Information-Theoretic Equilibration: The Appearance of Irreversibility under Complex Quantum Dynamics

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(Received 28 August 2012; published 20 August 2013)

The question of how irreversibility can emerge as a generic phenomenon when the underlying mechanical theory is reversible has been a long-standing fundamental problem for both classical and quantum mechanics. We describe a mechanism for the appearance of irreversibility that applies to coherent, isolated systems in a pure quantum state. This equilibration mechanism requires only an assumption of sufficiently complex internal dynamics and natural information-theoretic constraints arising from the infeasibility of collecting an astronomical amount of measurement data. Remarkably, we are able to prove that irreversibility can be understood *as typical* without assuming decoherence or restricting to coarse-grained observables, and hence occurs under distinct conditions and time scales from those implied by the usual decoherence point of view. We illustrate the effect numerically in several model systems and prove that the effect is typical under the standard random-matrix conjecture for complex quantum systems.

DOI: 10.1103/PhysRevLett.111.080403 PACS numbers: 05.30.−d, 03.67.−a, 05.45.Mt

There has been considerable recent interest in the sufficient conditions for equilibration [1–15]. These approaches normally assume a decoherence mechanism resulting from the entanglement between the system of interest and a larger environment, or else assume highly coarse-grained observables. In this work we describe a mechanism for equilibration that applies to isolated quantum systems in pure states, without assuming decoherence, restricting to subsystems, time averaging or coarse graining the observables. The mechanism for equilibration that we describe is an *information-theoretic* one that requires an assumption of complex internal dynamics coupled with realistic limitations to predicting the detailed evolution of the system and the experimental infeasibility of collecting an astronomically large amount of measurement data. This approach builds on earlier arguments by Peres [16] and Srednicki [17,18] who proposed that the statistical complexity of the system's eigenvectors could be responsible for equilibration in isolated quantum systems. We show that these conditions are sufficient to account for the effective (microcanonical) equilibration of the measurement statistics for natural choices of (even nondegenerate) observables, meaning that, after a finite equilibration time, the dynamical state becomes effectively indistinguishable from the microcanonical state. Hence, information-theoretic equilibration (ITE) accounts for microcanonical equilibration in a way that is directly analogous to how classical chaos (mixing) accounts for the microcanonical equilibration of classically chaotic systems [19,20]. Remarkably, we are able to prove that ITE is universal for complex systems under the standard random-matrix conjecture [21,22]. Specifically, we prove that information-theoretic equilibration occurs with high probability for individual Hamiltonians drawn from two physically relevant ensembles: the Gaussian unitary ensemble (GUE), which has a successful history of predicting universal features of complex quantum systems [21], and a random local Hamiltonian (RLH) ensemble consisting of many-body systems restricted to two-body interactions. We then illustrate ITE numerically in some surprisingly simple examples of Hamiltonian models under natural choices of (maximally fine-grained) observables: a two-field variant of the many-body Heisenberg Hamiltonian as well as the quantum kicked top [22], which is a single-body, classically chaotic system.

Consider a pure state evolving under a Hamiltonian H, $\rho(t) = \exp(-iHt/\hbar)|\psi(0)\rangle\langle\psi(0)|\exp(iHt/\hbar)$. The dynamical state $\rho(t)$ cannot reach the true equilibrium state $\sigma_\infty := \lim_{\tau\to\infty}(1/\tau)\int_0^\tau \rho(t)dt$ [1,13] because the state remains pure. In particular, the trace distance $\|\rho(t) - \sigma_\infty\|$, which characterizes the distinguishability under an *optimal* choice of measurement operator, can be large throughout the evolution. However, for a given complex system H in a large Hilbert space, even a suboptimal measurement that enables distinguishability of these two states at any time t may neither be known theoretically nor easily engineered experimentally. For example, for a cubic lattice of dipolarly coupled spins, which is an analytically intractable system that has been probed experimentally for decades, only recently was a measurement procedure devised that revealed long-lived (multiple-quantum) coherence after equilibration of the free-induction decay [23].

Conceptually then we see that the appearance of equilibration can and does result from insufficient knowledge of, or control over, the choice of observable. Our contribution is to characterize and illustrate conditions under which the signatures of purity and coherence are provably "lost in Hilbert space," and hence unobservable due to realistic limitations on both theoretical and experimental abilities.

