All States are Universal Catalysts in Quantum Thermodynamics

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Quantum catalysis is a fascinating concept that demonstrates how certain transformations can only become possible when given access to a specific resource that has to be returned unaffected. It was first discovered in the context of entanglement theory, and since then, it has been applied in a number of resource-theoretic frameworks, including quantum thermodynamics. Although, in that case, the necessary (and sometimes also sufficient) conditions on the existence of a catalyst are known, almost nothing is known about the precise form of the catalyst state required by the transformation. In particular, it is not clear whether it has to have some special properties or be finely tuned to the desired transformation. In this work, we describe a surprising property of multicopy states: We show that in resource theories governed by majorization, all resourceful states are catalysts for all allowed transformations. In quantum thermodynamics, this means that the so-called "second laws of thermodynamics" do not require a fine-tuned catalyst; rather, any state, given sufficiently many copies, can serve as a useful catalyst. These analytic results are accompanied by several numerical investigations that indicate that neither a multicopy form nor a very-large-dimension catalyst is required to activate most allowed transformations catalytically.

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I. INTRODUCTION

The laws of physics are often expressed as limitations on what physical systems can and cannot do. The second law of thermodynamics is a cardinal example of this approach: It says which thermodynamic transformations can be performed under given conditions. Specifically, at a constant background temperature and volume, the transition between two equilibrium states can occur if and only if the Helmholtz free energy decreases during the process. The second law describes a relationship between average quantities (energy and entropy) and hence specifies the *typical* thermodynamic behavior, i.e., justified in the limit of a large number of identically distributed and weakly interacting systems.

Recent experiments provide evidence that, with our current technology, we can control and manipulate systems at much smaller scales than those governed by the second law [1–6]. Therefore, understanding thermodynamic behavior and, in particular, finding the correct way in which the standard laws of thermodynamics translate into this domain are of crucial practical and theoretical importance. Very recently, this translation into the microscopic

regime was made possible using powerful tools derived within the field of classical and quantum information theory [7–10].

One of the most striking differences between standard thermodynamics and its microscopic counterpart is that transformations between states can become significantly more demanding. More specifically, there are paradigms where they are no longer described by a single second law but by an entire family of conditions, the so-called "second laws of quantum thermodynamics" [11]. In this way, the free energy loses its meaning as the unique indicator of which state transitions are possible—its role is replaced by a family of generalized free energies, a collection of information-theoretic quantities closely related to the Renyi entropies [12]. This captures the idea that for microscopic systems, more structure of the energy distribution must be specified in order to determine their thermodynamic properties. Importantly, by invoking typicality arguments, it can be shown that, in the limit of identically distributed and weakly interacting systems, all members of this family of quantities approach the Helmholtz free energy, thus recovering the standard second law as a special case.

However, these results rely on a specific assumption: that there exists some thermal machine or "catalyst" that is not consumed by the protocol but nonetheless makes the transformation possible. More specifically, if the second laws are satisfied for a pair of states ρ and σ, then there is a quantum state ω that is unchanged by the protocol but still

enables the joint transformation $\rho \otimes \omega \rightarrow \sigma \otimes \omega$. This additional assumption becomes more natural once we realize that standard treatments implicitly adopt an analogous assumption: To perform a thermodynamic transformation, one always needs to supply additional devices that can be cyclically reused (e.g., engines, refrigerators, or heat pumps). In this way, the ancillary state ω models the behavior of a thermal machine or an experimental apparatus, which facilitates or even enables the transformation. This phenomenon of "lifting restrictions without being consumed" is called quantum catalysis.

As may be expected, quantum catalysis is not exclusively related to thermodynamics. The basic idea was introduced for the first time by Jonathan and Plenio in the context of entanglement transformations using local operations and classical communication (LOCC) [13]. However, the ability to borrow an ancillary state (the catalyst) that remains unchanged can allow for otherwise impossible transformations regardless of the specific physical situation. Because of this generality, the scenario of catalysis can be effectively described using the general tools developed within the framework of quantum resource theories (QRTs) [14–32]. More precisely, the problem has a particularly elegant and conceptually simple description for a class of theories referred to as majorization-based quantum resource theories (MB-QRTs). In such theories, quantum states are represented by probability vectors, which encode their affiliation to the specific resource. The problem of conversion can then be formulated purely in terms of these vectors and solved using the concept of majorization [9]. Arguably, the most well-studied examples of such theories are the resource theories of entanglement [16,33,34], coherence [18,35–37], purity [38,39], asymmetry [26,40], and thermodynamics (or athermality) [11,22,41]. To focus our attention, we describe our findings in terms of the resource theory of quantum thermodynamics; however, the results that we present here are general, and they hold for any majorization-based resource theory.

Returning to quantum thermodynamics, the second laws emerge when the catalyst is returned perfectly undisturbed. In reality, however, every thermodynamic protocol will modify the catalyst's state, so a realistic notion of catalysis must be robust against such perturbations. This realization leads to the notion of inexact catalysis, where the catalyst is allowed to be returned up to some small error ϵ_C [21,42,43]. A natural and operationally motivated error quantifier is the trace distance, which also quantifies the best average probability of discriminating quantum states [44]. Surprisingly, states that are close in trace distance may have very different thermodynamic properties, which allows us to "cheat" when using such catalysts, e.g., returning them with a small error as quantified by the trace distance but also much lower work content [43]. Protocols acting in this way extract work from the catalyst in order to lift the limitations imposed by the second laws

and perform the transformation. In this sense, the catalyst is used as a work source (or an entropy sink) rather than a device genuinely catalyzing the transformation, leading to the phenomenon known as (thermal) embezzlement [43].

