of the ETH are needed to retain its presumed role as the fundamental mechanism behind thermalization.

An obvious precondition for basis-dependent ETH quantifiers is that the considered Hamiltonian H exhibits degeneracies. We showed that the vast majority of all eigenvalues indeed exhibit degeneracies if H is translationally symmetric as well as invariant under a spatial reflection. The relevance of this result becomes apparent by observing that translationally invariant models with broken reflection symmetry are actually very uncommon. Yet, they do exist, as exemplified by so-called ratchet models [60], or the models considered in Ref. [61]. An important implication is that previous results which have been obtained under the assumptions of translational invariance and absence of degeneracies, for instance in Refs. [21,22,38,62], are rigorously speaking restricted to such "uncommon" models (without reflection symmetry). Finally, even in those latter cases there still may exist some other symmetries from which one may again infer the existence of degeneracies along similar lines as in Sec. II.

In a next step, we demonstrated that the ETH quantifier from Eq. (2), or more generally from Eq. (22), assumes its maximally possible value if the basis is chosen such that the considered observable A is diagonal in every eigenspace of H. In turn, the ETH quantifier assumes its minimally possible value when choosing the basis such that the diagonal matrix elements of A are constant within every eigenspace of H.

The maximizing bases were also found to be of considerable importance in several other contexts: They must be chosen in order to express long-time averages in terms of a so-called diagonal ensemble [see Eq. (56)]. Likewise, they govern the long-time average of dynamical autocorrelation functions [see Eq. (60)]. The latter equation was demonstrated in Appendix C to be also very useful for numerical explorations of the ETH. Finally, the maximizing bases play a key role regarding the question of whether a system rethermalizes after a local quench [see Eq. (64)].

We furthermore showed that these physical consequences remain observable in weakly perturbed systems without degeneracies. In particular, one may draw the wrong physical conclusions if one evaluates the ETH by exploiting symmetries in systems with degeneracies. This insight is especially relevant for numerical studies of the ETH.

Since the values assumed by the ETH quantifiers (2) and (22) in the maximizing bases can be expressed in terms of basis-independent quantities [cf. Eqs. (18) and (23)], the latter suggest themselves as natural, unambiguous generalizations of weak ETH quantifiers. It will be important to characterize these objects in more detail and possibly derive conditions under which their vanishing in the thermodynamic limit can be guaranteed, extending such proofs for the traditional, basis-dependent quantifier (2) for translationally invariant eigenbases.

Specifically, for our above-mentioned example of a translationally invariant system which violates the weak ETH in some energy eigenbasis, it follows that the autocorrelation function does not decay to zero for asymptotically large times, and that the system does not rethermalize after a local quench. Since such behavior has not been commonly observed until now, it seems a quite interesting and challenging task to discover and explore larger classes of such examples in the future. Another formidable task may be to find analogous examples where the conventional (strong) ETH is fulfilled in one basis and violated in another basis.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [64].

APPENDIX A: DERIVATION OF EQ. (6)

In this Appendix, we provide the derivation of Eq. (6). In doing so, we tacitly employ the same notation and definitions as in Sec. II.

For any given system size $L \geqslant 2$, its unique prime factor decomposition (PFD) can be written in the form

$$L = \prod_{j=1}^{J} (p_j)^{\mu_j} \tag{A1}$$

for suitably chosen exponents $\mu_j \in \mathbb{N}$, prime numbers p_j, and $J \in \mathbb{N}$. Since $p_j \geqslant 2$ and $\mu_j \geqslant 1$ it follows that $(p_j)^{\mu_j} \geqslant 2$ for all $j \in \{1, \ldots, J\}$. Together with (A1) this yields $L \geqslant 2^J$

and thus

$$J \leqslant \ln L/\ln 2. \tag{A2}$$

Recalling the definitions (3) and (4), our next goal is to estimate the number of basis vectors $|\boldsymbol{\sigma}\rangle$ with the property that