We remark that our assumptions are conceptually similar and yet distinct from those of the usual decoherence argument, in which a system coupled to a reservoir appears to reach equilibrium (due to entanglement between the system and reservoir) although the joint state of the system plus reservoir remains pure. That conclusion holds only if one assumes that one cannot predict or perform the kind of (entangling) measurement across the combined system plus reservoir that would readily distinguish the actual state from the equilibrium one; that is, the argument goes through by restricting the set of observables to local ones. In contrast, our observation is that information-theoretic limitations alone are sufficient to account for the appearance of equilibration for accessible observables on complex systems and so, contrary to the usual assumption (see [1,24,25]), decoherence from a reservoir is not necessary from an explanatory point of view. More practically, whereas the time scale for equilibration under decoherence depends on the strength of the coupling to the reservoir, our mechanism does not and predicts equilibration on a distinct, and potentially shorter, time scale. Furthermore, our approach is a natural quantum analog of classical *microcanonical* equilibration [19,20].

We consider a quantum system with some kinematically accessible Hilbert space that is finite dimensional $\mathcal{H} = \mathbb{C}^D$. In order to show that we do not require coarse graining, we consider a maximally fine-grained (i.e., nondegenerate) observable A acting on $\mathcal{H}$, where $A = \sum_{k=1}^{D} a_k \hat{P}_k$ with rank-one orthogonal projectors $\hat{P}_k$. Our argument applies also to local or other coarse-grained observables (which can be represented by degeneracies). For simplicity of analysis we consider the (most adversarial) setting where the system starts in a pure state that is maximally localized with respect to A, i.e., $\rho_0 = |a_i\rangle\langle a_i|$, and then examine how the pure states spread out over the eigenbasis of A under a time evolution given a Hamiltonian H. The empirical question of whether the system appears to approach (microcanonical) equilibrium given some observable A corresponds to asking whether the experimental measurement statistics for the evolved pure state can be distinguished from those of the equilibrium state. Hence, the relevant quantities for this task are the probabilities over distinct outcomes k,

$$\Pr(k|\rho(t)) = \mathrm{Tr}[\hat{P}_k U(t) \rho_0 U^\dagger(t)], \tag{1}$$

and the goal is to distinguish $\rho(t)$ from σ_∞ by sampling the distribution in Eq. (1). For simplicity we focus on cases where $\sigma_\infty = \mathbb{1}/D$, but σ_∞ may differ from the microcanonical state $\rho_{\mathrm{mc}} := \mathbb{1}/D$ or any thermal state [3].

Definition 1.—A Hamiltonian H acting on $\mathcal{H} = \mathbb{C}^D$ exhibits ITE with respect to an observable A at a time t, if the outcome distribution $\Pr(k|\rho(t))$ can only be distinguished from the microcanonical distribution $\Pr_{\mathrm{mc}}(k)$ with probability at least $1 - O(1/\mathrm{poly}(D))$ by (a) taking a number of samples from $\Pr(k|\rho(t))$ that scales at least as $O(\mathrm{poly}(D))$ or (b) performing any information processing that requires at least $O(\mathrm{poly}(D))$ arithmetic or logical operations.

This definition emphasizes that although the exact quantum distribution for the system may be, *in principle*, distinguishable from the microcanonical distribution, the two are effectively indistinguishable if the resources needed to distinguish them exceed those practically available. We delineate the practical from the impractical by disallowing resources (the number of measurements taken and computational time used in their analysis) that grow polynomially with the Hilbert space dimension (and hence exponentially with the number of subsystems). Of course, for a different physical scenario, a different cutoff may be appropriate. Our condition (b) includes a restriction on computational resources because the two distributions could be distinguished using fewer samples if the $\Pr(k|\rho(t))$ can be precomputed. In other words, information-theoretic equilibration is relevant precisely when the system is in a sufficiently large Hilbert space that such a precomputation is infeasible. We represent our ignorance of $\Pr(k|\rho(t))$ by assuming that it is drawn from a distribution that is invariant under permutations of outcome labels. We now show in the following theorem that, without the ability to efficiently predict $\Pr(k|\rho(t))$, ITE with respect to a particular measurement occurs when the *outcome variance*,

$$\mathbb{V}_k\{\Pr(k)\} := D^{-1} \sum_{k=0}^{D-1} [\Pr(k) - D^{-1}]^2, \tag{2}$$

is sufficiently small, which is typical of cases where the underlying dynamics has no constants of motion. Proof is provided in the Supplemental Material [26].