As a result, the partial order quantified by the second laws vanishes and everything becomes possible—there are no longer any laws. One promising way to amend this situation is to quantify how the error on the catalyst scales with its dimension [45]. This approach naturally leads to two different regimes of catalysis: the embezzlement regime, in which the partial order between states completely vanishes, and the genuine catalysis regime, where the partial order collapses to a certain extent (so that only a subset of the second laws remains) or is even fully retained. The boundary between these two regimes in terms of the trace distance error has been studied in Ref. [43]. There, it was found that for systems with fully degenerate Hamiltonians, all state transformations become possible when the error exceeds a certain threshold that scales linearly with the number of catalyst particles n (or with the logarithm of the dimension). Furthermore, once the error scaling is better than linear in n, some of the generalized free energies are recovered, ultimately leading to a full partial order when no error is allowed.

Arguably, one of the most important problems within this approach to thermodynamics is how to find a catalyst that can be useful for a given transformation. Many of the existing results are based on constructing a very specific catalyst. However, this approach may be obscuring the true physical mechanism behind catalysis. Furthermore, it is still not well understood which properties of quantum states are relevant for catalysis. The second laws only guarantee the existence of the catalyst; even if they are satisfied by a pair of states, it may still be difficult to find which state catalyzes a particular process. This intuition comes from our macroscopic experience: Chemical reactions can be catalyzed only by appropriately chosen chemical compounds; similarly, thermal machines need to be carefully tuned so that the desired transformation may happen. In this way, a natural question arises: How can we find a state that catalyzes a given transformation, and how special are these states?

In this work, we push forward our understanding of catalysis by reporting a surprising property of multicopy catalysts, which we term catalytic universality. We show that any state, as long as enough copies of it are available, can serve as a catalyst for all allowable transformations. For the case of genuine catalysis, this means that if the two states obey the second laws, then a catalyst formed from sufficiently many copies of *any* state ω can catalyze the transformation from ρ to σ approximately, i.e., with a disturbance on the catalyst decreasing almost exponentially with the number of copies. Furthermore, by employing a recent result from quantum information theory called the convex-split lemma, we show that the universality

phenomenon also manifests into the embezzlement regime, i.e., when the partial order between states fully collapses. In this case, sufficiently many copies of any state can catalyze *any* state transformation with a vanishing disturbance, although much more slowly than in the regime of genuine catalysis.

We also emphasize that these results are valid for any QRT whose transitions are governed by majorization. In this way, the phenomenon of catalytic universality appears naturally in the resource theory of entanglement, coherence, or purity. Therefore, our results also lead to new insights into the theory of entanglement by characterizing new and broad families of universal embezzling states.

The paper is structured as follows. In Sec. II, we introduce the relevant framework for thermodynamics and the main mathematical tools used to prove our results. In Sec. III, we describe the general protocol and then specify it to the two catalysis regimes: embezzlement and genuine catalysis. Then, in Sec. IV, we provide numerical evidence that the phenomenon of catalytic universality can be even more general, and we conjecture that it holds for arbitrary states with a sufficiently large dimension. In Sec. V, we provide a brief summary of our main results, and finally, in Sec. VI, we discuss potential implications and describe several open problems that follow naturally from these findings.

II. FRAMEWORK

We begin by describing the resource theory of quantum thermodynamics. As a starting point, we define a restricted set of quantum operations known as thermal operations (TOs), which were introduced in Ref. [22] and subsequently studied in Refs. [11,21,46–58]. This established setting allows us to explore fundamental thermodynamic limitations by assuming perfect control over the environment. Furthermore, recent studies indicate that these operations can be achieved experimentally with a coarse-grained control [49]. A readable introduction to this field of quantum thermodynamics can be found in Refs. [59–61]. One of the main benefits of using this formal framework is that it readily allows us to apply the results of quantum and classical information theory in the thermodynamic context, which can then be adapted to a specific physical scenario by considering a more demanding dynamics.

The setting studied by the TO framework consists of a system S with Hamiltonian $H_S = \sum_{i=1}^{d_S} E_i |i\rangle\langle i|_S$ and a heat bath B at temperature T with Hamiltonian H_B satisfying a few reasonable assumptions about its energy spectrum (see Ref. [22] for details). We always assume that the heat bath starts in a thermal state $\tau_B = e^{-\beta H_B}/Z_B$, where $Z_B = \mathrm{Tr} e^{-\beta H_B}$ is the partition function and $\beta = 1/k_B T$ is the inverse temperature. The interaction of the system with the heat bath is modeled using a unitary U_{SB} that conserves the total energy, i.e., $[U_{SB}, H_S + H_B] = 0$. The map $\mathcal{T}_S$ arising from this unitary after tracing out the ancillary

