Eigenstate Thermalization for Degenerate Observables

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Under unitary time evolution, expectation values of physically reasonable observables often evolve towards the predictions of equilibrium statistical mechanics. The eigenstate thermalization hypothesis (ETH) states that this is also true already for individual energy eigenstates. Here we aim at elucidating the emergence of the ETH for observables that can realistically be measured due to their high degeneracy, such as local, extensive, or macroscopic observables. We bisect this problem into two parts, a condition on the relative overlaps and one on the relative phases between the eigenbases of the observable and Hamiltonian. We show that the relative overlaps are unbiased for highly degenerate observables and demonstrate that unless relative phases conspire to cumulative effects, this makes such observables verify the ETH. Through this we elucidate potential pathways towards proofs of thermalization.

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"Pure state quantum statistical mechanics" [1–21] aims at understanding under which conditions the use of statistical mechanics can be justified based on the first principles of standard quantum mechanics. One of its pillars is the eigenstate thermalization hypothesis (ETH) [22–34]: A hypothesis about properties of individual energy eigenstates of quantum many-body systems which was suggested by results in quantum chaos theory. The basic idea is that, for large and sufficiently complex systems, the energy eigenstates can be so entangled that their overlaps with the eigenstates of a physical observable can be effectively described by random variables. If the ETH is fulfilled, it guarantees thermalization for all observables that equilibrate on average. Depending on how broad one wants the class of initial states that thermalize to be, the fulfillment of the ETH is also a necessary criterion for thermalization [5,35]. The ETH is sometimes criticized for its lack of predictive power, as it leaves open at least three important questions: What precisely are "physical observables", What makes a system "sufficiently complex" to expect that ETH applies, How long will it take for such observables to reach thermal expectation values [17–21]. For this reason, a lot of effort has been focused on numerical investigations that validate the ETH in specific Hamiltonian models and for various observables, often including local ones. The ETH is generally found to hold in nonintegrable systems that are not many-body localized and equilibration towards thermal expectation values usually happens on reasonable time-scales [18,20,21,34]. A satisfactory analytical explanation for the ETH, however, is still missing. Recently [36], a formal notion of observables that satisfy the ETH, together with their algorithmic construction, was introduced and dubbed "Hamiltonian unbiased observables" (HUOs). Unfortunately this still leaves open the question of when physically relevant observables satisfy the ETH. In this Letter we make progress in this direction. Building on the connection between HUOs and the ETH, we present a theorem which can be used to investigate the emergence of the ETH. In order to show how it can be used, we present three applications: local observables, extensive observables, and macroobservables. We will give precise definitions for each of them later.

The Letter is organized as follows. First we setup the notation and state precisely what we mean by the ETH. We continue with a brief digression on physical observables and degeneracies and recall the concepts of the Hamiltonian unbiased basis and observables. We then present our main result, which elucidates the conditions under which highly degenerate observables are (approximately) HUOs. Eventually we discuss the consequences for local, extensive, and macroobservables.

Statement of the ETH.—Several versions of the ETH have appeared in the literature [37], making it necessary to define precisely what we mean by the ETH in this work. Throughout the Letter we assume all Hamiltonians H to be nondegenerate with eigenvalues E_m and eigenstates $|E_m\rangle$. For any given initial state of the form $|\psi_0\rangle = \sum_m c_m |E_m\rangle$ with $c_m \coloneqq \langle E_m|\psi_0\rangle$ we denote by $\rho_{\mathrm{DE}} \coloneqq \sum_m |c_m|^2 |E_m\rangle\langle E_m|$ the corresponding diagonal ensemble, also known as the dephased

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or time-averaged state. We now state the version of the ETH we will be using throughout the Letter.

