

On the generic increase of observational entropy in isolated systems

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Observational entropy – a quantity that unifies Boltzmann’s entropy, Gibbs’ entropy, von Neumann’s macroscopic entropy, and the diagonal entropy – has recently been argued to play a key role in a modern formulation of statistical mechanics. Here, relying on algebraic techniques taken from Petz’s theory of statistical sufficiency and on a Lévy-type concentration bound, we prove rigorous theorems showing how the observational entropy of a system undergoing a unitary evolution chosen at random tends to increase with overwhelming probability and to reach its maximum very quickly. More precisely, we show that for any observation that is sufficiently coarse with respect to the size of the system, regardless of the initial state of the system (be it pure or mixed), random evolution renders its state practically indistinguishable from the microcanonical distribution with a probability approaching one as the size of the system grows. The same conclusion holds not only for random evolutions sampled according to the unitarily invariant Haar distribution, but also for approximate 2-designs, which are thought to provide a more physically reasonable way to model random evolutions.

John von Neumann, in his book on the mathematical foundations of quantum theory [1], immediately after having introduced and operationally motivated the quantity that is now known as *von Neumann entropy*, notices however that such a quantity is not the right one to consider in the context of statistical mechanics. This is because, as he writes,

[von Neumann entropy] is invariant in the normal [i.e., Hamiltonian] evolution in time of the system, and only increases with measurements – in the classical theory (where the measurements in general played no role) it increased as a rule even with the ordinary mechanical evolution in time of the system [1]. (Square brackets added for clarity.)

In the above passage, von Neumann presumably refers to the free expansion of an ideal gas, in which there is a strict increase in the (macroscopic) thermodynamic entropy, although the (microscopic) von Neumann entropy associated with the state of the gas does not change as the gas undergoes Hamiltonian evolution.

To meet this challenge, von Neumann proposes the concept of *macroscopic entropy*, which takes into account not only the intrinsic uncertainty associated with the microscopic state of the system, but also the additional uncertainty associated with the coarse-grained, macroscopic observation with which the system is being monitored. As the gas expands, it is this latter aspect of uncertainty, arising from the limited capabilities of a macroscopic observer, that increases while the microscopic degrees of freedom evolve undisturbed.

Since von Neumann’s proposal, macroscopic entropy has been largely overshadowed by its more famous – and eponymous – sibling. A notable exception is Wehrl’s review paper [2], where macroscopic entropy (therein referred to as *coarse-grained entropy*) plays an important role. Nevertheless, von Neumann’s macroscopic entropy

and a generalization of it called *observational entropy* have recently been the subject of renewed interest [3–7], in connection with the mathematical and conceptual foundations of statistical mechanics [8] and various applications [9–21].

von Neumann brings the idea of macroscopic entropy to fruition by proving for it a powerful H-theorem [22–24], showing that macroscopic entropy tends to increase, even in Hamiltonian systems, and typically grows to its maximum value, regardless of the initial state of the system [25]. In the same spirit, in this paper we study the change of observational entropy in unitarily evolving systems, focusing in particular on its *generic* behavior when the evolution of the system is chosen at random. Motivated by Ref. [8], which shows that the observational entropy of an isolated¹ system initialized in a state fully known to the observer cannot decrease, we first provide an explicit characterization of all situations in which the observational entropy undergoes a *strict* increase with time. Such a characterization relies on Petz’s theory of statistical sufficiency [26–29].

We then move to the case of arbitrary initial states, for which, based on a Lévy-type concentration bound [30, 31] that we prove for the observational entropy, we arrive at a statement similar to von Neumann’s H-theorem: for any observation that is “sufficiently coarse-grained” with respect to the size of the system, under the action of Haar-random evolution, the observational entropy approaches its maximum, i.e., the state of the system becomes practically indistinguishable from the microcanonical distribution, regardless of the state it started from. Finally, by specializing several derandomization techniques [32–35], we show that the same conclusion holds when the

¹ Here we follow Ref. [8] and call a system *isolated* if it can only exchange work – its evolution is therefore unitary, but not necessarily energy conserving.

Haar distribution is replaced by an approximate 2-design, which represents a more reasonable model, both physically and computationally, for random evolutions.

Background.—Following the standard conventions in quantum information theory [36, 37], in this paper we consider a finite d -dimensional quantum system, with Hilbert space \mathcal{H} , whose states are represented by density operators $\rho \geq 0$, $\text{Tr}[\rho] = 1$. The maximally mixed (i.e., uniform) state, corresponding to the microcanonical ensemble, is denoted $u = \mathbb{1}/d$. The von Neumann entropy, i.e., the microscopic entropy, is defined by the formula $S(\rho) = -\text{Tr}[\rho \log \rho]$, which is zero if and only if the state ρ is pure, i.e., a rank-one projector on some unit vector $|\varphi\rangle \in \mathcal{H}$. Another central quantity is the Umegaki quantum relative entropy [38, 39], defined as $D(\rho\|\sigma) = \text{Tr}[\rho(\log \rho - \log \sigma)]$, where $\sigma > 0$ is an invertible reference (or *prior*) state. Whenever ρ and σ commute, the Umegaki relative entropy coincides with the Kullback–Leibler divergence [40]. An observation (measurement) on the system is mathematically represented by a positive operator-valued measure (POVM), i.e., a family $\mathbf{P} = \{P_x\}_x$ of positive semi-definite operators $P_x \geq 0$, labeled by a finite set $\mathcal{X} = \{x\}$ (the outcome set), and normalized so that $\sum_x P_x = \mathbb{1}$: given the state of the system ρ , the expected probability of observing outcome x is computed as $p_x = \text{Tr}[P_x \rho]$. Whenever all the elements of a POVM are projections, i.e., $P_x P_{x'} = \delta_{xx'} P_x$, we speak of a projection-valued measure, or PVM. A PVM is *trivial* if one of its elements is the identity operator $\mathbb{1}$ (and all the remaining elements are null). In what follows, as very often done in the literature, it will be convenient to think of an observation as a quantum-to-classical channel, i.e., a map $\mathcal{P}(\cdot) = \sum_x \text{Tr}[P_x \cdot] |x\rangle\langle x|$, where $|x\rangle$ are orthonormal vectors in an auxiliary Hilbert space with dimension equal to the size of the outcome set \mathcal{X} . Finally, we recall the idea of POVM post-processing [41, 42]: given two POVMs $\mathbf{P} = \{P_x\}_{x \in \mathcal{X}}$ and $\mathbf{Q} = \{Q_y\}_{y \in \mathcal{Y}}$, defined on the same Hilbert space \mathcal{H} but with possibly different outcome sets, we write $\mathbf{Q} \preceq \mathbf{P}$ whenever there exists a conditional probability distribution $p(y|x)$ such that $Q_y = \sum_x p(y|x) P_x$, for all $y \in \mathcal{Y}$.