degrees of freedom is called a thermal operation and can be written as

$$\mathcal{T}_S[\rho_S] = \mathrm{Tr}_{B'}[U_{SB}(\rho_S \otimes \tau_B)U_{SB}^\dagger], \qquad (1)$$

where the trace can be performed over any system B′ inside SB. In general, a complete characterization of the set of operations (1) is not known. However, for states ρ and σ, which are block-diagonal in the energy eigenbasis, there is a simple criterion determining when a TO exists such that $\mathcal{T}[\rho] = \sigma$. To present this criterion, let us first construct a resource representation of the two states, i.e.,

$$\boldsymbol{p} = (p_1, p_2, ..., p_{d_S}), \qquad \boldsymbol{q} = (q_1, q_2, ..., q_{d_S}), \quad (2)$$

where $p_i = \langle E_i|\rho|E_i\rangle$ and $q_i = \langle E_i|\sigma|E_i\rangle$ are the state's occupations in the energy eigenbasis. Similarly, we denote the system's thermal state by $\tau_S = \mathrm{diag}[\boldsymbol{g}] = (g_1, g_2, ..., g_{d_S})$, with $g_i = e^{-\beta E_i}/Z_S$. Let $\pi(i)$ be a permutation of the indices i, such that the vector with elements $p_{\pi(i)}/g_{\pi(i)}$ is sorted in a nonincreasing order (beta-ordered). Following Ref. [22], for such an ordered state, one then constructs a curve (thermo-majorization curve) by drawing points of the form

$$\left\{\left(\sum_{i=1}^k g_{\pi(i)}, \sum_{i=1}^k p_{\pi(i)}\right)\right\}_{k=1}^{d_S}, \qquad (3)$$

together with $\{(0,0)\}$, and connecting them piecewise linearly to form a convex curve. As proven in Ref. [22], transformation between block-diagonal states $\rho \to \sigma$ via thermal operations is possible if and only if the thermo-majorization curve of ρ_S is never below the curve of σ_S. This relation is known as thermo-majorization and will be denoted by "$\succ_T$." Notice that this notion also recovers, as a special case, the standard majorization relation, either by considering the limit of infinite temperature ($\beta \to 0$) or the fully degenerate system's Hamiltonian ($H_S \propto \mathbb{1}_S$).

The framework of thermal operations can naturally accommodate the phenomenon of catalysis. To do so, let us consider an ancillary system C prepared in a state ω_C of dimension d_C and Hamiltonian H_C. It turns out that any transformation between diagonal states which can be performed using a catalyst with a nontrivial energy spectrum can also be accomplished using a catalyst with a fully degenerate spectrum. In this sense, to describe all possible state transformations, without loss of generality, we can always choose a trivial Hamiltonian $H_C \propto \mathbb{1}_C$ [11]. Thus, we consider catalytic thermal operations (CTOs) to be transformations of the following form:

$$\mathcal{T}_{SC}[\rho_S \otimes \omega_C] = \sigma_S \otimes \omega_C, \qquad (4)$$

where now $\mathcal{T}_{SC}$ is a thermal operation (1), with S being replaced by the joint system SC. A fundamental question is when a catalyst ω_C that can facilitate a given transformation

$\rho \rightarrow \sigma$ exists. In this case, the necessary conditions for the existence of a transformation between two states is captured by a set of quantities called generalized or α-free energies F_α. An important result of Ref. [11] states that there exists a catalyst ω_C that enables the transformation $\rho_S \rightarrow \sigma_S$ as in Eq. (4) only if

$$F_\alpha(\rho_S, \tau_S) \geq F_\alpha(\sigma_S, \tau_S) \quad \forall \; \alpha \geq 0. \tag{5}$$

These relations are the second laws of thermodynamics, as stated in the Introduction. In fact, the precise statement of the second laws, which we give here, requires two additional technical assumptions. First, it assumes an arbitrarily small but nonzero error in the transformation. Second, it requires borrowing a qubit in a pure state that is given back with an arbitrarily small but, again, nonzero error [62]. The functions $F_\alpha(\rho_S, \tau_S)$ are defined as

$$F_\alpha(\rho_S, \tau_S) := \frac{1}{\beta}[D_\alpha(\rho_S || \tau_S) - \log Z_S], \tag{6}$$

with $D_\alpha(\rho || \tau)$ being the quantum Renyi divergences defined in Ref. [63]. Importantly, the conditions (5) become sufficient if the states ρ_S and σ_S are block diagonal in the energy basis determined by H_S. Thus, they commute with the operator τ_S, and hence, the quantum Renyi divergence $D_\alpha(\rho_S || \tau_S)$ for $\alpha \geq 0$ simplifies to

$$D_\alpha(\boldsymbol{p} || \boldsymbol{g}) = \frac{1}{\alpha - 1} \log \left[\sum_i p_i^\alpha g_i^{1-\alpha} \right]. \tag{7}$$

This result also allows the second laws to be written in a much simpler form and to see more clearly the connection between F_α and the nonequilibrium Helmholtz free energy, which is given by $F_1 = -k_B T \log Z_S$. It is important to note that the second laws (5) are *strictly* looser than the thermomajorization criteria, which means that there are transformations that cannot be realized via TO, i.e., without a catalyst, but can be performed when given access to a one. This realization is precisely the reason why catalysis is an important and highly nontrivial phenomenon in the resource theory of thermodynamics.