Hypothesis 1: (Complete ETH) The matrix elements $A_{m,n} := \langle E_m|A|E_n\rangle$ of any physically reasonable observable A with respect to the energy eigenstates $|E_m\rangle$ in the bulk of the spectrum of a Hamiltonian of a system with N particles satisfy

$$-\ln|A_{m+1,m+1} - A_{m,m}|, \qquad -\ln|A_{m,n}| \in \mathcal{O}(N). \quad (1)$$

This kind of ETH is what Srednicki argued to be fulfilled in a hard-sphere gas [25]. Similar variants appeared for example in Refs. [26,27,32,34,38]. As said above, several other versions of the ETH and related concepts have appeared in the literature [3,28,35,39–51]. In the Supplemental Material [52] we collect the most used ones.

The main reason why we refer to the formulation of the ETH given above is that it involves both diagonal A_{mm} and off-diagonal A_{mn} matrix elements. We believe it is important to highlight this aspect because the off-diagonal matrix elements contribute in a nontrivial way to the out-of-equilibrium dynamics of the observable [5,15,17–21,50]. Moreover, the equilibrium value can be physically meaningless if it is reached only after an astronomically large time or if fluctuations are too strong. This is what gives the off-diagonal ETH physical relevance. Hereafter, when we refer to the ETH we will always refer to the technical statement given above.

Physical observables.—An issue left open by the above definition is the identification of physical observables for which the ETH should hold. Here we focus on observables which can realistically be measured in a laboratory. Highly degenerate observables are good candidates as, already for a system of just 100 spin-$1/2$ particles, a nondegenerate observable would have 2^{100} different outcomes: an astronomically large number of 30 digits. This makes all nondegenerate observables impossible to measure and goes along with the idea behind statistical physics according to which, at the macroscopic scale, we cannot access the microscopic details of the system. We consider three scenarios: First, local observables have the property that each eigenvalue is exponentially degenerate in the size of the system on which they do not act. Second, extensive sums of nonoverlapping local observables, like the total magnetization, are, for combinatorial reasons, highly degenerate around the center of their spectrum. Third, macroobservables [9,12,13] as introduced by von Neumann [6,11]. Here the idea is that on macroscopic systems one can measure only a small number of observables and these can take only a number of values that is much smaller than the enormous dimension of the Hilbert space. Moreover, they commute either exactly or are very close to commuting observables. The classical position and momentum of a macroscopic system are examples. Such classical observables, hence, partition, in a natural way, the Hilbert space of a quantum system in a direct sum of subspaces, each corresponding to a vector of outcomes for all the macroobservables. Even by measuring all the available macroobservables one can only identify which subspace a quantum system is in, but never learn its precise quantum state. To get the impression that a system thermalizes it is hence sufficient that the overlap of the true quantum state with each of the subspaces from the partition is roughly constant in time and the average agrees with the suitable thermodynamical prediction. As in any realistic situation, the number of observables times the number of different subspaces is vastly smaller than the dimension of the Hilbert space, and one is again dealing with highly degenerate observables.

Hamiltonian unbiased observables.—Before we proceed with the main result of the Letter, it is important to summarize the results derived in Ref. [36]. Suppose $A := \sum_i a_i A_i$ is an observable with eigenvalues a_i and orthogonal projectors A_i. We say that A is a *thermal observable* with respect to the state ρ if its measurement statistics $p(a_i) := \mathrm{Tr}(\rho A_i)$ maximizes the Shannon entropy $S_A := -\sum_i p(a_i)\log p(a_i)$ under two constraints: normalization of the state $\mathrm{Tr}(\rho) = 1$ and fixed average energy $\mathrm{Tr}(\rho H)$.

In Ref. [36] it was proven that this is a generalization of the standard notion of thermal equilibrium: What we usually mean by thermal equilibrium is that the state of the system ρ is close to the Gibbs state ρ_G. A way to characterize ρ_G is via the constrained maximization of von Neumann entropy $S_{\mathrm{vN}} := -\mathrm{Tr}(\rho\log\rho)$. Now, for any state ρ, the minimum Shannon entropy S_A (among all the observables A) is the von Neumann entropy: $\min_A S_A = S_{\mathrm{vN}}$. Therefore, the Gibbs state is the one that maximizes the lowest among all Shannon entropies S_A. Hence the maximization of S_A is an observable dependent generalization of the usual notion of thermal equilibrium. By studying the emergence of thermal observables in a closed quantum system, it can be proven that for any given Hamiltonian there is a huge amount of observables satisfying the ETH: the Hamiltonian unbiased observables [36].