Observational entropy.—The observational entropy (OE) of a microscopic state ρ with respect to a POVM $\mathbf{P} = \{P_x\}_{x \in \mathcal{X}}$ is defined as [3–8]

$$\begin{aligned} S_{\mathbf{P}}(\rho) &= -\sum_x p_x \log \frac{p_x}{V_x} \\ &= \log d - D(\mathcal{P}(\rho)\|\mathcal{P}(u)), \end{aligned}$$

where $p_x = \text{Tr}[P_x \rho]$ and $V_x = \text{Tr}[P_x]$. Since $V_x = 0$ implies $P_x = 0$ and hence, in particular, $p_x = 0$, without loss of generality we can consider only POVMs with $V_x > 0$ for all $x \in \mathcal{X}$, so that the OE is always finite. The presence of both the probabilities p_x and the volume

terms V_x suggests that OE somehow “interpolates” between Boltzmann’s and Gibbs’ entropies. Indeed, when there exists one particular \bar{x} such that $p_{\bar{x}} = 1$, OE recovers the Boltzmann entropy $\log V_{\bar{x}}$, whereas when the volume terms are all equal to one, OE coincides with the Gibbs entropy $-\sum_x p_x \log p_x$. In the latter case, in particular, if the POVM consists of the orthogonal projectors on the energy eigenbasis, then OE recovers what is known as *diagonal entropy* [43].

The fundamental bound of OE, which is a consequence of the data-processing property of the Umegaki relative entropy, is $S_{\mathbf{P}}(\rho) \geq S(\rho)$, which holds for any choice of ρ and \mathbf{P} [6]. States that saturate the bound, i.e., states ρ such that $S_{\mathbf{P}}(\rho) = S(\rho)$ are called *macroscopic* for \mathbf{P} . The reason for such a name comes from the fact that the condition $S_{\mathbf{P}}(\rho) = S(\rho)$ holds if and only if [6]

$$\rho = \sum_x \text{Tr}[P_x \rho] \frac{P_x}{V_x}, \quad (1)$$

which means that the state ρ can be perfectly retrodicted [44–46] only from the knowledge of the measurement \mathbf{P} and its outcomes’ statistics p_x , i.e., information all available to the macroscopic observer [6]. Notice that the maximally mixed state u is always macroscopic, for any choice of POVM \mathbf{P} . Moreover, u always achieves the maximum value of OE, that is, $S_{\mathbf{P}}(u) = \log d$.

OE increase in macroscopic states.—As anticipated in the introduction, one of the main reasons to consider OE is that it can increase even in isolated systems, in contrast to von Neumann entropy, which instead remains constant. Motivated by Ref. [8], we begin our study by considering the behavior of OE when the initial state of the system is macroscopic. Such an assumption will be lifted in the rest of the paper.

Let us thus consider an isolated system evolving in time from $t = t_0$ to $t = t_1 > t_0$. Let ρ_0 be the initial state of the system, U describe the time evolution from t_0 to t_1 , and $\rho_1 = U \rho_0 U^\dagger$ be the state of the system at t_1 . Let us also assume that, at time t_0 , the system’s state is macroscopic for \mathbf{P} . While the von Neumann entropy $S(\rho_t)$ of the system remains constant (as a consequence of the fact that the von Neumann entropy only depends on the spectrum of the density operator, which does not change under unitary transformations), for the OE we have:

$$\begin{aligned} S_{\mathbf{P}}(\rho_1) &= -\sum_x \text{Tr}[P_x \rho_1] \log \frac{\text{Tr}[P_x \rho_1]}{\text{Tr}[P_x]} \\ &= \sum_x \text{Tr}[U^\dagger P_x U \rho_0] \log \frac{\text{Tr}[U^\dagger P_x U \rho_0]}{\text{Tr}[U^\dagger P_x U]} \\ &= S_{U^\dagger \mathbf{P} U}(\rho_0) \\ &\geq S(\rho_0) = S_{\mathbf{P}}(\rho_0) = S(\rho_1). \end{aligned} \quad (2)$$

The final inequality holds because ρ_0 is macroscopic for

\mathbf{P} , but may not be so for $U^\dagger \mathbf{P} U$. Thus, from the above, we immediately see that:

- i) the OE of an isolated system starting in a macroscopic state never decreases (cfr. Lemma 5 in [8]);
- ii) it remains constant if and only if ρ_1 is *also* macroscopic for the *same* \mathbf{P} as ρ_0 .

Given that, the question that we want to consider now is: when does the OE *strictly* increase? In order to answer this question, we first need to provide a characterization of all macroscopic states associated with a given POVM $\mathbf{P} = \{P_x\}$. While Eq. (1) provides an implicit characterization, the following theorem provides it *explicitly*.