The notion of catalysis can be naturally generalized to more physical scenarios if we allow for small perturbations in the final state of the catalyst. This relaxation leads to inexact catalysis, where the error on the catalyst ϵ_C is defined as

$$\epsilon_C := \|\mathrm{Tr}_S \mathcal{T}_{SC}[\rho_S \otimes \omega_C] - \omega_C\|_1, \tag{8}$$

where $\|M\|_1 := \max \{\mathrm{Tr}[PM] | 0 \leqslant P \leqslant \mathbb{1}\}$ is the trace distance or 1-norm. The case of exact catalysis can be recovered by (i) setting the error on the catalyst to zero, i.e., $\epsilon_C = 0$, and (ii) allowing no correlations between the system and the catalyst, i.e., demanding that the two

subsystems end up in a product form. This regime is also the one in which all of the second laws must be satisfied in order to transform one state into another. The case when $\epsilon_C = 0$ but arbitrary correlations between S and C are allowed to build up has been thoroughly studied in Ref. [56]. There, it was found that using a finely tuned catalyst, one can transform ρ_S into σ_S, as long as the free energy of ρ_S is higher than the free energy of σ_S. This result leads to the conclusion that only one of the families of second laws remains, namely, the nonequilibrium Helmholtz free energy F_1. Moreover, the authors of Ref. [11] showed that when the error on the catalyst scales *linearly* with the number of particles (up to a constant factor) $n = \log d_C$—that is, when $\epsilon_C \sim 1/n$—then the nonequilibrium Helmholtz free energy F_1 again completely describes all possible transformations. Finally, in Ref. [43], it was found that the second laws completely vanish (meaning that all state transitions are possible) when the error on the catalyst surpasses a certain threshold, which is determined by

$$\epsilon_C^{\mathrm{bnd}} = \frac{d_S - 1}{1 + (d_S - 1) \log d_C} \sim \frac{1}{n}. \tag{9}$$

In other words, this is the minimal error that can be achieved under the assumption that all states can be converted between each other. This error sets a boundary between the embezzlement and genuine catalysis regime; whenever the error on the catalyst scales with its dimension better than Eq. (9), then there are state transitions that are not allowed; thus, the partial order induced by the second laws is recovered to a certain degree. Whenever the scaling of ϵ_C is worse than or equal to Eq. (9), we refer to the corresponding regime of catalysis as the embezzlement regime. On the contrary, we use the term genuine catalysis to indicate that transformations are still governed by the second laws (or some nonempty subset of them). In order to simplify notation in what follows, we indicate the type of scaling using the big-$\mathcal{O}$ notation; i.e., $\mathcal{O}(1/n)$ means that the error scales as $1/n$ up the leading order.

Importantly, even if the second laws are satisfied, there is no general method of choosing catalysts for a given transformation. Moreover, not much is known about thermodynamic properties of such catalysts, like their average energy, entropy, or dimension. As such, there is still a lot to be understood about catalysis. In what follows, we show that, in fact, any catalyst composed of sufficiently many copies of an arbitrary state can catalyze any state transformation that is allowed by the transformation laws. We refer to this phenomenon as "catalytic universality" and demonstrate its appearance in the case of genuine catalysis and embezzlement.

III. RESULTS

In this section, we present our main result; i.e., we prove that all multicopy states can act as catalysts for all allowed
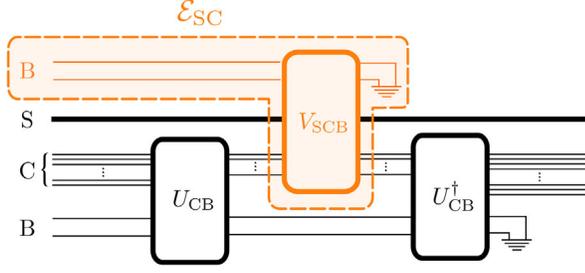
FIG. 1.   Main protocol. The catalyst C is processed using the unitary U_{CB}, and then, along with the system S, it is used as an input for the operation $\mathcal{E}_{SC}(\cdot) := \mathrm{Tr}_B[V_{SCB}((\cdot)_{SC} \otimes \tau_B)V^\dagger_{SCB}]$. The resulting state of the catalyst is then transformed back using the unitary $U^\dagger_{CB}$. As long as the backaction of the map $\mathcal{E}_{SC}$ on the catalyst is small, the protocol as a whole leaves the state of the catalyst approximately undisturbed.

transformations. We prove the result by constructing a general protocol (see Fig. 1), which will then be adapted to a specific regime of catalysis (embezzlement or genuine) by appropriately choosing the corresponding parameters.

A. Intuition

Before we describe our main protocol in full detail, let us first qualitatively argue why multicopy states can be seen as useful for catalysis.

Consider the catalyst to be an n-copy state $\omega_C^{\otimes n}$, where the single-copy state ω_C is an arbitrary state that is diagonal in the energy eigenbasis. Because of the law of large numbers [64,65] in the asymptotic regime ($n \to \infty$), there exists a subset of eigenvalues of $\omega_C^{\otimes n}$, the so-called typical set, which carries almost the whole probability weight and is almost uniformly occupied. Such a state can be approximately, reversibly converted into other states at a rate quantified by the relative entropy. Importantly, this conversion can happen with a negligible error, which vanishes quickly as the number of copies n increases.