The name originates from the notion of mutually unbiased basis (MUB). Two sets of normalized vectors, $\{|u_j\rangle\}_j$ and $\{|v_k\rangle\}_k$, are mutually unbiased if the inner product between any pairs satisfies $|\langle u_i|v_k\rangle| = 1/\sqrt{D}$, where D is the dimension of the Hilbert space. A basis is called a Hamiltonian unbiased basis (HUB) if it is unbiased with respect to the Hamiltonian basis. Accordingly, a HUO is an observable which is diagonal in a HUB. The concept of a MUB has been studied in depth in quantum information theory [53–58]. For our purposes, the most important result is the following: In any Hilbert space there are at least three MUBs [56–58].

By studying the matrix elements of a HUO, in the Hamiltonian basis, it is not too difficult to see that sufficiently degenerate HUOs should satisfy the ETH (under some additional conditions that we discuss in the following). Suppose a HUO has the spectral decomposition

$$O^{\mathrm{HUO}} := \sum_{j=1}^{n_A} \lambda_j \Pi_j \qquad \Pi_j := \sum_{s=1}^{d_j} |j,s\rangle\langle j,s|, \qquad (2)$$

where $\{|j,s\rangle\}$ is the HUB whose elements have been labeled with two indices: j runs over the distinct eigenvalues λ_j while s runs over the d_j degeneracy of each eigenvalue. It is easy to see that one has $O^{\rm HUO}_{mm} = \mathrm{Tr}(O^{\rm HUO})/D$ and the average value at equilibrium, i.e., computed from the diagonal ensemble, is microcanonical $\mathrm{Tr}(O^{\rm HUO}\rho_{\rm DE}) = \langle O^{\rm HUO}\rangle_{\rm mc}$, where $\langle\cdots\rangle_{\rm mc}$ is the expectation value computed in the maximally mixed state $\mathbb{1}/D$. Of course reality is more refined and realistic observables are not exactly HUOs, but, as our theorem below shows, they are often approximately HUOs.

Because of the MUB condition we have $\langle E_m|j,s\rangle = e^{i\theta^m_{js}}/\sqrt{D}$, which means that the off-diagonal matrix elements are given by

$$\mathcal{O}^{\rm HUO}_{mn} = \frac{1}{D}\sum_{j=1}^{n_A}\lambda_j\sum_{s=1}^{d_j}e^{i\gamma^{mn}_{js}} \qquad \gamma^{mn}_{js} \coloneqq (\theta^m_{js} - \theta^n_{js}). \quad (3)$$

In Ref. [36] a numerical study on the phases γ^{mn}_{js} was performed. It was argued that the γ^{mn}_{js}, when constructed with the standard algorithm to build MUBs, have certain features of pseudo-random variables with uniform distribution in $[-\pi,\pi]$. Whenever each eigenvalue has a large degeneracy, i.e., $d_j \gg n_A \geq 2$, we can apply the central limit theorem to argue that

$$\mathcal{O}^{\rm HUO}_{mn} \approx \sum_{j=1}^{n_A} X^{(j)}_{mn}X^{(j)}_{mn} \sim \mathcal{N}\left[0, \left(\frac{\lambda_j\sqrt{d_j}}{D}\right)^2\right], \quad (4)$$

where $X^{(j)}_{mn} \sim \mathcal{N}[\mu,\sigma^2]$ means that the $X^{(j)}_{mn}$ behave like complex random variables, normally distributed, with mean μ and variance σ^2. Under the additional assumption that the $X^{(j)}_{mn}$ are independent, one finds that, because Eq. (4) is a finite sum of normally distributed random variables, we have $\mathcal{O}^{\rm HUO}_{mn} \sim \mathcal{N}[0,\sigma^2_{n_A}]$ with variance $\sigma^2_{n_A} = (1/D)\langle(\mathcal{O}^{\rm HUO})^2\rangle_{\rm mc}$, which means that $\mathcal{O}^{\rm HUO}$ satisfies Hypothesis 1.

