

Von Neumann Entropy from Unitarity

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The von Neumann entropy is a key quantity in quantum information theory and, roughly speaking, quantifies the amount of quantum information contained in a state when many identical and independent (i.i.d.) copies of the state are available, in a regime that is often referred to as being asymptotic. In this Letter, we provide a new operational characterization of the von Neumann entropy which neither requires an i.i.d. limit nor any explicit randomness. We do so by showing that the von Neumann entropy fully characterizes single-shot state transitions in unitary quantum mechanics, as long as one has access to a catalyst—an ancillary system that can be reused after the transition—and an environment which has the effect of dephasing in a preferred basis. Building upon these insights, we formulate and provide evidence for the *catalytic entropy conjecture*, which states that the above result holds true even in the absence of decoherence. If true, this would prove an intimate connection between single-shot state transitions in unitary quantum mechanics and the von Neumann entropy. Our results add significant support to recent insights that, contrary to common wisdom, the standard von Neumann entropy also characterizes single-shot situations and opens up the possibility for operational single-shot interpretations of other standard entropic quantities. We discuss implications of these insights to readings of the third law of quantum thermodynamics and hint at potentially profound implications to holography.

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In quantum information theory, it is common to distinguish tasks as falling in one of two regimes: Either (i) one deals with situations in which many identically and independently distributed (i.i.d.) quantum systems appear. This regime is usually referred to as the *asymptotic regime*. Such tasks include, for example, Schumacher compression [1], entanglement distillation [2], and quantum hypothesis testing [3,4]. Or, in sharp contrast, (ii) one deals with situations that involve only a single quantum system, the so-called *single-shot* regime. Examples of protocols that have been analyzed in the single-shot setting include the decoupling of quantum systems [5], hypothesis testing [6], and state transitions in quantum thermodynamics [7].

Common wisdom has it that different quantities characterize these two regimes. In the first regime, the von Neumann entropy (VNE) or quantities directly related to it prevail, such as the standard quantum relative entropy or mutual information, while in the second regime quantities such as quantum Rényi divergences [8–11] and smoothed versions of the above [12,13] become important. This common wisdom is, however, recently being challenged [14–19], as it has been shown that the VNE determines possible single-shot state transitions in quantum mechanics—under unitary evolutions—provided that three assumptions hold [18]: (i) One can prepare a suitable auxiliary system that does not change its state during the

process but might become correlated with the system on which the transition is performed; (ii) one has access to an environment, or source of randomness, that is modeled as a large system in the maximally mixed state; and (iii) one has full control over the system, auxiliary system, and environment, in the sense that one can implement any unitary on the joint system. Assumption (ii) assigns an undesirably special role to maximally mixed systems, while assumption (iii) is in conflict with the common experience that environments cannot practically be accessed with a full degree of control.

In this work, we provide an operational characterization of the von Neumann entropy in terms of single-shot state transitions that, remarkably, does without assumptions (ii) and (iii). Instead, our characterization builds upon two natural classes of dynamics in quantum mechanics: controlled unitary evolution and uncontrolled decoherence to some given preferred basis. We also apply this characterization to a notion of cooling that is usually considered in the context of quantum readings of the *third law of thermodynamics* and discuss possible implications of our results for recent work on the decoupling of systems and the AdS/CFT correspondence in the context of *holography*. Finally, we formulate, and provide evidence for, a conjecture, which states that not even decoherence is necessary to single out VNE and, if true, would show that the von

Neumann entropy can be derived directly from unitary quantum mechanics alone.

Main result.—We will now present our main result and then discuss its implications. To state the result, let \mathcal{D}_J be the quantum channel that decoheres a system in a given orthonormal basis $J := \{|j\rangle\}$ of its Hilbert space, according to

$$\mathcal{D}_J[\sigma] = \sum_j \langle j|\sigma|j\rangle |j\rangle\langle j|.$$

Density matrices diagonal in $\{|j\rangle\}$ will be called *quasiclassical*. Our main result can be stated as follows.

Theorem 1: Single-shot characterization of the von Neumann entropy.—Let ρ and ρ' be two density matrices of the same finite dimension and with different spectra. Then the following two statements are equivalent: (i) $S(\rho') > S(\rho)$ and $\text{rank}(\rho') \geq \text{rank}(\rho)$. (ii) There exists a finite-dimensional Hilbert space, for any basis J of which there exists a quasiclassical density matrix σ and a unitary U such that

$$\text{Tr}_2[U(\rho \otimes \sigma)U^\dagger] = \rho', \quad (1)$$

$$\mathcal{D}_J[\text{Tr}_1[U(\rho \otimes \sigma)U^\dagger]] = \sigma. \quad (2)$$

The proof is presented in Sec. I in Supplemental Material [20]. Note first that if one has $S(\rho') > S(\rho)$ but $\text{rank}(\rho') < \text{rank}(\rho)$, then by Theorem 1 the transition is not possible exactly. However, it can be done to an arbitrary precision, since any state can be arbitrarily well approximated by a state with full rank. From a physical point of view, the condition on the rank is therefore not important.