In this way, when we have access to a large number n of copies of the state $\omega_C^{\otimes n}$, we can convert it almost reversibly into m copies of another state, which we can then fine-tune to our desired transformation. Once the catalyst is appropriately "preprocessed," we can apply the actual catalytic transformation and map ρ_S into σ_S with the help of the converted catalyst. Using the fact that for large n the error is negligible and the conversion is almost reversible, we can approximately recover the initial state of the catalyst by applying a suitable reverse map, i.e., by "postprocessing" it. Such a combined transformation consisting of these three steps can be equivalently viewed as a valid thermal operation on the system and the catalyst.

The surprising fact is that, for states that satisfy respective transformation laws, it is always possible to find an explicit intermediate state that can be used to catalyze a given state transformation with a sufficiently small or even

no error. This possibility is far from being obvious, and it solves one of the biggest problems of catalysis by explicitly determining the state that can catalyze a given transformation.

We now present the two main theorems of this paper. Their proofs are based on constructing a specific protocol that formalizes the above reasoning and adapting it to the respective regime of catalysis. When the error on the catalyst goes to zero with $n \to \infty$ slower than Eq. (9), the partial order between states vanishes and marks the emergence of the embezzlement regime. In this case, any multicopy state, provided that n is large enough, can act as a catalyst—or, more precisely, an embezzler—for any state transformation. This case is formalized by the following theorem:

Theorem 1. For any two states ρ_S and σ_S and any catalyst state ω_C, there exists a thermal operation $\mathcal{T}_{SC}$ such that

$$\mathcal{T}_{SC}[\rho_S \otimes \omega_C^{\otimes n}] = \sigma'_{SC}, \qquad (10)$$

so that the following equations hold:

$$\epsilon_C := \|\mathrm{Tr}_S[\sigma'_{SC}] - \omega_C^{\otimes n}\|_1 \leq \mathcal{O}\left(\frac{1}{\sqrt{n}}\right), \qquad (11)$$

$$\epsilon_S := \|\mathrm{Tr}_C[\sigma'_{SC}] - \sigma_S\|_1 \leq \mathcal{O}\left(\frac{1}{n}\right). \qquad (12)$$

The constants can be explicitly computed and are provided in Appendix B. The next theorem is more interesting as it relates to the regime when the partial order between states does not fully vanish. In this case, as long as the second laws are satisfied, a sufficient number of copies of any state can catalyze any state transformation, with an error scaling subexponentially with the number of catalyst particles, i.e., genuine catalysis regime:

Theorem 2. Let ρ_S and σ_S be two states with corresponding representations $\boldsymbol{p} = \mathrm{diag}[\rho_S]$ and $\boldsymbol{q} = \mathrm{diag}[\sigma_S]$, which satisfy

$$F_\alpha(\boldsymbol{p}, \boldsymbol{g}) > F_\alpha(\boldsymbol{q}, \boldsymbol{g}) \quad \forall \ \alpha \geq 0, \qquad (13)$$

where $\boldsymbol{g} = \mathrm{diag}[\tau_S]$. Then, for any catalyst state ω_C with $\boldsymbol{c} = \mathrm{diag}[\omega_C]$ and sufficiently large n, there exists a thermal operation $\mathcal{T}_{SC}$ such that

$$\mathcal{T}_{SC}[\rho_S \otimes \omega_C^{\otimes n}] = \sigma'_{SC}, \qquad (14)$$

and the errors on the system and the catalyst satisfy

$$\epsilon_C := \|\mathrm{Tr}_S[\sigma'_{SC}] - \omega_C^{\otimes n}\|_1 \leq \mathcal{O}(e^{-n^\kappa}), \qquad (15)$$

$$\epsilon_S := \|\mathrm{Tr}_C[\sigma'_{SC}] - \sigma_S\|_1 = 0, \qquad (16)$$

where $\kappa \in (0, 1)$ can be chosen arbitrarily. The explicit constants are provided in Appendix.

The complete proofs of Theorems 1 and 2 are provided in the next section, with a few technical steps that we postpone to the Appendix B.

B. Protocol

Preprocessing.—Let ρ_S denote the initial state of the system. Our goal is to transform it into another state σ_S using n copies of a catalyst ω_C via thermal operations. The total state of the system, the catalyst, and the heat bath is given by the product state

$$\rho_{SCB}^{(0)} = \rho_S \otimes \omega_C^{\otimes n} \otimes \tau_B. \qquad (17)$$

In the first step, we transform n copies of the catalyst ω_C into m copies of an arbitrary state η_C. The particular form of this intermediate state will be specified later, as it crucially depends on which regime of catalysis we choose. As we stated in the previous section, this conversion step can be accomplished with a subexponential error on the catalyst. To see this explicitly, let us invoke the following result from Ref. [66]:

Lemma 1. (Multicopy state conversion). There is a thermal operation $\mathcal{T}_C$ that performs the transformation

$$\mathcal{T}_C[\omega^{\otimes n}] = \tilde{\eta}_m, \qquad (18)$$

such that

$$\delta(n) := \|\tilde{\eta}_m - \eta^{\otimes m}\|_1 \le e^{-n^\kappa}, \qquad (19)$$

where $\kappa \in (0, 1)$ can be chosen arbitrarily and $m = n \cdot r_n$, with the conversion rate given by

$$r_n = \frac{D(\omega\|\tau)}{D(\eta\|\tau)} - \mathcal{O}\left(\frac{1}{\sqrt{n^{1-\kappa}}}\right), \qquad (20)$$

and $D(\rho\|\sigma) := \mathrm{Tr}[\rho \log \rho] - \mathrm{Tr}[\rho \log \sigma]$ is the relative entropy.