$$T^l|\boldsymbol{\sigma}\rangle = |\boldsymbol{\sigma}\rangle \tag{A3}$$

for some suitably chosen $l \in \{1,\ldots,L-1\}$. Therefore, let $|\boldsymbol{\sigma}\rangle$ be an arbitrary but fixed basis vector for which there exists an $l \in \{1,\ldots,L-1\}$ with the property (A3). Without loss of generality we furthermore assume that l has been chosen as small as possible. Since $1 \leqslant l < L$ and $L \geqslant 2$ one can conclude that there must exist an integer $m \geqslant 2$ with the property $ml = L + r$ and $0 \leqslant r < l$. Recalling $T^L = 1$ we thus can infer that $T^r|\boldsymbol{\sigma}\rangle = T^{r+L}|\boldsymbol{\sigma}\rangle = T^{ml}|\boldsymbol{\sigma}\rangle = |\boldsymbol{\sigma}\rangle$. Since l is the smallest integer within $\{1\ldots.,L-1\}$ with the property (A3) we can infer that $r = 0$ and thus $ml = L$. Since the PFD of L in (A1) is unique, and likewise for the PFD of $m \geqslant 2$ and of l, the relation $ml = L$ implies that at least one p_j must also appear in the PFD of m and hence $m' := m/p_j$ must be a positive integer. It follows that $m'l = L/p_j$ must be a positive integer satisfying $T^{L/p_j}|\boldsymbol{\sigma}\rangle = T^{m'l}|\boldsymbol{\sigma}\rangle = |\boldsymbol{\sigma}\rangle$. In other words,

$$q_j := L/p_j \tag{A4}$$

must be an integer with $1 \leqslant q_j \leqslant L/2$, where we exploited that $p_j \geqslant 2$ in the last step. The overall conclusion is that for every $|\boldsymbol{\sigma}\rangle$ with the property (A3) for some $l \in \{1,\ldots,L-1\}$ there exists at least one $j \in \{1,\ldots,J\}$ with the property

$$T^{q_j}|\boldsymbol{\sigma}\rangle = |\boldsymbol{\sigma}\rangle. \tag{A5}$$

Recalling that there are D^L orthonormalized basis vectors of the form (3), there must exist exactly D^{q_j} different basis vectors $|\boldsymbol{\sigma}\rangle$ with the property (A5) for the following reason: For each l with $1 \leqslant l \leqslant q_j$ we can choose σ_l arbitrarily in $\{1,\ldots,D\}$, while all σ_l with $l > q_j$ are then uniquely fixed via (A5). Denoting by N_{per} the total number of all $|\boldsymbol{\sigma}\rangle$ satisfying (A3) for some $l \in \{1,\ldots,L-1\}$, we can conclude that $N_{\mathrm{per}} \leqslant \sum_{j=1}^{J} D^{q_j}$. [The inequality is a consequence of the fact that some $|\boldsymbol{\sigma}\rangle$ may satisfy (A5) simultaneously for several different $j \in \{1,\ldots,J\}$.] Since $q_j \leqslant L/2$ [see below (A4)] it follows that $N_{\mathrm{per}} \leqslant JD^{L/2}$ and with (A2) that

$$N_{\mathrm{per}} \leqslant D^{L/2}\ln L/\ln 2. \tag{A6}$$

The above considerations imply that $\bar{N}_{\mathrm{per}} := D^L - N_{\mathrm{per}}$ is the number of all basis vectors $|\boldsymbol{\sigma}\rangle$ with the property

$$T^l|\boldsymbol{\sigma}\rangle \neq |\boldsymbol{\sigma}\rangle \quad \text{for all } l \in \{1,\ldots,L-1\}. \tag{A7}$$

Moreover, it follows with (A6) that

$$\bar{N}_{\mathrm{per}} = (1-\delta)\,D^L \tag{A8}$$

for some suitably chosen δ with

$$\delta \leqslant \frac{\ln L}{D^{L/2}\ln 2}. \tag{A9}$$

Altogether, we thus can conclude that for large L the vast majority of all the D^L basis vectors $|\boldsymbol{\sigma}\rangle$ satisfies (A7).