Theorem 1 (Macroscopic states). *Given a POVM $\mathbf{P} = \{P_x\}$, a state \mathbf{m} is macroscopic for \mathbf{P} , i.e., satisfies Eq. (1), if and only if there exists a PVM $\mathbf{\Pi} = \{\Pi_y\}_y$, with $\mathbf{\Pi} \preceq \mathbf{P}$, together with coefficients $c_y \geq 0$, such that*

$$\mathbf{m} = \sum_y c_y \Pi_y. \quad (3)$$

The full proof of Theorem 1, which is based on the theory of statistical sufficiency [28, 29], can be found in the Supplemental Material; here we only comment on its consequences. We first note that, since the maximally mixed state u is macroscopic for any POVM but remains invariant, the interesting situations, i.e., those in which a strict increase of OE can occur, may arise only if non-uniform macroscopic states exist. As a consequence of Theorem 1, a necessary condition for a state \mathbf{m} to be macroscopic for a POVM $\mathbf{P} = \{P_x\}_{x \in \mathcal{X}}$, is that $[\mathbf{m}, P_x] = 0$ for all $x \in \mathcal{X}$. This fact, whose proof can be found in the Supplemental Material, immediately tells us that, in the case of an isolated system initially prepared in a non-uniform macroscopic state, only a very restricted set of unitary operators, i.e., those that satisfy the conservation-like relation

$$[U \mathbf{m} U^\dagger, P_x] = 0, \quad \forall x,$$

can preserve the observer’s information about the system, whereas a generic evolution, such as one uniformly sampled from the entire set of unitary operators, will necessarily cause a strict increase in OE. In such cases, although the microscopic evolution is perfectly reversible, from the macroscopic observer’s point of view, information is irreversibly lost.

OE increase in arbitrary states.—In the above discussion, we used algebraic arguments to treat the case of isolated systems that are initially prepared in non-uniform macroscopic states. In what follows, we instead apply measure-theoretic ideas, in particular Lévy-type concentration bounds, to show that, under appropriate assumptions, no matter what the initial state of the system is (macroscopic or not, pure or mixed), if the observation

is “sufficiently coarse” with respect to the size of the system, the probability that a random unitary evolution will bring the OE of the system close to its maximum value $\log d$, so that the state of the system becomes macroscopically indistinguishable from the microcanonical distribution, is close to one.

In order to formalize this intuition we begin with the simplest, although highly idealized, case of a random evolution sampled from the Haar (unitarily invariant) distribution. (Proof in the Supplemental Material.)

Theorem 2 (Haar-random case). *Let us consider a d -dimensional system in an arbitrary (but fixed) state ρ , a POVM $\mathbf{P} = \{P_x\}$ with finite outcomes, and a value $\delta > 0$. For a unitary operator U sampled at random according to the Haar (unitarily invariant) distribution, the probability that the system’s observational entropy $S_{\mathbf{P}}(U \rho U^\dagger)$ is δ -far from the maximum value $\log d$ can be bounded as follows:*

$$\begin{aligned} \mathbb{P}_H \{S_{\mathbf{P}}(U \rho U^\dagger) \leq (1 - \delta) \log d\} \\ \leq \frac{4}{\kappa(\mathbf{P})} e^{-C \delta \kappa(\mathbf{P})^2 d \log d}, \end{aligned} \quad (4)$$

where $\kappa(\mathbf{P}) = \min_x \text{Tr}[P_x u]$ is an “effective coarseness” parameter and $C = \frac{1}{18\pi^3} \approx 0.0018 > 2^{-10}$.

In other words, after a random unitary evolution, under any sufficiently coarse observation, the system will essentially look as if it were in the microcanonical (i.e., maximally mixed) state, no matter what its actual initial state was. Looking at Eq. (4), the parameter that decides whether the POVM is sufficiently coarse with respect to given dimension d and tolerance δ is the effective coarseness parameter $\kappa(\mathbf{P})$. For the probability to be small, $\kappa(\mathbf{P})$ has to be large enough to compensate for C and δ . This also puts a bound on the number of outcomes $N(\mathbf{P})$, since $N(\mathbf{P}) \kappa(\mathbf{P}) \leq \sum_x \text{Tr}[P_x u] = 1$. This condition is reminiscent of von Neumann’s condition on the minimum size of the phase cells in his proof of the H-theorem [22]:

The number of states (quantum orbits) in each phase cell has to be not only very large, but also on average quite large compared to the number of phase cells.

In our notation, the role of the “number of states in each phase cell” is played by $\min_x \text{Tr}[P_x] = d \kappa(\mathbf{P})$, while the “number of phase cells” is $N(\mathbf{P})$. We can thus summarize von Neumann’s condition as

$$\frac{N(\mathbf{P})}{d \kappa(\mathbf{P})} \ll 1. \quad (5)$$

But how restrictive is it? As the following back-of-the-envelope calculation shows, the above condition is not difficult to meet, even for systems of moderate size: for example, in a system comprising 128 qubits, i.e., $d =$

2^{128} , with $\delta = 2^{-5}$ and $\min_x \text{Tr}[P_x] = 2^{90} \ll 2^{128}$, the exponent is bounded as

$$C\delta\kappa(\mathbf{P})^2 d \log d > 2^{-10} 2^{-5} \frac{2^{180}}{2^{128}} 2^7 = 2^{44},$$

so that the probability that the OE, after a Haar-random evolution, does *not* exceed $(1 - 2^{-5}) \times 128 = 124$ bits is less than $2^{50} \times \exp[-2^{44}] \approx 10^{-10^{12}}$. This means that there is an overwhelming probability that the OE will be greater than 124 bits, regardless of its value before random evolution took place.