In what follows, we are not directly interested in the thermal operation $\mathcal{T}_C$ but in the unitary U_{CB} that generates it as in Eq. (1). In particular, we compose this unitary alongside unitaries from the other two steps of the protocol to form a single thermal operation (which is different from just composing the thermal operations of the steps). Moreover, recall that we are working with block-diagonal states; for such states, any thermal operation can be realized using a "gentle" unitary, which (i) permutes energy levels inside the subspaces of equal energy and (ii) leads to the same error on C and the joint system CB (see Appendix C for details). In particular, this second observation will allow us to reverse the action of the unitary in order to recover the original catalyst with a sufficiently small error.

It is important to emphasize that Lemma 1 *does not* require that the number of catalyst particles n goes to infinity. In fact, the lemma is valid in the intermediate regime, i.e., when the number of copies is large but still finite. In that case, the conversion rate r_n will generally be smaller than the asymptotic one (r_∞). However, this discrepancy can be quantified by looking at the second-order corrections (see Appendix B and Ref. [66] for more details). For our purposes, in order to achieve the rate $r_n \approx r_\infty$ and the error scaling of approximately e^{-n^κ}, it is enough to consider large, but not infinitely large, n. What "large" here means depends on the states involved in the transformation and can be found by estimating the second-order corrections in Eq. (20); i.e., we can say that n is large when $\mathcal{O}(1/\sqrt{n^{1-\kappa}}) \ll 1$. Naturally, including more terms in the expansion would allow for a better estimate of the exact rate and even smaller numbers of copies comprising the catalyst.

Let us now consider the unitary U_{CB} that implements the map that performs the transformation (18). There are many unitaries that can implement this map—for our purposes, we use the one that does not propagate the error to the environment, i.e., that satisfies property (ii). This approach, in turn, implies

$$\|\mathrm{Tr}_B \mathcal{U}_{CB}[\omega_C^{\otimes n} \otimes \tau_B] - \eta_C^{\otimes m}\|_1 \le \delta(n), \qquad (21)$$

where $\mathcal{U}_{CB}[\cdot] := U_{CB}(\cdot)U_{CB}^\dagger$. The state of the system, the catalyst, and the environment after the first step of the protocol is given by

$$\rho_{SCB}^{(1)} = (\mathcal{I}_S \otimes \mathcal{U}_{CB})[\rho_{SCB}^{(0)}]. \qquad (22)$$

If we now trace out the bath, the state of the system and the catalyst for large n will be close to $\rho_S \otimes \eta_C^{\otimes m}$, with $m = r_n \cdot n$ being linearly proportional to n. In other words, the conversion rate r_n up to the leading order depends only on the states ω_C, η_C, and their respective thermal states. The precise form of the state η_C will be specified later when we focus on specific regimes of catalysis.

Catalytic transformation.—In the next step, we use the preprocessed catalyst state to facilitate the main thermal operation $\mathcal{E}_{SC}$, which transforms ρ_S into σ_S and (potentially) perturbs the state of the catalyst. Depending on the acceptable size of the backaction on the catalyst, we construct the transformation $\mathcal{E}_{SC}$ differently. With this in mind, the total state of the system SCB after this step reads

$$\rho_{SCB}^{(2)} = (\mathcal{E}_{SC} \otimes \mathcal{I}_B)[\rho_{SCB}^{(1)}]. \qquad (23)$$

As this state can differ from our target state $\sigma_S \otimes \eta_C^{\otimes m}$, we also define the transformation error induced on the catalyst in this step to be

$$\nu(n) := \|\text{Tr}_S \mathcal{E}_{SC}[\rho_S \otimes \eta_C^{\otimes m}] - \eta_C^{\otimes m}\|_1. \qquad (24)$$

Let us note that this is also the only time in the protocol in which we modify the state of the system S. Hence, the transformation error on the system can be entirely associated with the map $\mathcal{E}_{SC}$.

Postprocessing.—In the last step, we apply the inverse of the unitary transformation, which we applied in the preprocessing stage. As a result, the initial state of the catalyst should be approximately recovered, given that it was not perturbed too much during the previous step. To do so, we simply apply the inverse unitary channel $\mathcal{U}_{CB}^\dagger$ to the joint state of the catalyst and the heat bath. Importantly, in order to do so, we use the part of the heat bath that had only interacted with the catalyst in the preprocessing stage (see Fig. 1). This approach allows the catalyst to be transformed back to its initial state again, with a small error. In this way, the final state of the three systems becomes

$$\rho_{SCB}^{(3)} = (\mathcal{I}_S \otimes \mathcal{U}_{CB}^\dagger)[\rho_{SCB}^{(2)}]. \qquad (25)$$

Notice that this reversal is possible only if we keep the state of the bath from the preprocessing step. This implies that the correlations with the heat bath that are created during the preprocessing step play an important role in the whole protocol and allow us to keep the final error on the catalyst acceptably small. Crucially, this three-step protocol is still a valid thermal operation.