Observing that $\langle\boldsymbol{\sigma}'|\boldsymbol{\sigma}\rangle$ is unity if $|\boldsymbol{\sigma}'\rangle = |\boldsymbol{\sigma}\rangle$ and zero otherwise, we can conclude that every $|\boldsymbol{\sigma}\rangle$ with the property (A7) satisfies $\langle T^m\boldsymbol{\sigma}|T^n\boldsymbol{\sigma}\rangle = \delta_{mn}$ for all $m,n \in \{0,\ldots,L-1\}$. In other words, the L vectors $\{T^l|\boldsymbol{\sigma}\rangle\}_{l=0}^{L-1}$ are normalized and pairwise orthogonal.

For any given $|\boldsymbol{\sigma}\rangle$ with the property (A7) we denote by $\mathcal{H}_{\boldsymbol{\sigma}}$ the subspace which is spanned by the L vectors $\{T^l|\boldsymbol{\sigma}\rangle\}_{l=0}^{L-1}$. Since $T^L|\boldsymbol{\sigma}\rangle = |\boldsymbol{\sigma}\rangle$ it follows that $\mathcal{H}_{\boldsymbol{\sigma}'} = \mathcal{H}_{\boldsymbol{\sigma}}$ whenever $|\boldsymbol{\sigma}'\rangle$ can be written as $T^l|\boldsymbol{\sigma}\rangle$ for some l. Hence, there must be $\bar{N}_{\mathrm{per}}/L$ pairwise orthogonal subspaces $\mathcal{H}_{\boldsymbol{\sigma}}$, and each $|\boldsymbol{\sigma}\rangle$ with the property (A7) is contained in exactly one of them.

For an arbitrary but fixed $|\boldsymbol{\sigma}\rangle$ with the property (A7) and any $\nu \in \{0,\ldots,L-1\}$ we define

$$|\boldsymbol{\sigma}_\nu\rangle := L^{-1/2}\sum_{l=0}^{L-1} e^{-2\pi i\frac{\nu l}{L}}\,T^l|\boldsymbol{\sigma}\rangle. \tag{A10}$$

Exploiting that the $\{T^l|\boldsymbol{\sigma}\rangle\}_{l=0}^{L-1}$ are orthonormalized (see above), a straightforward calculation yields

$$\langle\boldsymbol{\sigma}_\mu|\boldsymbol{\sigma}_\nu\rangle = \delta_{\mu\nu} \tag{A11}$$

for all $\mu,\nu \in \{0,\ldots,L-1\}$. Recalling that $\mathcal{H}_{\boldsymbol{\sigma}}$ is spanned by $\{T^l|\boldsymbol{\sigma}\rangle\}_{l=0}^{L-1}$, we thus can conclude that $\{|\boldsymbol{\sigma}_\nu\rangle\}_{\nu=0}^{L-1}$ is an orthonormal basis of $\mathcal{H}_{\boldsymbol{\sigma}}$. Moreover, one can infer from (A10) and $T^L = 1$ that

$$T|\boldsymbol{\sigma}_\nu\rangle = \gamma_\nu|\boldsymbol{\sigma}_\nu\rangle \tag{A12}$$

with γ_ν from Eq. (5).

Finally, $T^L = 1$ implies that all eigenvalues of T are of the form (5) with $\nu \in \{0,\ldots,L-1\}$. For an arbitrary but fixed $\nu \in \{0,\ldots,L-1\}$ we denote by $\mathcal{H}_\nu$ the eigenspace of T with eigenvalue γ_ν. Since each of the $\bar{N}_{\mathrm{per}}/L$ pairwise orthogonal subspaces $\mathcal{H}_{\boldsymbol{\sigma}}$ contributes one eigenvector of the form (A10) to $\mathcal{H}_\nu$ it follows that the dimension of $\mathcal{H}_\nu$ is lower bounded by $\bar{N}_{\mathrm{per}}/L$. Together with (A9) and (A8) we finally recover Eq. (6).

