Entropy and reversible catalysis

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I show that non-decreasing entropy provides a necessary and sufficient condition to convert the state of a physical system into a different state by a reversible transformation that acts on the system of interest and a further "catalyst" whose state has to remain invariant exactly in the transition. This statement is proven both in the case of finite-dimensional quantum mechanics, where von Neumann entropy is the relevant entropy, and in the case of systems whose states are described by probability distributions on finite sample spaces, where Shannon entropy is the relevant entropy. The results give an affirmative resolution to the (approximate) "catalytic entropy conjecture" introduced by Boes et al. [PRL 122, 210402 (2019)]. They provide a complete single-shot characterization without external randomness of von Neumann entropy and Shannon entropy.

A central question in quantum information theory is which quantum states on some physical system may be transformed into which other states on the same (or a different) physical system by a given set of operations. This question underlies quantum resource theories, such as entanglement [1–4], thermodynamics [5–10] or asymmetry [11–13] (see Ref. [14] for a review on quantum resource theories). Common to most resource theories is that they allow for probabilistic mixing of operations, i.e., to use a source of classical randomness (such as a coin toss) to decide on the operation that is implemented. This use of randomness immediately implies that the resource theory is *convex*, which greatly simplifies the mathematical analysis. While often a natural assumption due to the commonplace access to (quasi-)randomness and classical communication, one may ask what happens if either one considers the cost of classical or quantum randomness explicitly or simply disallows the use of classical or quantum randomness. In the most extreme limit one would then end up only allowing the use of unitary operations and the question of which states can be inter-converted becomes trivial: namely all those states which are unitarily invariant, or in other words, all states with the same spectrum (including multiplicities).

In many resource theories the use of a *catalyst* is operationally well motivated and may greatly enrich the set of possible state transitions [9, 15–22]. A catalyst is a system which remains invariant in a given process, but may or may not, depending on the resource theory, build up correlations to other systems. Since its state does not change in a process, no resources are used up and the catalyst may be used again to facilitate further state transitions on other systems – this is conceptually similar to catalysts in chemistry or the ubiquitous "periodically working machines" in thermodynamics. One may therefore wonder what happens if we consider only unitary operations together with the possibility for catalysts. Interestingly, Ref. [22] found that in this setting the von Neumann entropy plays a special role due to its sub-additivity property (see below). It was in fact conjectured that the von Neumann entropy is the *only* constraint for state-transitions once one allows for arbitrary small errors on the system (but not the catalyst). This conjecture was called "catalytic entropy conjecture" and can also be formulated in the classical setting as a conjecture connecting Shannon entropy to catalytic permutations of probability distributions. The ideas behind this conjecture already have found application in the context of thermodynamics and fluctuation theorems [23].

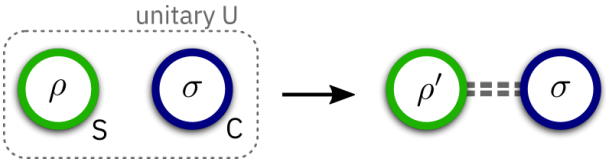

FIG. 1. A catalytic transition: A unitary operation U is applied to systems S and C in the state $\rho \otimes \sigma$. The resulting reduced state on S is (arbitrarily close to) ρ', while the reduced state on C is preserved exactly, but correlated to S (indicated by the dashed lines). The main result of this paper shows that a matching σ and U can be found if and only if $H(\rho') \geq H(\rho)$.

The special role of von Neumann entropy is surprising for several reasons: Typically, the Shannon or von Neumann entropy appears in settings involving many weakly correlated systems due to the phenomenon of *typicality* [24–26]. It was therefore long believed that the von Neumann entropy only plays a special role in asymptotic settings, such as the thermodynamic limit in physics or the limit of many identically and independently distributed signals in information theory. In particular, in resource theories involving free randomness and allowing for catalysts (that however may not become correlated to the system of interest), state transitions are usually characterized by an infinite set of constraints [9, 18–20]. It was only very recently first conjectured and then proven that these conditions may collapse to the von Neumann entropy (or similar quantities, such as relative entropy or free energy) if one allows for catalysts that become correlated to the system [27–33]. However, these settings still made use of external randomness – either by allowing for classical randomness explicitly or allowing free access to systems such as heat baths, which can be seen as sources of randomness. It is thus interesting that the catalytic entropy conjecture posits that von Neumann entropy plays such a special role in situations that neither allow for the use of external randomness, nor require an asymptotic limit. This paper provides an affirmative resolution of the catalytic entropy conjecture.

The catalytic entropy conjecture can also be formulated in full analogy in the classical case by replacing finite dimensional density matrices with probability distributions on finite sample spaces, unitary operations with permutations (reversible transformations on the sample space) and von Neu-

mann entropy with Shannon entropy. In the main text of this paper we will only consider the quantum case and only briefly comment on how to proof the classical version of our main result. A full proof of the classical result is given in the Appendix. While the proof of the classical result also implies the quantum result, it has the drawback of requiring a larger catalyst in general.