Before we proceed, we expand on the mechanism behind the emergence of the ETH for a highly-degenerate HUO. Equation (4) will hold whenever we can apply the central limit theorem within each subspace at a fixed eigenvalue. As was argued in Ref. [36], for a fixed pair of indices (m,n), the phases γ^{mn}_{js} behave as if they were pseudorandom variables and their number is exponentially large in the system size. The labels (j,s) provide a partition of these D phases into n_A groups, each made of d_j elements. In the overwhelming majority of cases each group will exhibit the same statistical behavior as the whole set. In this case, Eq. (4) will behave as a sum of independent random variables and it will give the exponential decay of the off-diagonal matrix elements. It may happen that the index j, labeling different eigenvalues, samples the phases in a biased way and prevents some of the off-diagonal matrix elements from being exponentially small. This can induce coherent dynamics, preventing the observable from thermalizing. This can happen, for example, in an integrable quantum system for observables which are close to being conserved quantities.

The point can also be seen from the perspective of random matrix theory. Given the Hamiltonian eigenbasis, if we perform several random unitary transformations, in the overwhelming majority of cases we obtain a basis that is almost a HUB, up to corrections which are exponentially small in the system size [53,54]. Hence, for large system sizes, if we pick a basis at random, most likely it will be almost a HUB [53,54].

We now present the main result of the Letter: a theorem that can be used to study under which conditions highly degenerate observables are (almost) HUOs.

Theorem 1: Let $\{|\psi_m\rangle\}_{m=1}^M \subset \mathcal{H}$ be a set of orthonormal vectors in a Hilbert space $\mathcal{H}$ of dimension D. Let $A = \sum_{j=1}^{n_A} a_j\Pi_j$ be an operator on $\mathcal{H}$ with $n_A \leq D$ distinct eigenvalues a_j and corresponding eigenprojectors Π_j. Decompose $\mathcal{H} = \bigoplus_{j=1}^{n_A}\mathcal{H}_j$ into a direct sum such that each $\mathcal{H}_j$ is the image of the corresponding Π_j with dimension D_j. For each j for which $D_j(D_j-1) \geq M+1$ there exists an orthonormal basis $\{|j,k\rangle\}_{k=1}^{D_j} \subset \mathcal{H}_j$ such that for all k, m

$$|\langle\psi_m|j,k\rangle|^2 = \langle\psi_m|\Pi_j|\psi_m\rangle/D_j. \quad (5)$$

A detailed proof is provided in the Supplemental Material [59]. If the condition $D_j(D_j-1) \geq M+1$ is fulfilled for all j, then the set of all $\{|j,k\rangle\}_{j,k}$ is an orthonormal basis for $\mathcal{H}$ which diagonalizes A. So, as long as the degeneracies D_j of A are all high enough with respect to M, A has an eigenbasis whose overlaps with the states $|\psi_m\rangle$ are given by the right-hand side of Eq. (5).

A particularly relevant case is when A is a local observable acting nontrivially only on some small subsystem S of dimension D_S of a larger N-partite spin system of dimension $D = d^N$, i.e., $A \coloneqq \sum_{j=1}^{D_S} a_j|a_j\rangle\langle a_j| \otimes \mathbb{1}_{\bar{S}}$ and $\{|\psi_m\rangle\}_{m=1}^M$ is taken to be an eigenbasis $\{|E_m\rangle\}_{m=1}^D$ of the Hamiltonian H of the full system. We summarize some nonessential details in the Supplemental Material [59]. In this case the degeneracies are $D_j \geq D/D_S = d^{N-|S|}$, so that the above results guarantee that for all observables on up to $|S| < N/2$ sites there exists a tensor product basis $\{|a_j,k\rangle\}_{j,k}$ for $\mathcal{H}$ which diagonalizes A and with the property that

$$|\langle E_m|a_j,k\rangle|^2 = \frac{1}{d^{N-|S|}}\langle a_j|\mathrm{Tr}_{\bar{S}}|E_m\rangle\langle E_m||a_j\rangle. \quad (6)$$