Taking the limit.—Theorem 2 above provides a bound on the probability of large deviations when all parameters are fixed. In what follows, following a common approach, we want to consider also the asymptotic behavior of OE in a sequence of systems and observations, in the limit of d (i.e., the system’s Hilbert space dimension) tending to infinity. To do this, we must first define exactly what it means for a sequence of observations to be “asymptotically coarse”.

Definition 1 (Asymptotic coarseness). *Consider a sequence of systems with increasing dimension d and, in each system, a POVM $\mathbf{P}^{(d)} = \{P_{x_d}^{(d)}\}_{x_d}$. For each d , define $\kappa(d) \equiv \kappa(\mathbf{P}^{(d)}) = \min_{x_d} \text{Tr}[P_{x_d}^{(d)} u]$. The sequence of POVMs $\{\mathbf{P}^{(d)}\}_{d \in \mathbb{N}}$ is said to be asymptotically coarse whenever there exists $\tau > 0$ such that*

$$\kappa(d) = \Omega(d^{-\frac{1}{2}+\tau}), \quad (6)$$

i.e., whenever $\exists M > 0$ and $\exists d_0$ such that

$$\kappa(d) \geq M \cdot d^{-\frac{1}{2}+\tau}, \quad \forall d > d_0. \quad (7)$$

The above definition can be justified starting from von Neumann’s condition (5) as follows. Let us assume that, in the limit $d \rightarrow \infty$, von Neumann’s condition becomes $N(\mathbf{P}^{(d)})/d\kappa(\mathbf{P}^{(d)}) \rightarrow 0$. For $\kappa(d) \sim d^\alpha$, we obtain

$$\frac{N(\mathbf{P}^{(d)})}{d\kappa(\mathbf{P}^{(d)})} \leq \frac{1}{d[\kappa(\mathbf{P}^{(d)})]^2} \sim d^{-2\alpha-1},$$

where for the first inequality we used the fact that the POVM is normalized, i.e., $N(\mathbf{P}^{(d)})\kappa(\mathbf{P}^{(d)}) \leq 1$. The above then goes to zero if and only if $\alpha > -1/2$, in agreement with Definition 1.

An alternative justification for Definition 1 can be derived from Theorem 2. For an asymptotically coarse sequence $\{\mathbf{P}^{(d)}\}_{d \in \mathbb{N}}$ of POVM, i.e., such that $\kappa(d) = \Omega(d^{-\frac{1}{2}+\tau})$, the right-hand side of Eq. (4) is of order $d^{\frac{1}{2}-\tau} e^{-C\delta d^{2\tau} \log d}$, which goes to zero for any $\delta > 0$ in the limit of $d \rightarrow \infty$. Therefore, for a system of sufficiently large dimension d , it holds that

$$\mathbb{P}_H\{S_{\mathbf{P}^{(d)}}(U\rho U^\dagger) \approx \log d\} \approx 1, \quad (8)$$

in line with what would be expected from a typical macroscopic observation.

Physical random evolutions.—The Haar distribution, while mathematically convenient, is often considered an unphysical model for random evolutions, because the amount of randomness required to sample from it grows exponentially with the dimension of the system. In what follows, we derive an alternative law of OE increase that also holds for generic, but now physically reasonable, random evolutions.

As is now common practice in theoretical condensed matter physics, in what follows we replace the continuous Haar distribution by ε -approximate 2-designs, i.e. finite sets \mathcal{E} of unitary operators which, if chosen at random, are able to reproduce, up to an error ε , many features of the Haar distribution that are of physical interest [32, 33]. The relevance of approximate 2-designs lies in the fact that it has recently been shown, using rigorous complexity-theoretic arguments [34, 35], that indeed ε -approximate 2-designs and, more generally, k -designs can be efficiently implemented as short random circuits, thus justifying them as a physically reasonable model for random evolutions. As shown in the Supplemental Material, we obtain the following theorem.

Theorem 3 (Approximate 2-design case). *For a unitary operator U sampled at random from an ε -approximate 2-design \mathcal{E} , regardless of the initial state ρ of the d -dimensional system at hand, we have*

$$\begin{aligned} \mathbb{P}_{\mathcal{E}}\{S_{\mathbf{P}}(U\rho U^\dagger) \leq (1 - \delta) \log d\} \\ \leq \frac{1}{\kappa(\mathbf{P})^3 d \log d} \frac{4(1 + \varepsilon)}{\delta}, \end{aligned} \quad (9)$$

for any value $\delta > 0$.

The upper bound given in Eq. (9) is weaker with respect to that given in Eq. (4), since the negative exponential rate in d that was present in (4) is now lost, replaced by $(d \log d)^{-1}$. This is due to the fact that the assumptions in Theorem 3 are weaker, in the sense that an ε -approximate 2 design is only an approximation of the ideal, but unphysical, Haar distribution. Again, we emphasize that while ε -approximate 2-designs are physically reasonable because they can be implemented efficiently with little randomness [34, 35], the Haar distribution is more of a mathematical abstraction.

Nevertheless, the right-hand side of Eq. (9) is still very small in a large window of parameter values. For example, using the same values of the parameters that we used in the back-of-the-envelope calculation that we did for the Haar-random case, the probability that the OE, after an evolution sampled at random from an ε -approximate 2-design ($\varepsilon < 1$), does not exceed 124 bits (when the maximum is 128) is again quite small:

$$\frac{1}{\kappa(\mathbf{P})^3 d \log d} \frac{4(1 + \varepsilon)}{\delta} < \frac{2^{258}}{2^{277}} \times 2^8 = 2^{-11}.$$

Crucially, the only parameter that depends on the POVM is again the effective coarseness $\kappa(\mathbf{P})$.