Setting and main result. Throughout we consider a system S described by density matrices ρ and ρ' on a Hilbert-space of dimension d. In the following we write $H(\rho)$ for von Neumann entropy, which is defined as

$$H(\rho) = -\mathrm{Tr}[\rho \log(\rho)]. \tag{1}$$

Von Neumann entropy is continuous in ρ and has several useful properties, such as unitary invariance ($H(\rho) = H(U\rho U^\dagger)$ for any unitary U), additivity ($H(\rho \otimes \sigma) = H(\rho) + H(\sigma)$) and sub-additvity: $H(\rho_{12}) \leq H(\rho_1) + H(\rho_2)$, where ρ_{12} is a bipartite quantum state with marginals ρ_1 and ρ_2. Finally, denote by $D(\rho, \rho') := \frac{1}{2}\|\rho - \rho'\|_1$ the trace-distance between two density-matrices. We then define catalytic state transitions formally as follows (see also Fig. 1).

Definition 1 (Approximate catalytic transformation)**.** *Consider two finite-dimensional density matrices ρ and ρ' on the same system S. We write $\rho \to_\epsilon \rho'$ if there exists a finite-dimensional density matrix σ on a system C and a unitary U on SC such that*

$$\mathrm{Tr}_S[U\rho \otimes \sigma U^\dagger] = \sigma \tag{2}$$

and

$$D\big(\mathrm{Tr}_C[U\rho \otimes \sigma U^\dagger], \rho'\big) \leq \epsilon. \tag{3}$$

The following main result of this paper then shows that the set of states that are reachable from a given state ρ is given exactly by the set of states with higher von Neumann entropy:

Theorem 2 (Catalytic transformations characterize von Neumann entropy)**.** *The following are equivalent:*

i) $\rho \to_\epsilon \rho'$ for all $\epsilon > 0$.

ii) $H(\rho') \geq H(\rho)$.

Before coming to the proof, let us briefly discuss the formal similarity between the theorem and the Second Law of Thermodynamics. While an isolated system that undergoes (micro-)reversible dynamics has constant entropy, the result shows that if a system plus its environment undergo reversible dynamics in such a way that the (statistical) state of the environment remains unchanged at the end of the process, then the systems entropy is non-decreasing. Moreover, *any state* with higher entropy may be reached by a suitable environment and reversible dynamics.

Proof of the result. The direction i) $\Rightarrow$ ii) follows directly from sub-additivity, unitary invariance and continuity of von Neumann entropy: For a given ϵ, denote by ρ'_ϵ the final state on S. Then we have

$$H(\rho'_\epsilon) + H(\sigma) \geq H(U(\rho \otimes \sigma)U^\dagger) = H(\rho) + H(\sigma) \tag{4}$$

and hence $H(\rho'_\epsilon) \geq H(\rho)$. By continuity we thus find $H(\rho') \geq H(\rho)$.

The converse direction ii) $\Rightarrow$ i) requires several Lemmas. First, we collect a combination of some standard results on typicality and majorization. We write $\rho \succeq \rho'$ if ρ *majorizes* ρ', meaning that there exists a probability distribution q_i over unitaries V_i such that $\rho' = \sum_i q_i V_i \rho V_i^\dagger$. Similarly, we write $\boldsymbol{a} \succeq \boldsymbol{b}$ for two vectors $\boldsymbol{a}, \boldsymbol{b} \in \mathbb{R}^d$ if there exists a probability distribution q_i over permutation-matrices π_i such that $\boldsymbol{a} = \sum_i q_i \pi_i \boldsymbol{b}$.

Lemma 3 (Typicality and majorization)**.** *Let ρ and ρ' be two finite-dimensional density matrices of dimension d with $H(\rho) < H(\rho')$. Then for any $\epsilon > 0$ and large enough n there exists a state $\rho'_{\epsilon,n}$ such that $\rho^{\otimes n} \succeq \rho'_{\epsilon,n}$ and $D(\rho'_{\epsilon,n}, \rho'^{\otimes n}) \leq \epsilon$. Moreover, the error ϵ can be bounded as*

$$\epsilon \leq O(\exp(-n\Delta H^2/4)) \tag{5}$$

with $\Delta H := H(\rho') - H(\rho)$.

A proof-sketch for Lemma 3 is given in the Appendix. It is clear that the given error bound is not optimal for every choice of ρ and ρ', since, for example, $\epsilon = 0$ is possible if $\rho \succeq \rho'$. However, Ref. [34] shows that the given error bound is essentially optimal up to constants as a bound that does not take into account detailed information about ρ and ρ'. We will later use this to estimate the size of the catalyst.