For subsystems with support on a small part of the whole system $|S| \ll N-|S|$, it is well known that the reduced states of highly entangled states are (almost) maximally mixed [8], i.e., proportional to the identity. Moreover, there is widespread agreement [60–68] that away from integrability, the energy eigenstates in the bulk of the spectrum have a large amount of entanglement. Thus, if the eigenstates $|E_m\rangle$ are highly entangled $\mathrm{Tr}_{\bar{S}}|E_m\rangle\langle E_m| \approx \mathbb{1}_S/d^{|S|}$ so that we have

$$|\langle E_m|a_j,k\rangle|^2 \approx 1/d^N. \tag{7}$$

This way of arguing shows how entanglement in the energy basis can lead to the emergence of the ETH in a local observable. If one is interested in a window $[E_a, E_b]$ with only $M \ll D$ eigenstates, the hypothesis of our theorem is fulfilled for observables supported on larger subsystems. While this result was expected for the diagonal matrix elements, we would like to stress that the HUO construction and Theorem 1 allows us to make nontrivial statement [such as Eq. (4)] about the off-diagonal matrix elements. Since their magnitude controls the dynamical fluctuations around the equilibrium, their suppression in increasing system size contributes to the emergence of thermal equilibrium on reasonable timescales.

We now turn our attention to the study of extensive sums of nonoverlapping local observables and assume that we are interested in a certain energy window $[E_a, E_b]$ which contains $M \leq D$ energy eigenstates. The details of the computations can be found in the Supplemental Material [69]. The paradigmatic case that we study is the global magnetization $M_z \coloneqq \sum_{i=1}^N \sigma_i^z$ with spectral decomposition $M_z = \sum_{j=-N}^N j\Pi_j$, where each eigenvalue has degeneracy $D_j \coloneqq \mathrm{Tr}\Pi_j = \{N/[(N-j)/2]\}$. We call $\mathcal{H}_j \subset \mathcal{H}$ the image of the projector Π_j. The inequality $D_j(D_j - 1) \geq M + 1$ selects a subset $j \in [-j_*(M), j_*(M)]$ of spaces $\mathcal{H}_j$ for which the conditions of our theorem are satisfied. The smaller M, the larger the set of subspaces $\mathcal{H}_j$ for which the hypothesis of Theorem 1 is satisfied. For the whole energy spectrum $M = D$, a rough estimation, supported by numerical calculations, shows that $j_*(D)$ scales linearly with system size: $j_*(D) \simeq 0.78N$. The physical intuition that we obtain is the following: Subspaces with "macroscopic magnetization," i.e., around the edges of the spectrum of M_z, have very small degeneracy and the theorem does not yield anything meaningful for them. However, in the bulk of the spectrum there is a large window $j \in [-j_*(D), j_*(D)]$ where the respective subspaces $\mathcal{H}_j$ meet the conditions for the applicability of the theorem. Therefore $\forall j \in [-j_*(D), j_*(D)]$ we have $|\langle E_m|j,s\rangle|^2 = (\langle E_m|\Pi_j|E_m\rangle / D_j)$. If, for some physical reason, one is not interested in the whole energy spectrum but only in a small subset, the window $[-j_*(M), j_*(M)]$ will increase accordingly. Using Stirling's approximation within $[-j_*(D), j_*(D)]$, M_z is a HUO if and only if

$$\forall m \quad \langle E_m|\Pi_j|E_m\rangle \approx 2^{-NH_2(p(j)\|p(0))}, \tag{8}$$

where $p(j) \coloneqq [\frac{1}{2} + (j/2N), \frac{1}{2} - (j/2N)]$ and we used the binary relative entropy $H_2(p\|q) \coloneqq \sum_{k=1,2} p_k \log_2(p_k/q_k)$. This relation has a natural interpretation in terms of large-deviation theory. Indeed, such a relation is a statement about the statistics induced by the energy eigenstates on the observable M_z. If such statistics satisfy large-deviation theory, as in Eq. (8), the observable will satisfy the ETH. A complete understanding of how this concretely happens goes beyond the purpose of the present work and it is left for future investigation.