Theorem 1.—Consider an unknown distribution that is promised to be with equal probability either (a) the uniform distribution on the set $\mathcal{S} = \{1, \ldots, M\}$ or (b) an unknown distribution $P(k)$ that is drawn from a distribution over probability distributions on $\mathcal{S}$ with outcome variances that scale as $O(M^{-2})$ such that $\Pr(P(k))$ is invariant with respect to permutations of $\mathcal{S}$. With high probability, the probability of correctly distinguishing between (a) and (b) after obtaining N samples is at most $1/2 + O(N/M^{1/4})$.

Theorem 1 shows that $N \geq O(M^{1/4})$ samples are needed to distinguish the distributions with probability substantially greater than $1/2$, which is prohibitively expensive in the case of a nondegenerate projective measurement because $M = D$. Similarly, if we consider a generalized measurement with $M > D$ (as is relevant in the case of symmetric informationally complete positive operator valued measures), Theorem 1 similarly shows that distinguishing the distributions is hard. Finally, it is straightforward to show that coarse-grained measurements with $M < D$ do not provide an advantage under the assumptions of Theorem 1 because the permutation invariance of the prior distribution over $\Pr(k)$ prevents such strategies from succeeding with high probability. Another consideration is that $\mathbb{V}_k\{\Pr(k)\} = O(M^{-2})$ does not imply that the fluctuations are negligible, in principle; in fact, it is consistent with $\| \Pr(k|\rho(t)) - 1/M \|_1$ being constant, which implies that an optimal measurement exists that can distinguish the two distributions efficiently [27]. Hence, Theorem 1 is only meant to give a hardness result for distinguishing two states given the induced distributions with respect to a fixed measurement, and does not apply to cases where the optimal measurement is both known *a priori* and experimentally accessible. Indeed the exceptions to our assumptions are relevant, e.g., when the system admits constants of the motion that are simple relative to the selected observable.

Which Hamiltonian systems satisfy the assumptions of Theorem 1 for natural choices of A, and hence exhibit information-theoretic equilibration? Pure-state fluctuations satisfying the scaling of Theorem 1 were observed already in the two-body, classically chaotic quantum system studied in Refs. [28,29], which motivated the question: Was the behavior of that complex system exceptional, or was it evidence of a universal equilibration behavior for closed chaotic systems? If the latter, does this effect carry over from chaotic quantum systems to sufficiently complex many-body quantum systems?

To answer these questions, we take the enormously successful approach of Wigner and Dyson and the army of theoretical physicists following them who have demonstrated that certain features of appropriate random-matrix ensembles can predict typical properties of complex quantum systems. This is known as the random-matrix conjecture, and it has provided accurate predictions of the spectral properties of heavy nuclei [21], spectral and eigenvectors statistics of quantum chaos models [30,31], and quantum transport in mesoscopic structures [32]. Consider any ensemble that has a mean that equilibrates information theoretically with respect to A and is sufficiently sharply peaked about that mean; then individual systems from the ensemble will satisfy Theorem 1 with (very) high probability. This phenomenon, known as *concentration of measure*, is central to the random-matrix conjecture, and it is important to note that our averages over the ensemble are not an implicit appeal to decoherence or mixing, but a method for estimating the *typical properties* of *individual systems* within the ensemble.