APPENDIX B: SYMMETRY CONSIDERATIONS FOR THE HAMILTONIAN H FROM EQ. (24)

This Appendix collects various symmetry properties of the specific spin-chain model from Eq. (24) and certain generalizations thereof. In particular, we will identify a large class of observables A, including $A = s_l^z$, for which the thermal expectation value in (1) vanishes for any choice of the microcanonical energy window. For the rest, we utilize the same notation as in the main paper without recalling all the pertinent definitions.

To make the paper self-contained, we begin with a re-derivation of the previously known identity

$$e^{i\pi s^x}s^{y,z} = -s^{y,z}e^{i\pi s^x} \tag{B1}$$

for spin operators $s^{x,y,z}$ with arbitrary integer or half-integer spins in units with $\hbar = 1$:

From the definition $e^X := \sum_{k=0}^{\infty} X^k/k!$ one can infer the so-called Hadamard lemma of the Baker-Campbell-Hausdorff formula, reading as

$$e^X Y e^{-X} = \sum_{m=0}^{\infty}\frac{1}{m!}\,[X,Y]_m, \tag{B2}$$

$$[X,Y]_0 := Y, \tag{B3}$$

$$[X,Y]_{m+1} := [X,[X,Y]_m], \tag{B4}$$

where $[\ldots,\ldots]$ denotes the usual commutator. Choosing

$$X := qs^x, \tag{B5}$$

$$Y := qs^y, \tag{B6}$$

$$Z := qs^z, \tag{B7}$$

with an arbitrary but fixed $q \in \mathbb{C}$, and exploiting the usual commutation relations for $s^{x,y,z}$ it follows that

$$[X,Y]_1 = [X,Y] = iqZ, \tag{B8}$$

$$[X,Y]_2 = [X,iqZ] = q^2Y = q^2[X,Y]_0, \tag{B9}$$

$$[X,Y]_3 = [X,q^2Y] = iq^3Z = q^2[X,Y]_1, \tag{B10}$$

and so on. Together with (B3) and (B4) one can conclude that

$$[X,Y]_m = q^mY \text{ for even } m, \tag{B11}$$

$$[X,Y]_m = iq^mZ \text{ for odd } m, \tag{B12}$$

and with (B2) that

$$e^XYe^{-X} = Y\cosh(q) + iZ\sinh(q). \tag{B13}$$

Exploiting (B5)–(B7) and setting $q = i\phi$ this yields

$$e^{i\phi s^x}s^ye^{-i\phi s^x} = s^y\cos(\phi) - s^z\sin(\phi). \tag{B14}$$

In the special case $\phi = \pi$ we thus recover (B1) for s^y. Analogously, one verifies (B1) for s^z.

For later use we also note the obvious relations

$$e^{i\pi s^x}s^x = s^xe^{i\pi s^x}, \tag{B15}$$

$$\left[e^{i\pi s^x}\right]^\dagger = e^{-i\pi s^x} = \left[e^{i\pi s^x}\right]^{-1}. \tag{B16}$$

Let us now consider any spin Hamiltonian on a lattice Λ of the general structure

$$H = \sum_\nu h_\nu, \tag{B17}$$

where each summand h_ν consists of a product of factors of the form s^a_l with indices $l \in \Lambda$ and $a \in \{x,y,z\}$ which may or may not be different for each factor. Our only requirement is that *the number of factors s^a_l with the property $a \in \{y,z\}$ must be even for each h_ν*. All further details, for instance concerning the lattice Λ, the set of indices ν, the boundary conditions, or translational and parity symmetries, will play no role in the following.