The next Lemma will be essential to construct a candidate catalyst by making use of Lemma 3. It is based on the *Schur-Horn theorem*, which states that for any $d \times d$ Hermitian matrix its vector of eigenvalues $\boldsymbol{\lambda}$ majorizes the vector of diagonal elements in every orthonormal basis. Conversely, every vector that is majorized by $\boldsymbol{\lambda}$ may be obtained as the diagonal elements in a suitable orthonormal basis. In the following we denote by $\mathcal{D}_{\rho'}$ the *dephasing channel* in the eigenbasis of ρ' that acts as

$$\mathcal{D}_{\rho'}[\rho] = \sum_i |i\rangle\langle i|\rho|i\rangle\langle i|, \tag{6}$$

where the $|i\rangle$ constitute an orthonormal eigenbasis of ρ'.

Lemma 4 (Basic lemma)**.** *Let $H(\rho) < H(\rho')$ and $\mathcal{D}_{\rho'}$ the dephasing channel in the eigenbasis of ρ'. Then for any $\epsilon > 0$ there exists an $n \in \mathbb{N}$ and a unitary U such that for any $1 \leq k \leq n$:*

$$D\big(\rho', \mathcal{D}_{\rho'}[\chi_k]\big) \leq \epsilon, \quad \chi := U\rho^{\otimes n}U^\dagger, \tag{7}$$

where $\chi_k := \mathrm{Tr}_{\{1,\ldots,n\}\setminus\{k\}}[\chi]$. The error ϵ scales as in Lemma 3.

Proof. We make use of the state $\rho'_{\epsilon,n}$ guaranteed by Lemma 3. By the Schur-Horn theorem we now know that there exists a unitary U such that

$$\rho'_{\epsilon,n} = \mathcal{D}_{\rho'}^{\otimes n}[\chi]. \tag{8}$$

However, we have that (writing $\overline{k} := \{1, \ldots, n\} \setminus \{k\}$)

$$\begin{aligned}\mathcal{D}_{\rho'}[\chi_k] &= \mathrm{Tr}_{\overline{k}}[(\mathcal{D}_{\rho'} \otimes \mathbf{1}_{\overline{k}}[\chi]] = \mathrm{Tr}_{\overline{k}}[\mathcal{D}_{\rho'}^{\otimes n}[\chi]] \\ &= \mathrm{Tr}_{\overline{k}}[\rho'_{\epsilon,n}]\end{aligned} \tag{9}$$

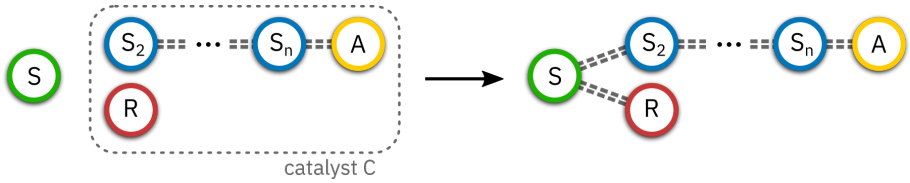

FIG. 2. The structure of the constructed catalyst C: It contains subsystems $S_2, \ldots, S_n$, which are copies of the target system S together with an auxiliary system A of dimension n as well as a catalytic source of randomness R. The dashed lines indicate possible correlations. The source of randomness is utilized to dilate the decoherence-channel $\mathcal{D}_{\rho'}$ on S in such a way that it does not become correlated to the systems $S_2, \ldots, S_n$ and A in the process.

by locality of quantum mechanics. But since the trace-distance non-increasing under partial traces, we then find

$$D\big(\rho', \mathcal{D}_{\rho'}[\chi_k]\big) \leq D\big(\rho'^{\otimes n}, \rho'_{\epsilon,n}\big) \leq \epsilon. \tag{10}$$

□

The final Lemma that we require provides a way to us to get rid of unwanted coherences (arising from Lemma 4) in the final state without correlating the catalyst internally (which would spoil the catalyst).

Lemma 5 (No propagation of correlations for mixed unitary channels)**.** *Consider a mixed unitary quantum channel $\mathcal{C}[\cdot] = \sum_i p_i V_i \cdot V_i^\dagger$ acting on a system S, where the p_i denote probabilities and the V_i are unitary operators. Dilate $\mathcal{C}$ using an auxiliary system C and state $\sigma = \sum_i p_i \, |i\rangle\langle i|$ using the unitary $V := \sum_i V_i \otimes |i\rangle\langle i|$ as*

$$\mathcal{C}[\rho] = \mathrm{Tr}_2\left[V \rho \otimes \sigma V^\dagger\right]. \tag{11}$$

Finally apply the dilation to a state $\rho_{S\overline{S}}$ on S and a further system $\overline{S}$. Then

$$\mathrm{Tr}_S\left[(V \otimes \mathbf{1}_{\overline{S}})\rho_{S\overline{S}} \otimes \sigma (V^\dagger \otimes \mathbf{1}_{\overline{S}})\right] = \rho_{\overline{S}} \otimes \sigma. \tag{12}$$

That is, the dilating system C is catalytic and remains uncorrelated to $\overline{S}$.