Analysis of the protocol.—We now move on to quantifying the total disturbance induced on the subsystems. The final state of the catalyst can be written as

$$\omega_C' = \text{Tr}_{SB}[\rho_{SCB}^{(3)}] \qquad (26)$$

$$= \text{Tr}_B[\mathcal{U}_{CB}^\dagger(\mathcal{E}_C^{(\rho)} \otimes \mathcal{I}_B)\mathcal{U}_{CB}[\omega_C^{\otimes n} \otimes \tau_B]], \qquad (27)$$

where we labeled the effective channel that acts on the catalyst with $\mathcal{E}_C^{(\rho)}[\omega] := \text{Tr}_S \mathcal{E}_{SC}[\rho_S \otimes \omega_C]$. In a similar way, we find the final state of the system S to be

$$\rho_S' = \text{Tr}_{CB}[\rho_{SCB}^{(3)}] = \text{Tr}_C \mathcal{E}_{SC}[\rho_S \otimes \mathcal{T}_C[\omega_C^{\otimes n}]], \qquad (28)$$

where $\mathcal{T}_C$ is the thermal operation that performs the conversion from Lemma 1 and it is related to the unitary U_{CB} via Eq. (1). With this in mind, we can now find the final transformation errors on the system S and the catalyst C. Recall that our main goal is to perform the transformation $\rho_S \to \sigma_S$ while keeping the n-copy catalyst state $\omega_C^{\otimes n}$ approximately undisturbed. Using the triangle inequality (see Appendix C for details) and standard algebraic manipulations, it can be shown that the errors on the system and the catalyst satisfy

$$\epsilon_S := \|\rho_S' - \rho_S\|_1, \qquad (29)$$

$$\epsilon_C := \|\omega_C' - \omega_C^{\otimes n}\|_1 \le 2\delta(n) + \nu(n), \qquad (30)$$

where $\delta(n)$ is related to the unitary U_{SB} used in the preprocessing and postprocessing steps in Eq. (21) and $\nu(n)$ comes from the channel $\mathcal{E}_{SC}$ in Eq. (24). Notice that the two contributions in Eq. (30) account for all possible types of error incurred on the catalyst during the main protocol. In particular, the term $\delta(n)$ quantifies the error due to the failure in preparing the desired intermediate state $\eta_C^{\otimes m}$ using unitary U_{CB} in the preprocessing step, as well as the failure in reversing the action of the unitary U_{CB} in the postprocessing step. This problem occurs, for example, when the action of the channel $\mathcal{E}_{SC}$ in the catalytic step significantly disturbs the catalyst. On the other hand, the term $\nu(n)$ is related solely to the disturbance applied to the catalyst in the catalytic step, and, as we shall see, it changes depending on the specific regime of catalysis one is interested in.

So far, we have treated the intermediate state η_C and the map $\mathcal{E}_{SC}$ as parameters of the main protocol. Depending on the specific choice of these parameters, we can now address different regimes of catalysis. In the remaining part of the paper, we first specialize the above protocol to the embezzlement regime and then to the regime of genuine catalysis.

C. Embezzlement regime

We begin by applying our protocol to the embezzlement regime, i.e., when the partial order between states completely vanishes and all transformations become possible. Even though embezzlement is not a proper form of catalysis, it is still an interesting phenomenon that has found several important applications, mostly in the resource theory of pure-state entanglement. The power of embezzling has been exploited in several areas of quantum information, such as coherent-state exchange protocols [67] or entangled projection games [68]. Moreover, embezzlement can also be viewed as a protocol that hides quantum states from external observers. With this interpretation, it was used to prove the quantum version of the reverse Shannon theorem [69,70].

Today, embezzlement is still a mysterious concept, and its full significance in a thermodynamic context still constitutes an important open problem. Even though its role is not well understood, quantifying which states can be used as embezzlers is a very relevant problem. Recent studies revealed a few families of universal embezzling states, both in the context of the resource theory of entanglement [67] and thermodynamics [43]. Such universal embezzlers have the power to "catalyze" any state transformation. In the case of the resource theory of entanglement, a further study exposed another family of universal embezzling states, and some of their properties were examined in Ref. [71]. In general, however, very few

such families of universal embezzlers are known, and the effects related to the dimension, entropy, or energy of the embezzler have hardly been studied.

The main technical tool we use in this section is the convex-split lemma, a recently discovered result from quantum communication theory. This important tool allows us to prove that n copies of *any* state can serve as a universal embezzler, i.e., can help in facilitating any state transformation. As we will see, in this case, the error on the catalyst, up to the leading order, is proportional to $1/\sqrt{n}$ and thus approaches zero as $n \to \infty$. Since this rate is slower than the boundary specified by Eq. (9), the transformation should be associated with the embezzlement regime.