To interpret this result, one can imagine a situation in which only a small region of space, say, the laboratory, can be controlled unitarily with a high degree of precision while any system outside this region is decohered very quickly in some given basis. This is a common situation in current experimental devices. Given these constraints, the goal is to transform a quantum system from ρ to ρ' by acting unitarily on this system together with an ancillary system in a quasiclassical state that one can “borrow” from the environment so long as, upon being returned to the environment, it decoheres back to its initial state and can hence be used to aid further transitions. Then, Theorem 1 says that the VNE fully characterizes possible transitions in this natural setup.

In general, the auxiliary system is clearly necessary to implement the transition $\rho \rightarrow \rho'$, since, otherwise, we would act unitarily on ρ and, therefore, could not change its spectrum. The same restriction would arise if we demanded that the auxiliary system is returned *uncorrelated* from the system. Finally, it can be reused to enable further transitions $\rho \rightarrow \rho'$ on independent copies of ρ . This is true even if correlations are established between the

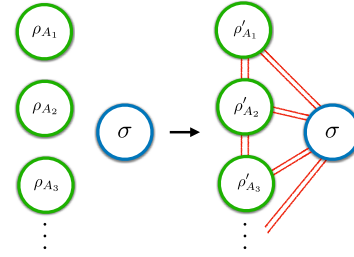


FIG. 1. Reusability of the auxiliary system for further transitions. Consider N subsystems in an uncorrelated state $\rho_{A_1, \dots, A_N} = \rho^{\otimes N}$. Because of Theorem 1, for any transition $\rho_{A_1} \rightarrow \rho'_{A_1}$ respecting the entropy and rank condition, it is possible to find an auxiliary system in state σ that enables this transition. When brought back in contact with the environment, it dephases and returns to its initial state while establishing correlations with A_1 . In spite of these correlations, it is reusable to implement the same transition on A_2 . This is true, since in the second step one applies a local operation on A_2 and the auxiliary system, whose outcome is independent of the correlations with A_1 . Repeating this process on the N subsystems results in having performed locally transitions $\{\rho_{A_i} \rightarrow \rho'_{A_i}\}_{i=1, \dots, N}$ while using a single auxiliary system. At the end of the process, all the subsystems are possibly correlated. However, these correlations do not play any role if one intends to use each subsystem A_i independently for further thermodynamic or information protocols, as is generally the case in a single-shot setting.

auxiliary system and the system of interest in each transition (see Fig. 1).

Thus, the auxiliary system acts like a *catalyst*, in the sense that it enables transitions that would otherwise be impossible without being degraded itself. The notion of catalysis we employ here, however, is different from the one commonly used in resource theories, where the catalyst is usually required to be returned uncorrelated to the system of interest (but may become correlated to other systems, e.g., heat baths in quantum thermodynamics). Finally, we emphasize that, as is usual for catalysts, the auxiliary system and its state σ depend on the transition $\rho \rightarrow \rho'$ and on the dephasing basis, which we think of as being determined by the environment (and, hence, can be expected to coincide with the energy eigenbasis).

Applications to notions of cooling and the third law.—We now discuss an application of Theorem 1 to one of the key problems in quantum thermodynamics. Namely, we analyze how it can be used as a protocol for *cooling to very low temperatures* beyond the i.i.d. setting. This is a situation usually captured in readings of the third law of thermodynamics or *Nernst’s unattainability principle* (UP), bounding achievable rates to cooling. Specifically, in this context, we consider the reading of the problem of preparing systems in a state which is arbitrarily close to being pure. Let us for simplicity take as an initial system two uncorrelated qubits $\rho = \rho \otimes \rho$ with $S(\rho) < 1/2$ (even the generalization to other systems is obvious). Theorem 1 then implies that it is possible to implement a transition