More importantly, Eq. (9) still allows us to prove an asymptotic result, although the notion of asymptotic coarseness given in Definition 1 must be modified with respect to that obtained before using Eq. (4). Now, in the case of ε -approximate 2-designs, we require that $\kappa(d) = \Omega(d^{-\frac{1}{3}+\tau})$ for some $\tau > 0$, which means that the number of states in the smallest cell has to grow with d as $d^{\frac{2}{3}+\tau}$. In other words, asymptotic coarseness for ε -approximate 2-designs is *coarser* than in Definition 1, which was introduced having in mind the case of Haar-random unitaries. But if the stricter requirement is satisfied, the right-hand side of Eq. (9) is of order $4(1+\varepsilon)/(\delta d^{3\tau} \log d)$, which goes to zero for any $\varepsilon, \delta > 0$ in the limit of $d \rightarrow \infty$. Therefore, for any sufficiently large d , even in the case where U is sampled from a ε -approximate 2-design \mathcal{E} , it holds that

$$\mathbb{P}_{\mathcal{E}}\{S_{\mathbf{P}}(U\rho U^{\dagger}) \approx \log d\} \approx 1. \quad (10)$$

Conclusions.—In this paper we have demonstrated three ways in which observational entropy tends to increase and reach its maximum in isolated systems undergoing a generic unitary evolution. First, we showed that if the system starts in a non-uniform macroscopic state, only unitary operators belonging to a subvariety of zero volume in the set of all unitaries keep OE invariant, otherwise OE strictly increases. Our proofs here were entirely algebraic, relying on Petz’s theory of statistical sufficiency. We then moved on to the problem of showing that the increase of OE, in sufficiently large systems and for sufficiently coarse observations, is a generic phenomenon, independent of the initial state of the system. We considered both Haar-random evolutions, which give better bounds but are not physically reasonable, and ε -approximate 2-designs, which give looser bounds but provide a realistic model of random physical evolutions. In both cases, we found that for sufficiently large systems and sufficiently coarse observations, the state of the system quickly becomes indistinguishable from the micro-canonical one.

An important open question is whether it is possible to show OE concentration inequalities for concrete Hamiltonians, such as the free-fermion chain [47]. Another possibility is to show an increase of the OE for random matrix product states and their long time averages [48].

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APPENDIX

Characterization of the macroscopic states (Proof of Theorem 1)

Lemma 1. *Suppose that $\mathbf{Q} = \{Q_y\}$ is sharp, i.e., there exists a unit vector $|\phi_y\rangle$ such that $Q_y|\phi_y\rangle = |\phi_y\rangle$ for all $y \in \mathcal{Y}$ [49]. Suppose also that there exists another POVM $\mathbf{P} = \{P_x\}$ such that $\mathbf{Q} \preceq \mathbf{P}$. Then, the post-processing transforming \mathbf{P} into \mathbf{Q} is deterministic, i.e., $p(y|x) \in \{0, 1\}$ for all x and y .*

Proof. Let us choose and fix some $\bar{y} \in \mathcal{Y}$ and let $|\phi_{\bar{y}}\rangle$ be such that $\langle\phi_{\bar{y}}|Q_{\bar{y}}|\phi_{\bar{y}}\rangle = 1$. Such a vector exists because Q is assumed to be sharp. Then,

$$1 = \langle\phi_{\bar{y}}|Q_{\bar{y}}|\phi_{\bar{y}}\rangle \quad (\text{S.1})$$

$$= \sum_{x:p(\bar{y}|x)>0} p(\bar{y}|x)\langle\phi_{\bar{y}}|P_x|\phi_{\bar{y}}\rangle \quad (\text{S.2})$$

$$\leq \sum_{x:p(\bar{y}|x)>0} \langle\phi_{\bar{y}}|P_x|\phi_{\bar{y}}\rangle \quad (\text{S.3})$$

$$\leq 1. \quad (\text{S.4})$$

Therefore, for all $x \in \mathcal{X}$, the probabilities $p(\bar{y}|x)$ must be either one or zero. Since the same holds for any choice of \bar{y} , the statement is proved. \square

Proof of Theorem 1. By definition, \mathbf{m} is a macroscopic state if and only if

$$D(\mathbf{m}||u) = D(\mathcal{P}(\mathbf{m})||\mathcal{P}(u)). \quad (\text{S.5})$$

As proved in [6], the above condition is equivalent to

$$\mathbf{m} = \sum_x \text{Tr}[P_x \mathbf{m}] \frac{P_x}{V_x}. \quad (\text{S.6})$$

The condition (S.6) is satisfied for $\mathbf{m}' := \sum_y c_y \Pi_y$. Indeed, we have

$$\sum_x \text{Tr}[P_x \mathbf{m}'] \frac{P_x}{V_x} = \sum_y c_y \sum_x \text{Tr}[P_x \Pi_y] \frac{P_x}{V_x} \quad (\text{S.7})$$

$$= \sum_y c_y \sum_{x:\text{supp}P_x \subset \text{supp}\Pi_y} \text{Tr}[P_x] \frac{P_x}{V_x} \quad (\text{S.8})$$

$$= \sum_y c_y \Pi_y \quad (\text{S.9})$$

$$= \mathbf{m}', \quad (\text{S.10})$$

where the second and the third line follows from Lemma 1.