Proof. The result immediately from the univary invariance of the (partial) trace:

$$\begin{aligned} &\mathrm{Tr}_S\left[(V \otimes \mathbf{1}_{\overline{S}})\rho_{S\overline{S}} \otimes \sigma (V^\dagger \otimes \mathbf{1}_{\overline{S}})\right] &(13)\\ &= \sum_i p_i \mathrm{Tr}_S\left[(V_i \otimes \mathbf{1}_{\overline{S}})\rho_{S\overline{S}}(V_i^\dagger \otimes \mathbf{1}_{\overline{S}})\right] \otimes |i\rangle\langle i| \\ &= \sum_i p_i \rho_{\overline{S}} \otimes |i\rangle\langle i| = \rho_{\overline{S}} \otimes \sigma. &(14)\end{aligned}$$

□

We are now in position to prove ii) ⇒ i) of Thoerem 2. The proof proceeds in two parts. First we construct a catalyst σ_1 for the exact transition from ρ to the equal mixture

$$\overline{\chi} := \frac{1}{n}\sum_{k=1}^n \chi_k \tag{15}$$

of the states $\chi_k = \mathrm{Tr}_{\overline{k}}[\chi]$, where χ is the state from Lemma 4. Then we use a second catalyst R in state σ_2 to implement the dephasing map and obtain $\mathcal{D}_{\rho'}[\overline{\chi}]$, which is ϵ-close to the target ρ'. The part R of the catalyst thus effectively acts as a source of randomness. By Lemma 5 and the fact that the dephasing map is a mixed unitary channel, this second part can be done in such a way that the two parts of the catalyst remain uncorrelated. From the results of [35] it follows that σ_2 only needs to have a dimension of the order of $\sqrt{d}$. Furthermore, note that by perturbing ρ' arbitrarily slightly, we can always ensure that $H(\rho) < H(\rho')$ since we allow for arbitrarily small errors and von Neumann entropy is continuous. We thus only need to prove that we can do the transition $\rho \to_{\epsilon=0} \overline{\chi}$ in the case $H(\rho') > H(\rho)$. To show this we make use of a trick that was used in recent work by Shiraishi and Sagawa [33]: We denote by $S = S_1$ the system and by $S_2, \ldots, S_n$ and A subsystems of the first part of the catalyst. The S_i all have the same Hilbert-space dimension as S and A has Hilbert-space dimension n (see Fig 2 for an illustration of the structure of the catalyst). Then define

$$\sigma_1 = \frac{1}{n}\sum_{k=1}^n \rho^{\otimes k-1} \otimes \chi_{1,\ldots,n-k} \otimes |k\rangle\langle k|_A, \tag{16}$$

where $\chi_{1,\ldots,i}$ denotes the reduced density matrix of χ consisting of the subsystems 1 to i and we define χ_0 and $\rho^{\otimes 0}$ to be the trivial state 1. We now apply the following sequence of unitaries on $\rho \otimes \sigma_1$ (see Fig. 3):

1. $U \otimes |n\rangle\langle n| + \mathbf{1} \otimes \sum_{k=1}^{n-1} |k\rangle\langle k|$, with U the unitary from Lemma 4.
2. The cyclic shift of sub-systems $S_i \to S_{i+1}$ with $S_n \to S_1$.
3. The cyclic shift on A, acting as $|i\rangle \to |i+1\rangle$ with $|n+1\rangle = |1\rangle$.

After the three steps the catalyst is back to its initial state. The state on the system, on the other hand, is given by $\overline{\chi}$ and, after applying the dephasing map using the system R, we find

$$D\big(\frac{1}{n}\sum_{k=1}^n \mathcal{D}_{\rho'}[\chi_k], \rho'\big) \leq \frac{1}{n}\sum_{k=1}^n D(\mathcal{D}_{\rho'}[\chi_k], \rho') \leq \epsilon$$

by Lemma 4. This finishes the proof.

Size of the catalyst. It is interesting to ask how the construction of the catalyst given above scales in certain limiting

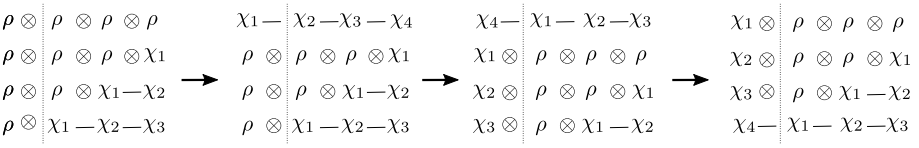

FIG. 3. Illustration of the steps in the first part of the proof for $n = 4$. The different columns denote the systems $S_1 \cdots S_n$ with $S_1 = S$ and the different rows indicate the state $|k\rangle$ of the auxiliary system A. The hyphen indicates that the corresponding subsystems may be correlated. This procedure is essentially identical to the one in Ref. [33]. In the proof of the classical result (see appendix), each of the subsystems with marginals called χ_i here is further correlated to the second part R of the catalyst which is not shown.