Our second key player will be the operator

$$U := \exp\left\{i\pi\sum_{l\in\Lambda}s^x_l\right\}. \tag{B18}$$

Since all s^x_l commute with each other, one readily infers from (B1), (B15), and (B16) that

$$Us^x_l = s^x_lU, \tag{B19}$$

$$Us^y_l = -s^y_lU, \tag{B20}$$

$$Us^z_l = -s^z_lU, \tag{B21}$$

$$U^\dagger = U^{-1} \tag{B22}$$

for any $l \in \Lambda$. Since we assumed that the number of factors s^a_l with the property $a \in \{y,z\}$ is even for each h_ν, one can infer that $Uh_\nu = h_\nu U$ and with (B17) that

$$UH = HU. \tag{B23}$$

Let $|n\rangle$ be an arbitrary but fixed eigenvector of H with eigenvalue E_n and define $|\tilde{n}\rangle := U|n\rangle$. It readily follows with (B23) that $H|\tilde{n}\rangle = E_n|\tilde{n}\rangle$ and with (B21) and (B22) that

$$\langle\tilde{n}|s^z_l|\tilde{n}\rangle = -\langle n|s^z_l|n\rangle \tag{B24}$$

for any $l \in \Lambda$. In conclusion, either $\langle n|s^z_l|n\rangle = 0$ or there must be a pair of degenerate eigenvectors with opposite diagonal elements of the observable s^z_l.

The remaining problem is that $\langle n|\tilde{n}\rangle$ may not be zero, meaning that $|n\rangle$ and $|\tilde{n}\rangle$ may not be members of the same orthonormal basis (ONB). The way out is as follows: Let us denote by $\mathcal{H}_E$ an arbitrary but fixed eigenspace of H and by E the corresponding eigenvalue. In the rest of this paragraph we temporarily restrict ourselves to eigenvectors $|n\rangle$ belonging to this eigenspace $\mathcal{H}_E$. For every such $|n\rangle \in \mathcal{H}_E$ we define its counterpart $|\tilde{n}\rangle := U|n\rangle$. As before, it follows that all those $|\tilde{n}\rangle$ are again eigenvectors of H with eigenvalue E and thus are contained in $\mathcal{H}_E$. Moreover, one finds that $\langle n|m\rangle = \langle\tilde{n}|\tilde{m}\rangle$, i.e., both the $|n\rangle$ and the $|\tilde{n}\rangle$ are an ONB of $\mathcal{H}_E$. As usual, the trace over the (sub)space $\mathcal{H}_E$ is basis independent, i.e.,

$$\mathrm{tr}_{\mathcal{H}_E}\left\{s^z_l\right\} = \sum_n\langle n|s^z_l|n\rangle = \sum_n\langle\tilde{n}|s^z_l|\tilde{n}\rangle. \tag{B25}$$

Together with (B24) it follows that

$$\mathrm{tr}_{\mathcal{H}_E}\left\{s^z_l\right\} = \sum_n\langle n|s^z_l|n\rangle = 0 \tag{B26}$$

for any $l \in \Lambda$ and for any eigenbasis $|n\rangle$ of $\mathcal{H}_E$.

Returning to the full Hilbert space $\mathcal{H}$ of H and the corresponding full ONB $|n\rangle$, we can conclude that the average of the diagonal elements $\langle n|s^z_l|n\rangle$ over any (arbitrarily small or large) energy interval is always zero. In other words, we recover the announced property that the thermal expectation value of $A = s^z_l$ in (1) vanishes for any choice of the microcanonical energy window. Likewise, one finds that the equilibrium expectation value A_{eq} from Eq. (21) must vanish for any such observable A and any equilibrium ensemble ρ_{eq} in Eq. (19).

The same line of reasoning can be readily extended to arbitrary observables of the general structure $A = \sum_\mu A_\mu$, where each A_μ consists of a product of factors of the form s^a_l so that the number of factors with $a \in \{y,z\}$ is *odd*.

Since H commutes with U [see Eq. (B23)], there exists a common set of eigenvectors $|n\rangle$, and since U is unitary, all its eigenvalues are of unit modulus, implying $\langle n|U^\dagger AU|n\rangle = \langle n|A|n\rangle$ for any Hermitian operator A. Choosing $A = s^z_l$, we moreover can conclude from (B21) that $\langle n|U^\dagger AU|n\rangle = -\langle n|A|n\rangle$ and thus $\langle n|A|n\rangle = 0$ for all n and all l, and likewise for the more general A's from the previous paragraph.