Conversely, suppose that \mathbf{m} satisfies Eq. (S.5) and let $\{|e_k\rangle\}_k$ be an eigenbasis of \mathbf{m} . Correspondingly, let us define the map

$$\text{diag}_{\mathbf{m}}(X) := \sum_k |e_k\rangle\langle e_k|X|e_k\rangle\langle e_k|.$$

As shown in [28, Section 4.2], Eq. (S.5) implies that

$$\mathbf{m}\Pi_y = c_y \Pi_y, \quad (\text{S.11})$$

where $\Pi_y := \sum_{x \in \mathcal{X}_y} \text{diag}_{\mathbf{m}}(P_x)$, for some partition of \mathcal{X} into disjoint subsets as $\mathcal{X} = \mathcal{X}_1 \cup \mathcal{X}_2 \cup \dots \cup \mathcal{X}_\ell$, such that $\text{diag}_{\mathbf{m}}(P_x)\text{diag}_{\mathbf{m}}(P_{x'}) = 0$ whenever x and x' do not belong to the same subset. Notice that, in general, such a partition is not uniquely defined.

It is easy to see that the operators Π_y are, by construction, positive semi-definite and orthogonal to each other. Moreover, since $\mathbb{1} = \text{diag}_{\mathbf{m}}(\mathbb{1}) = \text{diag}_{\mathbf{m}}(\sum_x P_x) = \sum_x \text{diag}_{\mathbf{m}}(P_x)$, the set $\mathbf{\Pi} = \{\Pi_y\}_y$ in fact constitutes a PVM. Thus, by summing (S.11) over y , we immediately obtain Eq. (3) in the main text, i.e.,

$$\mathbf{m} = \sum_y c_y \Pi_y .$$

We still need to show that, for any such a partition, the corresponding PVM $\mathbf{\Pi}$ satisfies $\mathbf{\Pi} \preceq \mathbf{P}$. This is due to the fact that, since $\text{Supp} \text{diag}_{\mathbf{m}}(P_x) \supseteq \text{Supp} P_x$, two POVM elements P_x and $P_{x'}$ must have orthogonal supports, whenever x and x' belong to different subsets. Thus, not only $\Pi_y = \sum_{x \in \mathcal{X}_y} \text{diag}_{\mathbf{m}}(P_x)$, but in fact $\Pi_y = \sum_{x \in \mathcal{X}_y} P_x$, that is $\mathbf{\Pi} \preceq \mathbf{P}$. \square

In particular, if \mathbf{m} is macroscopic for $\mathbf{P} = \{P_x\}$, then

$$[\mathbf{m}, P_x] = 0 ,$$

for all $P_x \in \mathbf{P}$. In order to show this, for any PVM $\mathbf{\Pi} = \{\Pi_y\}$ such that $\mathbf{\Pi} \preceq \mathbf{P}$, as a consequence of Lemma 1 we have $\Pi_y := \sum_{x \in \mathcal{X}_y} P_x$, where \mathcal{X}_y are disjoint subsets covering \mathcal{X} . Then, $\text{Supp} \Pi_y \supseteq \text{Supp} P_x$ for all $x \in \mathcal{X}_y$, and being Π_y a projection, we see that Π_y acts as the identity operator on the supports of all the P_x 's it comprises. Moreover, it acts as the null operator on the support of all remaining P_x 's. Thus, any Π_y commutes with any P_x , though we notice that the operators P_x need not commute with each other. As a consequence, since macroscopic states are just linear combinations of Π_y 's, they all commute with all P_x 's.

Concentration of observational entropy

The proof strategy that we use here is to show that, for a unitary sampled at random, the probability that $\text{Tr}[U\rho U^\dagger P]$ is “close” to $\text{Tr}[uP]$, for any density matrix ρ and any non-null effect $0 \leq P \leq \mathbb{1}$, is “high”. We then use this fact to bound the probability of large deviations in observational entropy.

From probability to observational entropy

Lemma 2. *Let ρ be a density operator and $\mathbf{P} = \{P_x\}_{x \in \mathcal{X}}$ a POVM such that $|\mathcal{X}| < +\infty$. Let ν denote a measure on the d -dimensional unitary group \mathcal{U}_d and \mathbb{P}_ν the corresponding probability of an event. Suppose that there exists a real-valued non-increasing function g such that*

$$\mathbb{P}_\nu \{ |\text{Tr}[U\rho U^\dagger P_x] - \text{Tr}[uP_x]| \geq \xi \} \leq g(\xi) , \quad (\text{S.12})$$

for all $x \in \mathcal{X}$ and $\xi > 0$. Then, it holds that

$$\mathbb{P}_\nu \{ S_{\mathbf{P}}(U\rho U^\dagger) \leq (1 - \delta) \log d \} \leq \frac{1}{\kappa(\mathbf{P})} g \left(\kappa(\mathbf{P}) \sqrt{\delta \log d} \right) , \quad (\text{S.13})$$

where $\kappa(\mathbf{P}) := \min_{x \in \mathcal{X}} \text{Tr}[uP_x]$.

Proof. Define probability distributions $\mathbf{p} = \{p_x\}_x$ and $\mathbf{q} = \{q_x\}_x$ by $p_x = \text{Tr}[U\rho U^\dagger P_x]$ and $q_x = \text{Tr}[uP_x]$. By the definition of the observational entropy, we have

$$\log d - S_{\mathbf{P}}(U\rho U^\dagger) = D_{\text{KL}}(\mathbf{p} \parallel \mathbf{q}) , \quad (\text{S.14})$$

where D_{KL} is the Kullback-Leibler divergence for classical probability distributions defined by $D_{\text{KL}}(\mathbf{p} \parallel \mathbf{q}) = \sum_x p_x \log(p_x/q_x)$. The condition $S_{\mathbf{P}}(U\rho U^\dagger) \leq (1 - \delta) \log d$ is thus equivalent to $D_{\text{KL}}(\mathbf{p} \parallel \mathbf{q}) \geq \delta \log d$. We will invoke the following upper bound on D_{KL} :

$$D_{\text{KL}}(\mathbf{p} \parallel \mathbf{q}) \leq \sum_x \frac{(p_x - q_x)^2}{q_x} \leq \frac{|\mathcal{X}| \max_x (p_x - q_x)^2}{\min_x q_x} , \quad (\text{S.15})$$

where the first inequality was proved in [50] (see Lemma A.3 therein). The condition $D_{\text{KL}}(\mathbf{p}||\mathbf{q}) \geq \delta \log d$ then implies

$$\frac{|\mathcal{X}| \max_x (p_x - q_x)^2}{\kappa(\mathbf{P})} \geq \delta \log d, \quad (\text{S.16})$$

which is equivalent to

$$\max_x |\text{Tr}[U\rho U^\dagger P_x] - \text{Tr}[uP_x]| \geq \sqrt{\frac{\kappa(\mathbf{P})\delta \log d}{|\mathcal{X}|}}. \quad (\text{S.17})$$