cases. The dimension of the catalyst is essentially controlled by the number of copies n required to achieve a certain precision ϵ in the construction of the catalyst, which in turn only depends on the error for majorization from Lemma 3. This error leads to a scaling of the required number of copies n as

$$n = O\left(\frac{\log(1/\epsilon)}{\Delta H^2}\right) \tag{17}$$

and hence the dimension of the catalyst diverges as $d_c = O(\exp(\log(1/\epsilon)/\Delta H^2))$. In particular, the catalyst dimension may in general diverge in a state transfer between two states with almost the same entropy. In Ref. [36] a lower bound for exact catalytic transitions was proven for state-transition with a fixed change of the *variance of surprisal* $V(\rho) = \mathrm{Tr}[\rho(-\log(\rho) - H(\rho))^2]$ but a small change of entropy. It was found that the dimension of the catalyst has to grow at least as as $O(\exp(\Delta H^{-1/8}))$, which is compatible with the above estimate. It is worth emphasizing, however, that these diverging catalysts sizes are only needed when ρ does not majorize ρ' already — if $\rho \succeq \rho'$ the catalyst can be very small, namely of dimension d in the classical case and $\sqrt{d}$ in the quantum case [35].

The classical case. As mentioned above, we can also formulate a the classical version of Theorem 2. To do that, we can define a catalytic transition $\boldsymbol{p} \to_\epsilon \boldsymbol{p}'$ between two probability vectors $\boldsymbol{p}, \boldsymbol{p}' \in \mathbb{R}^d$ as in the quantum case, but with the catalysts' density matrix replaced by a further probability vector $\boldsymbol{q} \in \mathbb{R}^{d_C}$ and the unitary U replaced by a permutation acting on the canonical basis vectors of $\mathbb{R}^d \otimes \mathbb{R}^{d_C}$. The corresponding theorem, which is fully proven in the appendix, can then be stated as follows:

Theorem 6. *Let $\boldsymbol{p}, \boldsymbol{p}' \in \mathbb{R}^d$ be two probability vectors with Shannon entropies $H(\boldsymbol{p})$ and $H(\boldsymbol{p}')$, respectively. The following are equivalent:*

1. *For all $\epsilon > 0$ we have $\boldsymbol{p} \to_\epsilon \boldsymbol{p}'$.*
2. *$H(\boldsymbol{p}) \leq H(\boldsymbol{p}')$.*

Let me briefly comment on the main difference in the proof as compared to the quantum case: The essential construction of the catalyst is quite similar to the quantum case, however clearly we cannot make use of the Schur-Horn theorem, since we do not have access to unitary operations. The proof therefore proceeds by building into the catalyst a source of randomness, which instead of being used to dephase the system, is already correlated with the first part of the catalyst $S_2 \cdots S_n A$ from the beginning and can be used to implement the transition $\boldsymbol{p}^{\otimes n} \to_{\varepsilon=0} \boldsymbol{p}'_{\epsilon,n}$ by a random permutation in the case that the auxiliary system A is in state n (note that the epsilons in $\to_{\varepsilon=0}$ and $\boldsymbol{p}'_{\epsilon,n}$ are different quantities here). This source of randomness in general needs to have a dimension of the order of d^n in the contrast to the source of randomness in the catalyst needed in the quantum case, which only requires a dimension of the order of $\sqrt{d}$.

Conclusion and open problems. We have seen that von Neumann entropy and Shannon uniquely characterize state transitions that allow for the use of a catalyst but are otherwise reversible. There are several natural open problems left for future work: First, in Ref. [22], an exact form of the quantum catalytic entropy conjecture was conjectured, where no error is allowed in the transition from ρ to ρ' at the expense of the additional constraint that the rank of ρ' has to be at least as large as that of ρ. This form of the conjecture seems much more difficult to prove and probably require methods that go beyond standard typicality results (which always yield asymptotic statements with vanishingly small, but finite error).

A second open problem is to investigate whether a similar result also holds for other standard entropic quantities, such as mutual information or relative entropy.

Finally, it will be worthwhile to explore the consequences of the given results for applications. Some immediate applications of an affirmative resolution of the catalytic entropy conjecture in the context of (quantum) thermodynamics have been explored in Refs. [22, 23], but more applications can be expected. In particular, it would be interesting to see whether there are useful applications in the context of (potentially entanglement-assisted) communication scenarios.