In other words, there exists at least one energy eigenbasis for which even the strong ETH is trivially fulfilled. Moreover, this property is simultaneously true for all the above specified observables A. We also recall that all so far conclusions do not require translational invariance of H [see below Eq. (B17)]. On the other hand, if H does commute with the translation

operator T, and since also U commutes with T, we can even choose a common eigenbasis of H, U, and T. In other words, there must exist even a translationally invariant basis for which the strong ETH is trivially fulfilled for a large class of observables. On the other hand, it also must be emphasized that the conventional understanding of the (strong and weak) ETH is that its claims must be fulfilled by *all* local observables.

As an example we finally turn to the spin-1 Hamiltonian from Eq. (24). The remaining task is to show that this Hamiltonian is as specified in and below Eq. (B17). Without loss of generality, we focus on the first summand with $l = 1$ on the right-hand side of (24):

$$Q := s_1^+ (s_2^-)^2 s_3^+. \tag{B27}$$

Recalling that $s_l^\pm := s_l^x \pm i s_l^y$ implies that the last two factors commute and thus

$$\begin{aligned} Q &= \left[\left(s_1^x + i s_1^y\right)\left(s_3^x + i s_3^y\right)\right]\left[s_2^x - i s_2^y\right]^2 \\ &= [B_1 + iB_2][B_3 - iB_4], \end{aligned} \tag{B28}$$

$$B_1 := s_1^x s_3^x - s_1^y s_3^y, \tag{B29}$$

$$B_2 := s_1^x s_3^y + s_1^y s_3^x, \tag{B30}$$

$$B_3 := \left(s_2^x\right)^2 - \left(s_2^y\right)^2, \tag{B31}$$

$$B_4 := s_2^x s_2^y + s_2^y s_2^x. \tag{B32}$$

It follows that

$$Q = Q_1 + iQ_2, \tag{B33}$$

$$Q_1 := B_1 B_3 + B_2 B_4, \tag{B34}$$

$$Q_2 := B_2 B_3 - B_1 B_4. \tag{B35}$$

One readily verifies that the operators $B_1, \ldots, B_4$ are Hermitian and that all products appearing on the right-hand side of (B34) and (B35) consist of commuting factors. It follows that also Q_1 and Q_2 are Hermitian and therefore $Q + Q^\dagger = 2Q_1$. Moreover, for both summands contributing to Q_1 in (B34), the number of factors s_l^a with the property $a \in \{y, z\}$ is even. Hence, the same must indeed be true for each summand appearing on the right-hand side of Eq. (24).

We finally remark that somewhat similar symmetry properties are also mentioned (but not derived) in Appendix A of Ref. [25] [see in and around Eq. (A2) therein].

APPENDIX C: NUMERICAL EVALUATION OF THE ETH QUANTIFIER VIA DYNAMICAL TYPICALITY

In this Appendix, we explain how we evaluated the ETH quantifier $\Delta^2_{A,\mathrm{eq}}(\beta)$ from (53) numerically for the two basis choices in Fig. 1: the maximally ETH-violating basis and a translationally invariant basis.

We adopt standard dynamical-typicality methods [29,30] to calculate canonical expectation values and correlation functions in high-dimensional Hilbert spaces, exploiting the symmetries of the problem. Concretely, the Hamiltonian (24) commutes with the translation operator T from (4), the total magnetization

$$M^z := \sum_{l=1}^{L} s_l^z, \tag{C1}$$

and the dipole moment

$$P^z := \sum_{l=1}^{L} (l - l_0) s_l^z, \tag{C2}$$

where l_0 is a fixed reference site. The magnetization commutes with both P^z and T, but $[P^z, T] \neq 0$, so we can use the eigenvalues of either (M^z, P^z) or (M^z, T) to label symmetry sectors by good quantum numbers. For the numerics in Sec. IV, we choose (M^z, P^z) because the product basis (3) is an eigenbasis for this pair, making it particularly convenient to define the associated subspaces. The magnetization M^z has $2L + 1$ distinct eigenvalues $m \in \{-L, -L + 1, \ldots, L\}$. Since the values of the dipole moment must be invariant under shifts of the reference site l_0 by multiples of L, the eigenvalues of P^z are defined modulo L, e.g., $p \in \{0, \ldots, L - 1\}$.