satisfying (1) and (2) so that the final state is $\rho' = \rho' \otimes \mathbf{1}_2$, where $\mathbf{1}_k$ represents a maximally mixed state of dimension k and ρ is any full-rank state with $S(\rho') = \epsilon$ for arbitrarily small $\epsilon > 0$, i.e., arbitrarily close, in trace distance, to a pure state. This is reminiscent of protocols of *algorithmic cooling* [24–27] which take a large number n of “warm” qubits ρ and distill from them $n_c = n[1 - S(\rho)]$ “cold” qubits having each a smallest eigenvalue $\lambda_{\min} = \mathcal{O}(\exp(-n))$ (see, in particular, Ref. [24]). The advantage of our protocol is that we can obtain *arbitrarily cold systems* using a small number of copies, $n = 2$ in this case, in contrast to the asymptotic i.i.d. setting considered in algorithmic cooling. Furthermore, the fact that the auxiliary systems remain invariant allows one to repeat the protocol for $n/2$ copies of ρ using a single auxiliary system. Taking $S(\rho) \approx 1/2$, we obtain $n_c \approx n/2$ qubits which are arbitrarily close to a pure state. This coincides with the bound given by algorithmic cooling, which in this case is $n_c = n[1 - S(\rho)] \approx n/2$ and that is the ultimate bound for any entropy nondecreasing protocol. Hence, our protocol not only distills arbitrarily cold qubits with few copies, but also has an optimal efficiency—in terms of the rate of almost pure qubits—when applied sequentially in the asymptotic limit. At the same time, however, our protocol establishes correlations among the cold qubits produced. Hence, although they can be used individually for further applications, it would be wrong to conclude that using our results one can prepare an arbitrary number $(\rho')^{\otimes n}$ of uncorrelated quasipure states using the same auxiliary system over and over (see Supplemental Material, Sec. III [20]). This again stresses the importance of correlations in the scheme.

The fact that one can produce systems in a state ρ' which is arbitrarily close to a pure state might, moreover, at first glance seem to be in contradiction with the third law of thermodynamics as formulated in the UP. The UP states that an infinite time is required to cool down a system to its ground state (see, e.g., Refs. [28–31] for recent approaches to quantum readings of the UP and their relation with pure state preparation). However, we note that preparing an arbitrarily pure ρ' also requires an arbitrarily large auxiliary system and might require a very large environment to implement the dephasing map \mathcal{D} , which, in turn, ensures that it cannot be prepared in a finite time.

Relation to previous work.—Let us now briefly discuss the relation of our results to previous work (see Fig. 2 for an overview). To begin with, we note that one can use previous results to fully characterize the possible state transitions $\rho \rightarrow \rho'$ for the special case in which the auxiliary system is constrained to be a maximally mixed state. Specifically, one can recast recent results [32,33] as the statement that there exists a d -dimensional Hilbert space such that for any basis J of it there exists a unitary U such that

$$\text{Tr}_2[U(\rho \otimes \mathbf{1}_d)U^\dagger] = \rho', \quad (3)$$

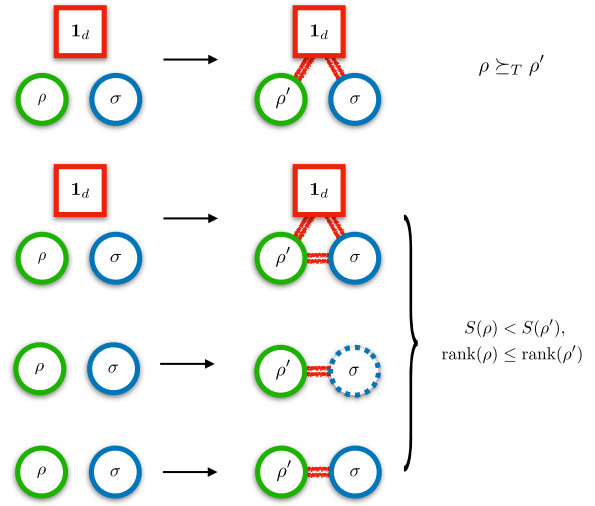


FIG. 2. Comparison of various settings and results. Top: State transitions implementable using a source of randomness and an uncorrelated catalyst σ are characterized by the trumping relations. Middle top: State transitions allowing for a source of randomness and a correlated catalyst, an auxiliary system that locally remains unchanged, are characterized by entropy and rank [18]. Middle bottom: By Theorem 1, state transitions using a correlated catalyst and a dephasing environment that acts on the catalyst (dashed boundary) are also characterized by entropy and rank. Bottom: State transitions using a correlated catalyst alone are characterized by entropy and rank. This is the content of Conjecture 1.