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Appendix A: Proof-sketch of Lemma 3

We here provide a sketch of the proof of Lemma 3. For any $\delta > 0$ and state $\rho = \sum_i p_i \, |i\rangle\langle i|$ define the typical subspace $\Pi_\delta^{\rho^{\otimes n}}$ as the subspace spanned by those states $|i_1\rangle \otimes \cdots \otimes |i_n\rangle$ such that

$$\left| \frac{1}{n} \sum_{j=1}^{n} \log(1/p_{i_j}) - H(\rho) \right| < \delta. \tag{A1}$$

We further identify $\Pi_\delta^{\rho^{\otimes n}}$ with the projector onto the subspace. It follows from Hoeffding's inequality that $\rho^{\otimes n}$ is approximated by

$$\hat{\rho}_{\delta,n} := \frac{\Pi_\delta^{\rho^{\otimes n}} \rho^{\otimes n} \Pi_\delta^{\rho^{\otimes n}}}{\mathrm{Tr}[\Pi_\delta^{\rho^{\otimes n}} \rho^{\otimes n}]} \tag{A2}$$

with an error in trace-distance of the order $\exp(-n\delta^2)$ and this error is essentially optimal up to constants for general density matrices [34] (but of course may deviate significantly for particular density matrices). Furthermore, the following properties are well-known [26]: i) For any $\varepsilon > 0$ and sufficiently large n, we have

$$(1-\varepsilon)\mathrm{e}^{n(H(\rho)-\delta)} \leq \mathrm{Tr}[\Pi_\delta^{\rho^{\otimes n}}] \leq \mathrm{e}^{n(H(\rho)+\delta)}. \tag{A3}$$

ii) The approximation $\hat{\rho}_{\delta,n}$ fulfills the operator inequality

$$\mathrm{e}^{-n(H(\rho)+\delta)} \Pi_\delta^{\rho^{\otimes n}} \leq \hat{\rho}_{\delta,n} \leq \mathrm{e}^{-n(H(\rho)-\delta)} \Pi_\delta^{\rho^{\otimes n}}. \tag{A4}$$

These conditions ensure that the approximation $\hat{\rho}_{\delta,n}$ majorizes the approximation $\hat{\rho}'_{\delta,n}$ if

$$\Delta H := H(\rho') - H(\rho) \geq 2\delta. \tag{A5}$$

We therefore now choose $\delta = \Delta H/2$. Since $\hat{\rho}_{\delta,n}$ approximates $\rho^{\otimes n}$ to an error of the order $\exp(-n\delta^2)$ and smilarly for $\hat{\rho}'_{\delta,n}$ and $\rho'^{\otimes n}$, we find that there exists an ϵ-approximation $\rho'_{\epsilon,n}$ of $\rho'^{\otimes n}$ such that $\rho^{\otimes n} \succeq \rho'_{\epsilon,n}$ with $\epsilon = O(\exp(-n\Delta H^2/4))$.

Appendix B: The classical result

In this section we formulate and prove Theorem 6. We continue to speak of systems, and a system S is described by a

probability vector $\boldsymbol{p} \in \mathbb{R}^{|S|}$, where $|S|$ denotes the number of distinct states of S. Joint states of two systems S and S' are described by probability vectors in $\mathbb{R}^{|S_1|} \otimes \mathbb{R}^{|S_2|} \simeq \mathbb{R}^{|S_1||S_2|}$. If $\boldsymbol{p}_{SS'} \in \mathbb{R}^{|S|} \otimes \mathbb{R}^{|S'|}$ is a probability vector describing a bipartite state, we continue to write

$$\boldsymbol{p}_S := \mathrm{Tr}_{S'}[\boldsymbol{p}_{SS'}] \tag{B1}$$

for the marginal on S, whose entries are given by

$$(\boldsymbol{p}_S)_i = \sum_{j=1}^{|S'|} (\boldsymbol{p}_{SS'})_{i,j}. \tag{B2}$$

Instead of unitary matrices acting on $\mathbb{C}^d$, we now continue permutation matrices π acting on $\mathbb{R}^d$ by re-shuffling the basis vectors:

$$(\pi \boldsymbol{p})_i = \sum_{j=1}^{d} \pi_{i,j} p_j, \tag{B3}$$

where π is a permutation matrix and $\boldsymbol{p} = (p_1, \ldots, p_d)^\top$. For two vectors $\boldsymbol{p}, \boldsymbol{p}' \in \mathbb{R}^d$ we have $\boldsymbol{p} \succeq \boldsymbol{p}'$ if and only if there exists a probability distribution q_α of permutations $\pi^{(\alpha)}$ such that

$$\boldsymbol{p}' = \sum_\alpha q_\alpha \pi^{(\alpha)} \boldsymbol{p}. \tag{B4}$$

The Shannon entropy of a probability vector $\boldsymbol{p} = (p_1, \ldots, p_d)^\top$ is defined as

$$H(\boldsymbol{p}) = -\sum_{j=1}^{d} p_j \log(p_j). \tag{B5}$$

Finally, the trace-distance is replaced by the total variation distance given by

$$D(\boldsymbol{p}, \boldsymbol{p}') := \frac{1}{2} \sum_{j=1}^{d} |p_j - p'_j|. \tag{B6}$$

A formal definition of catalytic transitions in the classical case can now be given in full analogy to the quantum case:

Definition 7 (Classical approximate catalytic transitions)**.** *For two probability vectors $\boldsymbol{p}, \boldsymbol{p}' \in \mathbb{R}^{|S|}$ on a system S we write $\boldsymbol{p} \to_\epsilon \boldsymbol{p}'$ if there exists a finite-dimensional probability vector $\boldsymbol{q} \in \mathbb{R}^{|C|}$ on a system C and permutation matrix π on $\mathbb{R}^{|S|} \otimes \mathbb{R}^{|C|}$ such that*

$$\mathrm{Tr}_S[\pi \boldsymbol{p} \otimes \boldsymbol{q}] = \boldsymbol{q} \text{ and } D\big(\mathrm{Tr}_C[\pi \boldsymbol{p} \otimes \boldsymbol{q}], \boldsymbol{p}'\big) \leq \epsilon. \tag{B7}$$

We are now in position to prove Theorem 6. The implication i) $\Rightarrow$ ii) follows as before from additivity, sub-additivity, continuity as well as invariance under permutations of Shannon entropy. We therefore only need to prove the converse direction. As all the results about typicality transfer unchanged (up to notation) we will freely use them in the proof. In particular Lemma 3 implies that for sufficiently large n we have

$$\boldsymbol{p}^{\otimes n} \succeq \boldsymbol{p}'_{\epsilon,n} \tag{B8}$$

with $D\big(\boldsymbol{p}'^{\otimes n}, \boldsymbol{p}'_{\epsilon,n}\big) \leq \epsilon$ and the same error scaling as before. Let $(q_\alpha, \pi^{(\alpha)})$ be the corresponding distribution over permutations required for the majorization in (B8). We again introduce $n-1$ systems $S_2 \cdots S_n$, an auxiliary system A with $|A| = n$ and a source of randomness R whose dimension now coincides with the number of permutations in the collection $(q_\alpha, \pi^{(\alpha)})$ (at most d^n by Caratheodory's theorem). Fig. 4 illustrates the structure of the catalyst. We denote the canonical basis vectors on A by $\boldsymbol{a}_k$ and those on R by $\boldsymbol{r}_\alpha$ for clarity of notation. Finally, define

$$\boldsymbol{x}^{(\alpha)}_{1,\ldots,i} := \mathrm{Tr}_{S_{i+1}\cdots S_n}\left[\pi^{(\alpha)} \boldsymbol{p}^{\otimes n}\right] \tag{B9}$$

with $\boldsymbol{x}^{(\alpha)}_0 = 1$ the trivial state. We then define the catalyst state

$$\boldsymbol{q} := \frac{1}{n} \sum_{k=1}^{n} \sum_\alpha q_\alpha \boldsymbol{p}^{\otimes k-1} \otimes \boldsymbol{x}^{(\alpha)}_{1,\ldots,n-k} \otimes \boldsymbol{a}_k \otimes \boldsymbol{r}_\alpha \tag{B10}$$

and the permutation matrix on $S_1 \cdots S_n A R$ with $S = S_1$ given by

$$\pi := \sum_\alpha \pi^{(\alpha)} \otimes (\boldsymbol{a}_n \boldsymbol{a}_n^\top) \otimes (\boldsymbol{r}_\alpha \boldsymbol{r}_\alpha^\top) + \mathbf{1}_{S_1 S_2 \cdots S_n} \otimes P_A \otimes \mathbf{1}_R, \tag{B11}$$

where P_A denotes the orthonormal projector onto $\mathrm{span}\{\boldsymbol{a}_1, \ldots, \boldsymbol{a}_{n-1}\}$. Note that $\boldsymbol{r}_\alpha \boldsymbol{r}_\alpha^\top$ is simply the orthonormal projector onto the span of $\boldsymbol{r}_\alpha$ and similarly for $\boldsymbol{a}_k \boldsymbol{a}_k^\top$. It is worth to take a pause to understand the structure of the catalyst state $\boldsymbol{q}$: If A is in state $\boldsymbol{a}_k$ it consists of $k-1$ copies of $\boldsymbol{p}$ together with the first $n-k$ marginals of the state $\boldsymbol{p}'_{\epsilon,n}$. However, these latter marginals are correlated with the source of randomness R whose marginal is such that it is in state α with probability q_α. Thus, the source of randomness is correlated with all the other systems, but in a well controlled way. The permutation π has the effect of applying $\pi^{(\alpha)}$ to the systems $S_1 \cdots S_n$ if system A is in state n and system R is in state α. If these conditions are not met, it does nothing.