Thus, we have

$$\mathbb{P}_\nu \{S_{\mathbf{P}}(U\rho U^\dagger) \leq (1 - \delta) \log d\} \leq \mathbb{P}_\nu \left\{ \max_x |\text{Tr}[U\rho U^\dagger P_x] - \text{Tr}[uP_x]| \geq \sqrt{\frac{\kappa(\mathbf{P})\delta \log d}{|\mathcal{X}|}} \right\} \quad (\text{S.18})$$

$$\leq \sum_x \mathbb{P}_\nu \left\{ |\text{Tr}[U\rho U^\dagger P_x] - \text{Tr}[uP_x]| \geq \sqrt{\frac{\kappa(\mathbf{P})\delta \log d}{|\mathcal{X}|}} \right\} \quad (\text{S.19})$$

$$\leq |\mathcal{X}| g \left(\sqrt{\frac{\kappa(\mathbf{P})\delta \log d}{|\mathcal{X}|}} \right) \quad (\text{S.20})$$

$$\leq \frac{1}{\kappa(\mathbf{P})} g \left(\kappa(\mathbf{P}) \sqrt{\delta \log d} \right), \quad (\text{S.21})$$

where the last line is due to $|\mathcal{X}|\kappa(\mathbf{P}) \leq 1$. □

Concentration with Haar-random unitaries (Proof of Theorem 2)

Lemma 3. (Lemma 3.2 in [33], see also [30, 51]) Let f be a Lipschitz function on \mathcal{U}_d , with the Lipschitz constant η defined by

$$\eta = \sup_{U_1 \neq U_2 \in \mathcal{U}_d} \frac{|f(U_1) - f(U_2)|}{\|U_1 - U_2\|_2}. \quad (\text{S.22})$$

Then

$$\mathbb{P}_H(|f - \mathbb{E}_H[f]| \geq \xi) \leq 4 \exp \left(-\frac{2d}{9\pi^3 \eta^2} \xi^2 \right), \quad (\text{S.23})$$

where \mathbb{P}_H denotes the probability computed with respect to the Haar (unitarily invariant) measure on \mathcal{U}_d , and $\mathbb{E}_H[f]$ denotes the corresponding mean of f .

Lemma 4. Let ρ be a density operator and let P be a positive semidefinite operator such that $P \leq \mathbf{1}$. For a Haar-distributed random unitary, it holds that

$$\mathbb{P}_H \{ |\text{Tr}[U\rho U^\dagger P] - \text{Tr}[uP]| \geq \xi \} \leq 4 \exp \left(-\frac{d\xi^2}{18\pi^3} \right). \quad (\text{S.24})$$

Proof. Due to Lemma 3, it suffices to prove that the Lipschitz constant of the function $f : U \mapsto \text{Tr}[U\rho U^\dagger P]$ is bounded above by 2. By the triangle inequality and the Cauchy–Schwarz inequality, we have

$$\left| \text{Tr}[U_1\rho U_1^\dagger P] - \text{Tr}[U_2\rho U_2^\dagger P] \right| = \left| \frac{1}{2} \text{Tr}[(U_1 + U_2)\rho(U_1 - U_2)^\dagger P] + \frac{1}{2} \text{Tr}[(U_1 - U_2)\rho(U_1 + U_2)^\dagger P] \right| \quad (\text{S.25})$$

$$\leq \frac{1}{2} \left| \text{Tr}[(U_1 + U_2)\rho(U_1 - U_2)^\dagger P] \right| + \frac{1}{2} \left| \text{Tr}[(U_1 - U_2)\rho(U_1 + U_2)^\dagger P] \right| \quad (\text{S.26})$$

$$\leq \|U_1 - U_2\|_2 \cdot \|P(U_1 + U_2)\rho\|_2. \quad (\text{S.27})$$

Taking a diagonal decomposition $\rho = \sum_i \lambda_i |e_i\rangle\langle e_i|$, the second term in the last line can be bounded as

$$\|P(U_1 + U_2)\rho\|_2^2 = \text{Tr}[\rho(U_1 + U_2)^\dagger P^2(U_1 + U_2)\rho] \quad (\text{S.28})$$

$$\leq \text{Tr}[\rho(U_1 + U_2)^\dagger (U_1 + U_2)\rho] \quad (\text{S.29})$$

$$= \sum_{i=1}^d \lambda_i^2 \langle e_i | (U_1 + U_2)^\dagger (U_1 + U_2) | e_i \rangle \quad (\text{S.30})$$

$$\leq \sum_{i=1}^d \lambda_i^2 \|(U_1 + U_2)\|_\infty^2 \quad (\text{S.31})$$

$$\leq 4 \text{Tr}[\rho^2] . \quad (\text{S.32})$$

This implies

$$\frac{|\text{Tr}[U_1 \rho U_1^\dagger P] - \text{Tr}[U_2 \rho U_2^\dagger P]|}{\|U_1 - U_2\|_2} \leq 2\sqrt{\text{Tr}[\rho^2]} \leq 2 , \quad (\text{S.33})$$