The result agrees with the intuition that, in the thermodynamic limit, macroscopically large values of an extensive sum of local observables should be highly unlikely. In a recent work by Biroli *et al.* [30] it was argued that in a chain of interacting harmonic oscillators, the measurement statistics of the average of the nearest-neighbor interactions, given by the diagonal ensemble, satisfies a large-deviation statistics. This allows for the presence of rare, nonthermal, eigenstates which can account for the absence of thermalization in some integrable systems. Our result goes along with such intuition. Indeed, if it is possible to show that a large-deviation bound emerges at the level of each energy eigenstate, for all of them, this would imply an argument for ETH, as discussed before.

We now come to the last application of our theorem: von Neumann's macroobservables. More details are available in the Supplemental Material [59]. As explained before, macroobservables induce a partition of the Hilbert space into subspaces in which such classical-like observables have all well-defined eigenvalues. A *macrostate* is characterized by a choice of the eigenvalues of all these observables and the index j runs over different macrostates. Each macrostate $j = 1, \ldots, n$ corresponds to a highly degenerate subspace $\mathcal{H}_j \subset \mathcal{H}$ to which we can apply our theorem. According to the result by von Neumann [6] and Goldstein *et al.* [9] it can be proven that the following relation holds for a given partition, for most Hamiltonians, in the sense of the Haar measure: $\langle E_m|P_j|E_m\rangle \approx (D_j/D)$. The P_j's are the projectors onto the subspaces $\mathcal{H}_j$. Our theorem tells us that there exists a basis $\{|j,s\rangle\}$ which diagonalizes all the macroobservables such that $\langle E_m|P_j|E_m\rangle = D_j|\langle E_m|j,s\rangle|^2$. Using it in synergy with the previously mentioned result we find $|\langle E_m|j,s\rangle|^2 \approx (1/D)$. Hence, for most Hamiltonians, those macroobservables have a common basis that is almost a HUB. Given the huge degeneracy of the spaces $\mathcal{H}_j$ this allows us to state the following: for most Hamiltonians, in the sense of the Haar measure, the macroobservables are degenerate almost HUOs and therefore can be expected to satisfy ETH.

The validity of ETH for von Neumann's macroobservables was previously argued for in Ref. [70]. Our result confirms that macroobservables are expected to satisfy the ETH and it strengthens the intuition that the proposed notion of HUOs could underlie the emergence of the ETH in physically relevant cases.

While this gives an intuitive insight into the emergence of the ETH, it reinforces the idea that physical systems are not drawn according to the Haar measure. Indeed, for physically relevant observables, this would imply complete insensitivity to the energy, which is not what we observe in the real world. To resolve this matter, our Theorem 1 is in fact more refined and the right-hand side of Eq. (5) leaves room for energy sensitivity of observables.

Conclusions.—The ETH captures the widespread and numerically very well corroborated intuition that the eigenstates of sufficiently complicated quantum many-body system have thermal properties. Its importance stems from the fact that, together with the results that constitute the framework of pure state quantum statistical mechanics, a proof of the ETH would yield a very general argument for the emergence of not just equilibration, but thermalization towards the prediction of equilibrium statistical mechanics from quantum mechanics alone. Such a rigorous proof is still missing, despite the progress in recent years. Here we contribute to this program by bisecting the problem of proving the ETH into two subproblems related to the relative phases and the overlaps between the eigenstates of the Hamiltonian and an observable. We argue that the ETH can fail because of the former only through conspiratorial correlations in the phases. Our main result concerns the second half of the problem. Here we prove a rigorous result that shows when highly degenerate observables become almost Hamiltonian unbiased observables and thus satisfy this part of the ETH. We illustrate our results with three types of physical observables: local, extensive, and macroscopic observables. Our approach allows us in particular to make statements about the off-diagonal elements that are prominent in the original version of the ETH.

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