The final procedure now again consists of three steps (see again Fig. 3 in the main text):

1. Apply π to the initial state $\boldsymbol{p} \otimes \boldsymbol{q}$, obtaining the state

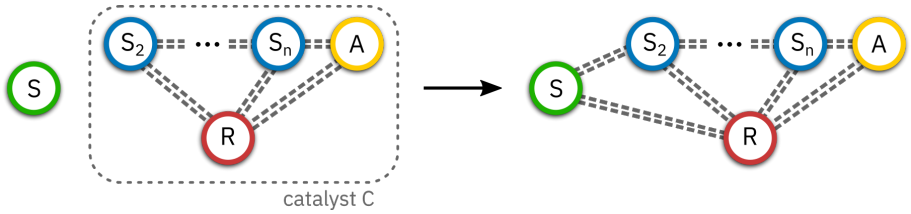

FIG. 4. The structure of the constructed catalyst C in the classical case: It contains subsystems $S_2, \ldots, S_n$, which are copies of the target system S together with an auxiliary system A and a catalytic source of randomness R. The dashed lines indicate possible correlations. The source of randomness is now utilized to fuel a random permutation on $S_1 \cdots S_n$ to make use of majorization. The catalyst and global permutation π are constructed in such a way that the correlations between all sub-systems of the catalyst remain invariant.

$$\pi \boldsymbol{p} \otimes \boldsymbol{q} = \frac{1}{n} \sum_{\alpha} q_\alpha \pi^{(\alpha)} \boldsymbol{p}^{\otimes n} \otimes \boldsymbol{a}_n \otimes \boldsymbol{r}_\alpha + \frac{1}{n} \sum_{k=1}^{n-1} \sum_{\alpha} q_\alpha \boldsymbol{p}^{\otimes k} \otimes \boldsymbol{x}^{(\alpha)}_{1,\ldots,n-k} \otimes \boldsymbol{a}_k \otimes \boldsymbol{r}_\alpha \tag{B12}$$

2. Apply the cyclic shift $\mathbb{S}$ which acts as $S_k \mapsto S_{k+1}$ among the subsystems S_i.

3. Apply the cyclic shift $\boldsymbol{a}_k \mapsto \boldsymbol{a}_{k+1}$ on the system A.

Observe that all steps correspond to permutation matrices, and therefore their composition is also a permutation matrix. Noting that $\mathrm{Tr}_{S_1}[\mathbb{S}\,\cdot\,] = \mathrm{Tr}_{S_n}[\,\cdot\,]$, the final state on the catalyst is then given by

$$\mathrm{Tr}_{S_n}\Big[\frac{1}{n} \sum_{\alpha} q_\alpha \pi^{(\alpha)} \boldsymbol{p}^{\otimes n}\Big] \otimes \boldsymbol{a}_1 \otimes \boldsymbol{r}_\alpha + \frac{1}{n} \sum_{k=1}^{n-1} \sum_{\alpha} q_\alpha \mathrm{Tr}_{S_n}[\boldsymbol{p}^{\otimes k} \otimes \boldsymbol{x}^{(\alpha)}_{1,\ldots,n-k}] \otimes \boldsymbol{a}_{k+1} \otimes \boldsymbol{r}_\alpha \tag{B13}$$

$$= \frac{1}{n} \sum_{\alpha} q_\alpha \boldsymbol{x}^{(\alpha)}_{1,\ldots,n-1} \otimes \boldsymbol{a}_1 \otimes \boldsymbol{r}_\alpha + \frac{1}{n} \sum_{k=2}^{n} \sum_{\alpha} q_\alpha \mathrm{Tr}_{S_n}[\boldsymbol{p}^{\otimes k-1} \otimes \boldsymbol{x}^{(\alpha)}_{1,\ldots,n-k+1}] \otimes \boldsymbol{a}_k \otimes \boldsymbol{r}_\alpha \tag{B14}$$

$$= \frac{1}{n} \sum_{\alpha} q_\alpha \boldsymbol{x}^{(\alpha)}_{1,\ldots,n-1} \otimes \boldsymbol{a}_1 \otimes \boldsymbol{r}_\alpha + \frac{1}{n} \sum_{k=2}^{n} \sum_{\alpha} q_\alpha \boldsymbol{p}^{\otimes k-1} \otimes \boldsymbol{x}^{(\alpha)}_{1,\ldots,n-k} \otimes \boldsymbol{a}_k \otimes \boldsymbol{r}_\alpha \tag{B15}$$

$$= \frac{1}{n} \sum_{k=2}^{n} \sum_{\alpha} q_\alpha \boldsymbol{p}^{\otimes k-1} \otimes \boldsymbol{x}^{(\alpha)}_{1,\ldots,n-k} \otimes \boldsymbol{a}_k \otimes \boldsymbol{r}_\alpha \tag{B16}$$

$$= \boldsymbol{q}. \tag{B17}$$

Similarly, it is easy to check that the final state on the system S is given by

$$\mathrm{Tr}_{S_2 \cdots S_n AR}[\pi \boldsymbol{p} \otimes \boldsymbol{q}] = \frac{1}{n} \sum_{k=1}^{n} \mathrm{Tr}_{\overline{k}}[\boldsymbol{p}'_{\epsilon,n}], \tag{B18}$$

where $\mathrm{Tr}_{\overline{k}}$ again denotes taking the marginal of subsystem S_k. Again we find

$$D\big(\boldsymbol{p}', \frac{1}{n} \sum_{k=1}^{n} \mathrm{Tr}_{\overline{k}}[\boldsymbol{p}'_{\epsilon,n}]\big) \leq \epsilon. \tag{B19}$$

This finishes the proof.