and completes the proof. \square

Proof of Theorem 2. It follows from Lemma 4 that

$$\mathbb{P}_H \{ |\text{Tr}[U \rho U^\dagger P_x] - \text{Tr}[u P_x]| \geq \xi \} \leq 4 \exp\left(-\frac{d\xi^2}{18\pi^3}\right) \quad (\text{S.34})$$

for all x . Applying Lemma 2, we obtain

$$\mathbb{P}_H \{ S_{\mathbf{P}}(U \rho U^\dagger) \leq (1 - \delta) \log d \} \leq \frac{4}{\kappa(\mathbf{P})} \exp\left(-\frac{\delta}{18\pi^3} \kappa(\mathbf{P})^2 d \log d\right) , \quad (\text{S.35})$$

where $\kappa(\mathbf{P}) := \min_{x \in \mathcal{X}} \text{Tr}[u P_x]$. \square

Concentration with approximate unitary designs (Proof of Theorem 3)

Next, we consider the concentration of observational entropy by approximate designs. Various definitions of approximate unitary designs have been proposed, depending on what measure is used to define ‘‘approximate’’. We adopt the following version proposed in [34]:

Definition 2. (Definition 4 in [34]) Fix $\varepsilon > 0$ and $t \in \mathbb{N}$. A unitary ensemble $\mathcal{E} := \{p_i, U_i\}_{i=1}^N$ is an ε -approximate (unitary) t -design in the diamond distance if

$$\left\| M_{\mathcal{E}}^{(t)} - M_H^{(t)} \right\|_\diamond \leq \frac{t!}{d^{2t}} \varepsilon . \quad (\text{S.36})$$

Here, $M_{\mathcal{E}}^{(t)}(X) := \sum_{i=1}^N p_i U_i^{\otimes t} X (U_i^\dagger)^{\otimes t}$ and $M_H^{(t)}(X) := \mathbb{E}[U^{\otimes t} X (U^\dagger)^{\otimes t}]$.

Lemma 5. Let ρ be a density operator and let P be a positive semidefinite operator such that $P \leq \mathbf{1}$. It holds that

$$\mathbb{P}_{\mathcal{E}} \{ |\text{Tr}[U \rho U^\dagger P] - \text{Tr}[u P]| \geq \xi \} \leq \frac{1}{\xi^t} (1 + \varepsilon) \left(\frac{t^2}{d}\right)^{\frac{1}{2}} . \quad (\text{S.37})$$

Here, U is sampled from an ε -approximate t -design in the diamond distance.

Proof. By Markov’s inequality, we have

$$\mathbb{P}_{\mathcal{E}} \{ |\text{Tr}[U \rho U^\dagger P] - \text{Tr}[u P]| \geq \xi \} = \mathbb{P}_{\mathcal{E}} \left\{ |\text{Tr}[U \rho U^\dagger P] - \text{Tr}[u P]|^t \geq \xi^t \right\} \quad (\text{S.38})$$

$$\leq \frac{1}{\xi^t} \mathbb{E}_{\mathcal{E}} \left[|\text{Tr}[U \rho U^\dagger P] - \text{Tr}[u P]|^t \right] . \quad (\text{S.39})$$

Due to the convexity of $f(z) = |z|^t$, with $\sum_{i=1}^r \lambda_i |i\rangle\langle i|$ be the spectral decomposition of ρ , we have

$$\mathbb{E}_{\mathcal{E}} \left[\left| \text{Tr}[U\rho U^\dagger P] - \text{Tr}[uP] \right|^t \right] = \mathbb{E}_{\mathcal{E}} \left[\left| \sum_{i=1}^r \lambda_i (\text{Tr}[U|i\rangle\langle i|U^\dagger P] - \text{Tr}[uP]) \right|^t \right] \quad (\text{S.40})$$

$$\leq \sum_{i=1}^r \lambda_i \mathbb{E}_{\mathcal{E}} \left[\left| \text{Tr}[U|i\rangle\langle i|U^\dagger P] - \text{Tr}[uP] \right|^t \right]. \quad (\text{S.41})$$

We will invoke Corollary 24 in [34]: Given a pure state $|\phi\rangle$ and a positive semidefinite operator $P \leq \mathbb{1}$, it holds

$$\mathbb{E}_{\mathcal{E}} \left[\left| \text{Tr}[U|\phi\rangle\langle\phi|U^\dagger P] - \text{Tr}[uP] \right|^t \right] \leq (1 + \varepsilon) \left(\frac{t^2}{d} \right)^{\frac{t}{2}}, \quad (\text{S.42})$$

where U is sampled from an ε -approximate (in the diamond measure) t -design \mathcal{E} . Applying this to each term in (S.41), we complete the proof. \square

Proof of Theorem 3. It follows from Lemma 2 and Lemma 5 that

$$\mathbb{P}_{\mathcal{E}} \left\{ S_{\mathbf{P}}(U\rho U^\dagger) \leq (1 - \delta) \log d \right\} \leq \frac{1 + \varepsilon}{\kappa(\mathbf{P})} \left(\frac{t^2}{\kappa(\mathbf{P})^2 \delta d \log d} \right)^{\frac{t}{2}}, \quad (\text{S.43})$$

with U being randomly sampled from an ε -approximate t -design \mathcal{E} in the diamond distance. Substituting $t = 2$ yields Ineq. (9). \square

Remark 4. It was proved in [35] that approximate unitary designs can be implemented on D -dimensional lattices by a local random quantum circuit of depth polynomial in the lattice size. Though the measures adopted in [35] to define “ ε -approximate” are different from Definition 2 above, it affects the circuit depth only polynomially. Hence, we conclude that the concentration of observational entropy occurs even under random unitaries generated by random polynomial-depth quantum circuits, which is often regarded as a physically more realistic model of local quantum chaotic dynamics.