If $q = (m, p)$ denotes the (pair of) quantum numbers identifying a symmetry sector, we define P_q as the projector onto this sector and

$$\mathrm{tr}_q A := \mathrm{tr}(P_q A) \tag{C3}$$

as the trace of an arbitrary observable A within the sector. In particular, $N_q := \mathrm{tr}_q \mathbb{1}$ is the sector dimension (number of states in the sector). Note that some of the so-defined sectors [e.g., $(\pm L, p)$ with $p > 0$] are empty ($N_q = 0$).

We can now decompose canonical expectation values into contributions from the symmetry sectors

$$\langle A \rangle_{\rho_\beta} := Z_\beta^{-1} \mathrm{tr}(e^{-\beta H} A) = Z_\beta^{-1} \sum_q \mathrm{tr}_q(e^{-\beta H} A), \tag{C4}$$

where

$$Z_\beta := \mathrm{tr}\, e^{-\beta H} = \sum_q Z_{\beta,q}, \tag{C5}$$

$$Z_{\beta,q} := \mathrm{tr}_q\, e^{-\beta H}. \tag{C6}$$

Within every symmetry sector, we employ dynamical typicality as usual to approximate traces by expectation values of Haar-random pure states: If $|\phi_q\rangle$ is a normalized Haar-random state in the sector q, then

$$\mathbb{P}(|\langle \phi_q | A | \phi_q \rangle - \mathrm{tr}_q A / N_q| \geqslant \varepsilon) \leqslant \frac{\|A\|_{\mathrm{op}}^2}{\varepsilon^2 N_q}, \tag{C7}$$

hence $\mathrm{tr}_q A \simeq N_q \langle \phi_q | A | \phi_q \rangle$ if $N_q \gg 1$ [65,66].

Defining

$$|\phi_{\beta,q}\rangle := e^{-\beta H/2} |\phi_q\rangle \tag{C8}$$

and recalling Eqs. (C4)–(C6), we can calculate

$$\langle A \rangle_{\rho_\beta} \simeq \frac{\sum_q N_q \langle \phi_{\beta,q} | A | \phi_{\beta,q} \rangle}{\sum_q N_q \langle \phi_{\beta,q} | \phi_{\beta,q} \rangle}. \tag{C9}$$

To calculate correlation functions $\langle A\, B(t) \rangle_{\rho_\beta}$, where $B(t) := e^{iHt} B e^{-iHt}$ is the time-evolved observable B in the Heisenberg picture, we furthermore introduce

$$|\phi^A_{\beta,q}\rangle := A |\phi_{\beta,q}\rangle \tag{C10}$$

and

$$|\phi_{\beta,q}(t)\rangle := e^{-iHt}|\phi_{\beta,q}\rangle, \quad \left|\phi^A_{\beta,q}(t)\right\rangle := e^{-iHt}\left|\phi^A_{\beta,q}\right\rangle. \quad \text{(C11)}$$

Replacing A by $AB(t)$ in (C9) and adopting Eqs. (C10) and (C11), we obtain

$$\langle AB(t)\rangle_{\rho_\beta} \simeq \frac{\sum_q N_q \langle\phi^A_{\beta,q}(t)|B|\phi_{\beta,q}(t)\rangle}{\sum_q N_q \langle\phi_{\beta,q}|\phi_{\beta,q}\rangle}. \quad \text{(C12)}$$

This leaves us with a recipe to calculate canonical expectation values:

(1) we generate a Haar-random pure state $|\phi_q\rangle$ in every symmetry sector q;

(2) we calculate all $|\phi_{\beta,q}\rangle$ by imaginary-time Suzuki-Trotter propagation of $|\phi_q\rangle$ with Hamiltonian H from imaginary time 0 to $\frac{\beta}{2}$;

(3) we calculate all $\langle\phi_{\beta,q}|A|\phi_{\beta,q}\rangle$ and $\langle\phi_{\beta,q}|\phi_{\beta,q}\rangle$;

(4) we combine the results from all sectors according to (C9) to obtain $\langle A\rangle_{\rho_\beta}$.