$$\mathcal{D}_J[\text{Tr}_1[U(\rho \otimes \mathbf{1}_d)U^\dagger]] = \mathbf{1}_d, \quad (4)$$

if and only if ρ majorizes ρ' , denoted by $\rho \succeq \rho'$ [32]. Clearly, the above is a special case of Eqs. (1) and (2). Majorization captures the state transitions that are possible under random unitary evolution, and, hence, the above establishes the intuitive result that every random unitary evolution can be implemented with a sufficiently large source of randomness without affecting the latter’s state. To compare this result with Theorem 1, it should be noted that $\rho \succeq \rho'$ is, as a constraint, much stronger than $S(\rho') > S(\rho)$. Indeed, one can see that Rényi entropies S_α , defined as

$$S_\alpha(\rho) = \frac{1}{1-\alpha} \log \text{Tr}(\rho^\alpha), \quad (\alpha \in \mathbb{R} \setminus \{1\}), \quad (5)$$

cannot decrease for transitions $\rho \rightarrow \rho'$ with $\rho \succeq \rho'$, where the VNE is given by the particular case of $S \equiv S_1 := \lim_{\alpha \rightarrow 1} S_\alpha$. The infinite set of conditions given by the Rényi entropies

$$S_\alpha(\rho') \geq S_\alpha(\rho) \quad \forall \alpha \in \mathbb{R} \quad (6)$$

become both necessary and sufficient for the existence of a further auxiliary system σ such that $\rho \otimes \sigma \succeq \rho' \otimes \sigma$ —an important relation known as *trumping* [34,35] in quantum

information theory. The trumping constraints lie, in strength, strictly between those imposed by majorization and the VNE alone. Lastly, in Ref. [18], it is shown that by allowing for correlations between both systems it is possible to collapse the infinite set of conditions for the trumping conditions to essentially the VNE. In particular, it is shown that condition (i) in Theorem 1 is equivalent to the existence of σ and U so that $\rho \otimes \sigma \succeq \rho'\sigma$, where $\rho'\sigma$ denotes a density matrix such that $\text{Tr}_2(\rho'\sigma) = \rho'$ and $\text{Tr}_1(\rho'\sigma) = \sigma$. This statement differs from Theorem 1 in that one needs to make use of a maximally mixed system over which one has full unitary control, while Theorem 1 includes external randomness only in the form of an uncontrolled dephasing map (see Fig. 2 for a comparison).

Catalytic entropy conjecture.—The discussion above raises the natural question whether an external environment, being modeled as a maximally mixed state or a dephasing map as above, is at all necessary to implement all transitions which do not decrease the VNE. This is what we capture in the following conjecture.

Conjecture 1: Catalytic entropy conjecture.—Let ρ and ρ' be two density matrices of the same finite dimension and with different spectra. Then the following two statements are equivalent: (a) $S(\rho') > S(\rho)$ and $\text{rank}(\rho') \geq \text{rank}(\rho)$. (b) There exists a density matrix σ and a unitary U such that

$$\text{Tr}_2[U(\rho \otimes \sigma)U^\dagger] = \rho' \quad \text{and} \quad \text{Tr}_1[U(\rho \otimes \sigma)U^\dagger] = \sigma. \quad (7)$$

The implication (b) \Rightarrow (a) follows directly from the subadditivity of the VNE and S_0 ; hence, the real content of the conjecture is that (a) are the only constraints on transitions of the form (b). If true, this conjecture implies that the von Neumann entropy characterizes correlated catalytic state transitions in unitary quantum mechanics in full generality, without the need to introduce noise or i.i.d. limits (see Fig. 2).

Let us now discuss why we believe this conjecture to be true. To begin with, it is easy to generate counterexamples that rule out the possibility that transitions of the form (b) are constrained by the aforementioned trumping relations. In Supplemental Material [20], we provide such a counterexample together with a method to construct further examples. But, in fact, we can rule out more general constraints than (6) with the help of the following lemma.

Lemma 2: Weak solution to catalytic entropy conjecture.—Let ρ and ρ' be two density matrices of the same, finite dimension and with different spectra. Then the following two statements are equivalent: (I) $S(\rho') > S(\rho)$ and $\text{rank}(\rho') \geq \text{rank}(\rho)$. (II) There exists a density matrix σ , a unitary U , and some finite dimension d such that

$$\text{Tr}_2[U(\rho \otimes \mathbf{1}_d \otimes \sigma)U^\dagger] = \rho' \otimes \mathbf{1}_d, \quad (8)$$

$$\text{Tr}_1[U(\rho \otimes \mathbf{1}_d \otimes \sigma)U^\dagger] = \sigma. \quad (9)$$

This result, which is proven in Supplemental Material [20], supports the conjecture in two ways: First, it shows that the catalytic entropy conjecture is true up to an additional maximally mixed system that remains uncorrelated to the system of interest but not to the auxiliary system. It can also be seen as an instance of the full catalytic entropy conjecture for the specific states $\rho \otimes \mathbf{1}_d$ and $\rho' \otimes \mathbf{1}_d$. Second, and more importantly, it allows us to prove the following corollary.