The system must be allowed to evolve for a sufficient amount of time for the state to spread out from a distribution with support on initial eigenstate of A to one that obeys $\Pr(k|\rho(t)) \approx 1/D$ for our result to hold (see Fig. 1). We refer to the earliest such time as the equilibration time, which we denote t_{eq}. For an individual system, we also require that for most $t \geq t_{\mathrm{eq}}$ that $\Pr(k|\rho(t))$ is nearly

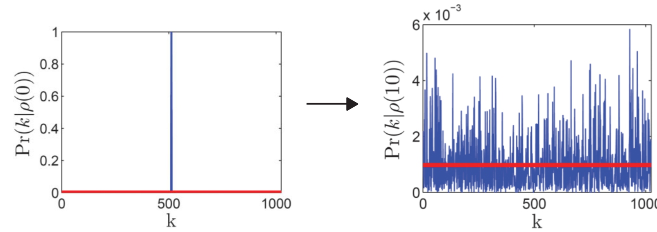

FIG. 1 (color). We plot $\Pr(k|\rho(t))$ for Pauli-Z measurements given by quantum theory (blue) and the uniform distribution (red) for a random local Hamiltonian acting on 10 qubits at $t = 0$ and for $t > t_{\mathrm{eq}}$. ITE arises from the difficulty in distinguishing quantum fluctuations from sampling errors for $t > t_{\mathrm{eq}}$.

maximally spread out. If the Hamiltonian is drawn from an ensemble, it is then possible to define an equilibration time such that almost all Hamiltonians drawn from the ensemble achieve ITE with respect to A and $t \geq t_{\mathrm{eq}}$:

Lemma 1.—Almost all Hamiltonians sampled from an ensemble of Hamiltonians equilibrate information theoretically with respect to a fixed observable A and time $t > t_{\mathrm{eq}}$, in the limit as $D \to \infty$, if the ensemble average and variance (denoted $\mathbb{E}_{E_H}$ and $\mathbb{V}_{E_H}$, respectively) of the outcome variance obey for all $t \geq t_{\mathrm{eq}}$,

$$\mathbb{E}_{E_H}[\mathbb{V}_k\{\Pr(k|\rho(t))\}] \leq O(D^{-2}), \tag{3}$$

$$\mathbb{V}_{E_H}[\mathbb{V}_k\{\Pr(k|\rho(t))\}] \leq O(D^{-4}). \tag{4}$$

Proof is given in the Supplemental Material [26].

We now give our first evidence for universality by proving that ITE is typical for the important GUE, which defines an invariant measure on the set of Hamiltonians. The GUE is the appropriate model, a highly successful model for many properties of complex physical systems with no hidden symmetries [21].

Theorem 2.—Take a nondegenerate observable A acting on $\mathcal{H} = \mathbb{C}^D$, and an initial pure state $\rho_0 = |x\rangle\langle x|$ which is an eigenstate of A. Almost all Hamiltonians drawn from GUE then equilibrate information theoretically with respect to A and $t \geq t_{\mathrm{eq}}$ in the limit as $D \to \infty$ for $t_{\mathrm{eq}}(D) = O(D^{-1/6})$.

The proof is in the Supplemental Material [26]. This theorem implies the remarkable result that, as D increases, the overwhelming majority of Hamiltonians will cause an initially pure, localized state to spread out over the nondegenerate eigenbasis of A in a sufficiently uniform manner, to become practically indistinguishable from the microcanonical state for any $t \geq t_{\mathrm{eq}}$. Thanks to decades of numerical studies of GUE as a model of complex many-body systems [32] and few-body quantum chaos systems [22], it is known that GUE is a good predictor of short-range spectral fluctuations [33], and low-order moments of eigenvector components [30,31], but not a good predictor of long-range spectral fluctuations [22]. Our proof of the smallness of the fluctuations using GUE (for $t > t_{\mathrm{eq}}$)

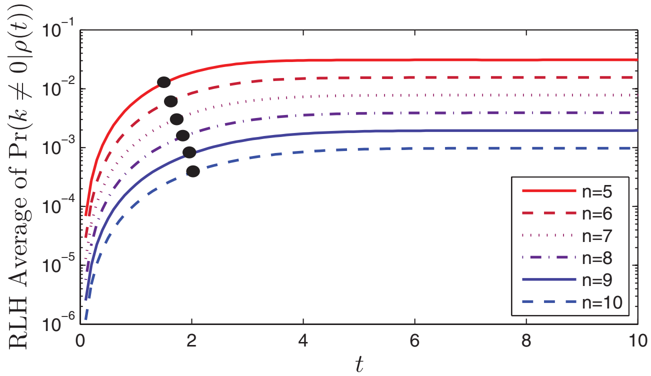

FIG. 2 (color). The RLH ensemble average of the probabilities $\Pr(k \neq 0|e^{-iHt}|0\rangle\langle 0|e^{iHt})$ of the evolved state for 250 random Hamiltonians plotted as a function of time for 5,…,10 qubit systems. The circles show $t_{\rm eq}$ for each n, which scale roughly as $O(\log(D))$.