To calculate correlation functions, we proceed and

(5) calculate $|\phi^A_{\beta,q}\rangle$ according to (C10) for every sector q and inverse temperature β of interest;

(6) calculate all $|\phi_{\beta,q}(t)\rangle$ and $|\phi^A_{\beta,q}(t)\rangle$ by real-time Suzuki-Trotter propagation of $|\phi_{\beta,q}\rangle$ and $|\phi^A_{\beta,q}\rangle$, respectively, with Hamiltonian H from time 0 to t;

(7) calculate all $\langle\phi^A_{\beta,q}(t)|B|\phi_{\beta,q}(t)\rangle$;

(8) combine the results from all sectors according to (C12) to obtain $\langle AB(t)\rangle_{\rho_\beta}$.

To increase and estimate the accuracy, we repeat this procedure for eight (four) independent sets of Haar-random states $|\phi_q\rangle$ for the systems with $L \leqslant 11$ ($L > 11$) in Figs. 1 and 3 and calculate the standard error (shown as error bars). In Fig. 4, the Hilbert space dimensions are smaller because we inspect symmetry sectors, hence, we used larger sets of 1000, 200, and 16 Haar-random states, respectively, for the systems with $L = 9$, 11, and 13.

Turning to the ETH quantifier $\Delta^2_{A,\mathrm{eq}}(\beta)$, we first inspect the maximizing energy eigenbasis, i.e., the basis in which A is diagonal in every degenerate subspace. As derived in Sec. VI B, $\Delta^2_{A,\mathrm{eq}}(\beta)$ is equal to the time-averaged autocorrelation function $\overline{C_A(t)}$ in this case [cf. Eq. (60), in particular]. Explicitly, we thus have

$$\Delta^2_{A,\mathrm{eq}}(\beta) = \overline{\langle AA(t)\rangle_{\rho_\beta}} - \langle A\rangle^2_{\rho_\beta}. \quad \text{(C13)}$$

Following the recipe outline above, we compute $\langle AA(t)\rangle_{\rho_\beta}$ and $\langle A\rangle_{\rho_\beta}$ via dynamical typicality, and time average the former in the interval $t \in [10, 20]$ to eventually obtain $\Delta^2_{A,\mathrm{eq}}(\beta)$ from (C13).

To evaluate $\Delta^2_{A,\mathrm{eq}}(\beta)$ for a translationally invariant basis $\{|n\rangle\}$, we observe that the diagonal matrix elements A_{nn} of the local observable A coincide with those of the corresponding intensive observable $B := \frac{1}{L}\sum_{l=1}^{L} T^l A T^{-l}$, i.e., $A_{nn} = B_{nn}$. Focusing on the special case $A = s^z_1$ of interest in Fig. 1, we furthermore recall that $A_{\mathrm{eq}} = 0$. We also observe that $B = M^z$ is the total z magnetization from (C1), which commutes with H from (24) and T from (4), meaning that we can choose the specific T-invariant energy eigenbasis $\{|n\rangle\}$ such that B is diagonal, too. The ETH quantifier $\Delta^2_{A,\mathrm{eq}}(\beta)$ can then be expressed in this basis as

$$\Delta^2_{A,\mathrm{eq}}(\beta) = \sum_n p_n A^2_{nn} = \sum_n p_n B^2_{nn} = \langle B^2\rangle_{\rho_\beta}, \quad \text{(C14)}$$

where we used $A_{\mathrm{eq}} = 0$ in the first equality and the fact that B is diagonal in the chosen T-invariant basis in the last equality. Since the last representation is just a canonical expectation value, we can evaluate it as before using dynamical typicality and imaginary-time evolution in the (M^z, P^z) symmetry sectors.

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