Corollary 3: Characterization of entropy functions.—Let f be a function from the set of density matrices to the real numbers such that, for every transition of the form (b) between full-rank density matrices, $f(\rho') > f(\rho)$. Then exactly one of the following two statements is true: (1) $S(\rho') > S(\rho) \Leftrightarrow f(\rho') > f(\rho)$, (2) f is nonadditive or discontinuous.

Corollary 3 follows from Lemma 2 by showing that any such function f has to be a linear function of the VNE (see Supplemental Material, Sec. V [20]). Thus, for full-rank density matrices, if Conjecture 1 was false, any additional constraint on transitions of the form (b) would have to be given by exotic entropic functions that are not additive or are discontinuous. For instance, this corollary immediately implies that none of the functions S_α , $\alpha \neq 0, 1$, can be a monotone for transitions of the form (b), since they all satisfy none of the two conditions in the corollary.

Discussion and open questions.—In this Letter, we have provided a new operational characterization of von Neumann entropy which adds significant support to recent proposals that, contrary to common wisdom, the standard von Neumann entropy characterizes not only the i.i.d. limit but also single-shot protocols in quantum information theory. We have done so by showing that the von Neumann entropy fully determines the possibility of single-shot state transitions in unitary quantum mechanics, as long as one has access to a catalyst, which may build up correlations, and environmental dephasing in a preferred basis. Furthermore, we have formulated the catalytic entropy conjecture which essentially states that the above result holds true even in the absence of decoherence. We have also presented evidence for the truth of this conjecture by ruling out alternatives.

Our work suggests that there might be a novel, hitherto unexplored sector of quantum information theory in which operations on *single* copies of a quantum state are characterized directly in terms of standard entropic quantities like VNE. For example, one may ask what happens in Theorem 1 or Conjecture 1 if we introduce another reference system R that is initially correlated or entangled with the system 1 (let us denote system 1 by A for now, and let C be the catalytic auxiliary system 2). Applying a unitary $U_{A,C}$ on A and C , denoting the new states of the systems by R' , A' , and C' , we obtain $R' = R$, by construction $C' = C$, and $S(A') \geq S(A)$, since A becomes correlated with C . Furthermore, the mutual information

$I(R:A)=S(R)+S(A)-S(R,A)$ satisfies $I(R':A')\leq I(R:A)$. Are these necessary conditions also *sufficient* for the existence of a transformation of that form—in particular, can A retain almost all of its correlations with R under correlating-catalytic transformations? A positive answer to this or other similar questions would yield a new single-shot interpretation of the standard mutual information which could potentially be useful in the context of *decoupling* [5,36–38] or merging of quantum states.

The results also hint at the insight that entanglement in single many-body systems can well be captured in terms of the von Neumann entropy. Ideas on *single-copy entanglement* have been considered in situations where each specimen consists of a many-body system, already naturally featuring asymptotically many constituents [39]. Then it can be unreasonable to capture entanglement of subsystems in yet another asymptotic limit of many copies of identical quantum many-body systems. The results laid out here give substance to the intuition that, even in single specimens of quantum many-body systems, entanglement can in this context be quantified in terms of the familiar von Neumann entanglement entropy.

Results of this kind would also have implications in the context of *holographic approaches* to quantum gravity, as in the AdS/CFT correspondence (see, for example, Refs. [40–47]). In these approaches, standard von Neumann (entanglement) entropies of boundary regions turn out to correspond to geometric quantities of a dual gravity theory in the bulk. In fact, it is exactly the mutual information that we have just discussed which is believed to be directly related to geometric quantities like area also in other (non-AdS/CFT) approaches to emergent spacetime [48–50]. To shed some light on this correspondence, it is therefore natural to consider operational interpretations of entropy in the boundary theory and to “dualize” them to obtain corresponding interpretations of geometric quantities in the bulk. A difficulty in doing so, however, is that the protocols on the boundary theory either involve many copies of the state (which seems unphysical given that there is a unique spacetime) or lead to quantification in terms of single-shot entropies (see, e.g., Ref. [44]) which do not always have a direct dual interpretation. The proven and conjectured results of this letter could therefore resolve this difficulty, by supplying a direct single-shot interpretation of standard entropic quantities which might ultimately shed some light on the operational basis of geometric quantities.

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