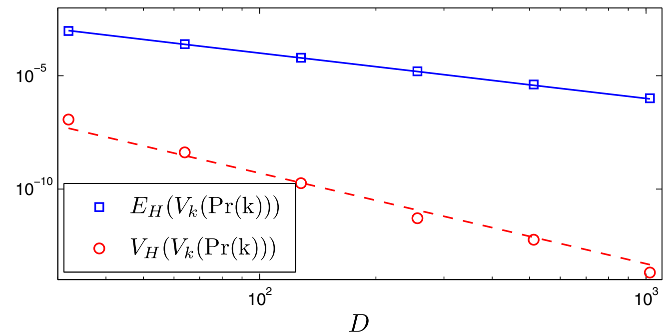

FIG. 3 (color online). Numerically computed expectation values and variances over the RLH ensemble of the outcome variance computed at $t = 10$ where $t_{\rm eq} \lesssim 2$ for $\rho(0) = |0\rangle\langle 0|$. The data were obtained for 250 randomly chosen Hamiltonians, and show that $\mathbb{V}_{E_H}[\mathbb{V}_k\{\Pr(k|\rho(t))\}] \approx 0.05D^{-4}$ and $\mathbb{E}_{E_H}[\mathbb{V}_k\{\Pr(k|\rho(t))\}] \approx D^{-2}$.

depends only on low-order moments of the eigenvector components, i.e., a unitary t-design condition with $t = 8$ [34] (see Supplemental Material for details [26]). Hence, we expect this aspect of the GUE model to be reflected in physically relevant Hamiltonian systems. However, we do not expect the GUE prediction for the equilibration time scale to be physically relevant (clearly the value of $t_{\rm eq}$ for GUE is unrealistically short) because it depends on long-range spectral fluctuations. We now confirm both of these expectations for two random-matrix ensembles consisting of many-body spins with two-body interactions, and conclude by demonstrating ITE with respect to tensor product measurements on a physically relevant time scale in some example model systems.

We construct an ensemble of RLH on n spins, consisting of two-body interactions between two-level quantum systems, as follows:

$$H = \|H\|^{-1}\left(\sum_{i=1}^{n}\sum_{p} a_{i,p}\sigma_p^{(i)} + \sum_{i<j}\sum_{p,p'} b_{i,j,p,p'}\sigma_p^{(i)}\sigma_{p'}^{(j)}\right),$$

where $p,\ p' \in \{X, Y, Z\}$, and each $a_{i,p}$ and $b_{i,j,p,p'}$ is a Gaussian random variable with mean 0 and variance 1. We consider the observable $A = \sum_{j=0}^{D-1} a_j|j\rangle\langle j|$, corresponding to a nondegenerate projective measurement in the eigenbasis of $\sigma_z^{\otimes n}$. RLH is clearly invariant under the permutation of qubit labels and local rotations of each qubit, and therefore our results also apply to any A' that differs from A by local rotations. Figure 2 shows that pure states evolving under individual elements of RLH approach equilibrium as D increases. We estimate the equilibration time using the location of the inflection points of the curves in Fig. 2, and find it scales as $O(\log(D))$, which is characteristic of quantum chaotic systems [22,28,29]. Figure 3 shows that the outcome variance for a typical Hamiltonian chosen uniformly from the RLH ensemble satisfies the requirements of Lemma 1, which implies that almost all RLH Hamiltonians will equilibrate information theoretically with respect to any nondegenerate measurement in the class A' as $D \to \infty$ for any $t \geq t_{\rm eq}$. We further strengthen the physical relevance of this result by showing that ITE still holds for $t \geq t_{\rm eq}$ when the two-local Hamiltonians are constrained to have nearest-neighbor interactions in one and two dimensions (see Supplemental Material [26]).

We now give two simple examples of individual model systems that exhibit information-theoretic equilibration: a many-body system that is a two-field variant of the Heisenberg Hamiltonian and a one-body chaotic model, the quantum kicked top. The two-field variant of the Heisenberg mode consists of n spins arranged in a line with periodic boundary conditions:

$$H = \frac{1}{\|H\|}\left(\sum_{i\leq n/2}\sigma_z^{(i)} + \sum_{i>n/2}\sigma_x^{(i)} + \sum_i \vec{\sigma}^{(i)}\cdot\vec{\sigma}^{(i+1)}\right). \quad (5)$$

We choose this Hamiltonian because it is highly structured local Hamiltonian that is not typical of RLH and yet it is unstructured enough to be nonintegrable so there are no

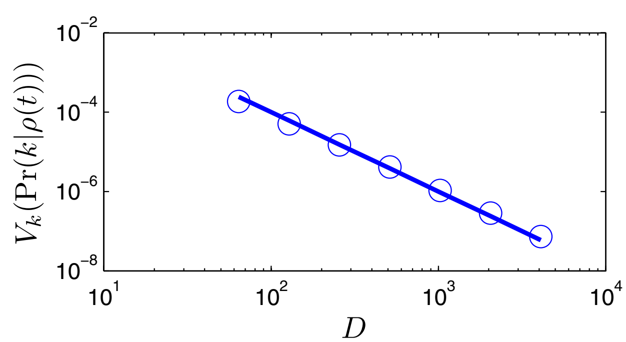

FIG. 4 (color online). Evidence of ITE for $t \geq t_{\rm eq}$ in an extremely simple many-body system with nearest-neighbor interactions for increasing number of spins n $(D = 2^n)$. The measurement consists of readout of each spin along the z axis. The plot shows $\mathbb{V}_k\{\Pr(k|\rho(t))\} \approx 1.6D^{-2}$ for the Hamiltonian, Eq. (5), with $t = 20$ where $t_{\rm eq} \simeq 15$ (see Supplemental Material [26]).

constants of motion that prevent equilibration on the full Hilbert space (otherwise ITE would be limited to the invariant subspaces fixed by the constants of motion). Figure 4 shows that the outcome variance of the probability distribution indeed scales as $O(D^{-2})$ with respect to $A = \sum_{j=0}^{D-1} a_j |j\rangle\langle j|$, corresponding to a readout of all spins in the computational basis. Hence, Theorem 1 implies that information-theoretic equilibration occurs for this simple many-body Hamiltonian with respect to a natural observable. This is evidence that our equilibration mechanism is not just a mathematical feature of random Hamiltonian ensembles but occurs also in a simple, physically accessible many-body model. We also demonstrate ITE for the quantum kicked top in a regime of global chaos with respect to nondegenerate measurements in the J_z basis (see Supplemental Material [26]) and physically accessible times.

Conclusion.—We have demonstrated a novel mechanism for equilibration that holds very broadly for the probability distributions of even maximally fine-grained measurements on pure quantum states of closed Hamiltonian systems. Remarkably, this information-theoretic equilibration is observed to hold without requiring any form of decoherence or restricting to local or otherwise coarse-grained measurements. This is because, in the typical case of a complex system, the dynamical pure-state quantum fluctuations, though finite, do *not* lead to a breakdown of correspondence with the equilibrium state (contrary to a common implicit assumption, see Refs. [1,24,25]) because they become unobservably small under purely statistical considerations (in the limit of large D) after the equilibration time scale. Our key insight is that although dynamical pure states of complex systems exhibit coherent fluctuations away from true microcanonical equilibrium, their detection in practice requires extraordinary experimental resources, such as collecting $O(D^{1/4})$ measurement outcomes from repetitions of the experiment, or precomputation of the location of the dynamical state in a D-dimensional Hilbert space, or performing joint (entangling) measurements on identical copies of the system. In the absence of such resources, by Theorem 1 we see that after some finite time, the empirical probability distributions for dynamical pure states of complex quantum systems cannot be distinguished from the microcanonical equilibrium state.

We thank Fernando Brandão, Carl Caves, David Cory, Patrick Hayden, Daniel Gottesman, and Victor Veitch for insightful comments. We acknowledge funding from CIFAR, Ontario ERA, NSERC, US ARO/DTO, and thank the Perimeter Institute for Theoretical Physics where this work was brought to completion.

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