We begin by specifying the preprocessed catalyst state η_C. We choose it to be precisely equal to the target state of the system σ_S, that is,

$$\eta_C^{\otimes m} = \sigma_C^{\otimes m}. \tag{31}$$

In order to specify the channel for the catalytic step, $\mathcal{E}_{SC}$, let us consider the following mixing process acting on an $(m+1)$-partite system:

$$\mathcal{T}^{(\mathrm{mix})}[\cdot] = \frac{1}{m+1}\sum_{i=0}^{m} S_{(0,i)}(\cdot)S_{(0,i)}^{\dagger}, \tag{32}$$

where $S_{(i,j)}$ is a unitary that swaps subsystems i and j, leaving all the remaining subsystems untouched, i.e.,

$$S_{(i,j)}|\ldots a_i, \ldots a_j, \ldots\rangle = |\ldots a_j, \ldots a_i, \ldots\rangle. \tag{33}$$

This type of operation naturally preserves the thermal state (or any other state that is a combination of identically distributed and independent copies); hence, it is also a valid thermal operation. We apply this map to the state of the system ρ_S (treated as the zeroth subsystem) and m copies of the preprocessed catalyst state $\eta_C = \sigma_C$ (treated as the remaining m subsystems). The resulting state is

$$\mathcal{T}_{SC}^{(\mathrm{mix})}[\rho_S \otimes \sigma_C^{\otimes m}] = \frac{1}{m+1}(\rho_S \otimes \sigma_{C_1} \otimes \ldots \otimes \sigma_{C_m} \\ + \cdots + \sigma_S \otimes \sigma_{C_1} \otimes \ldots \otimes \rho_{C_m}), \tag{34}$$

where now $C = C_1 C_2 \ldots C_m$. It can be easily verified (see Appendix C) that choosing this particular transformation in the main protocol, i.e., $\mathcal{E}_{SC} = \mathcal{T}_{SC}^{(\mathrm{mix})}$, allows us to bound the error term $\nu(n)$ as

$$\nu(n) \le \|\mathcal{T}_{SC}^{(\mathrm{mix})}[\rho_S \otimes \sigma_C^{\otimes m}] - \sigma_S \otimes \sigma_C^{\otimes m}\|_1. \tag{35}$$

Let us now present the main technical tool of this section, that is, the convex-split lemma adapted from Ref. [72]:

Lemma 2. (Convex split). Let ρ and σ be two quantum states satisfying $\mathrm{supp}(\rho) \subseteq \mathrm{supp}(\sigma)$. Then, for any $m \ge 1$, it holds that

$$\|\mathcal{T}_{SC}^{(\mathrm{mix})}[\rho_S \otimes \sigma_C^{\otimes m}] - \sigma_S \otimes \sigma_C^{\otimes m}\|_1^2 \le \frac{2^{D_\infty(\rho\|\sigma)}}{m}, \tag{36}$$

where $D_\infty(\rho\|\sigma)$ is the max-relative entropy corresponding to $\alpha \to \infty$ in the definition (7).

Using the lemma from above, we can bound the error term from Eq. (35) as

$$\nu(n) \le \sqrt{\frac{2^{D_\infty(\rho\|\sigma)}}{r_n}} \frac{1}{\sqrt{n}} \tag{37}$$

$$= c_n \frac{1}{\sqrt{n}}, \tag{38}$$

where c_n for fixed input and output states ρ and σ is effectively constant for large n. Consequently, the error term $\nu(n)$ scales with n as $\nu(n) \sim n^{-1/2}$, and using Eq. (30), we find that

$$\epsilon_C \le \mathcal{O}\left(\frac{1}{\sqrt{n}}\right). \tag{39}$$

Note that this procedure does not assume anything particular about the states ρ, σ, and ω. The only technical assumption is that $\mathrm{supp}(\rho) \subseteq \mathrm{supp}(\sigma)$, which can be achieved for any states ρ and σ by an arbitrarily small perturbation. Thus, by choosing sufficiently large n, we can carry out *any* state transformation on the system, at the same time keeping an arbitrarily small error on the catalyst. In this way, we have proven Theorem 1 from the beginning of this section.

D. Genuine catalysis regime

Let us now consider the other regime of inexact catalysis, that is, when the error scales with the catalyst dimension slowly enough to maintain the partial order between states. We again apply our main protocol, with a specific choice of the intermediate state η_C and transformation $\mathcal{E}_{SC}$.

Recall that we can represent the states ρ_S and σ_S with probability vectors $\boldsymbol{p}$ and $\boldsymbol{q}$ as described in Eq. (2). We assume that these two states satisfy the second laws of thermodynamics, Eq. (5), which means that there exists a catalyst that can be used to transform $\boldsymbol{p}$ into $\boldsymbol{q}$ without any disturbance on the catalyst. Interestingly, this implication is not the only one guaranteed by the second laws. It turns out that these families of conditions also provide a sufficient condition for a multicopy state transformation between ρ_S and σ_S, which was captured by a recent result from majorization theory [73] (Proposition 3.2.7). For our purposes, this result can be adapted to the thermodynamic

case by using the so-called embedding map introduced in Ref. [11]. Intuitively, the embedding map is an operation which facilitates the translation between the microcanonical and macrocanonical descriptions of a thermodynamic system. Leaving the technical details of the proof to Appendix C, here we just present the lemma, which we adapted from Ref. [73]:

Lemma 3. Let $\rho_S = \mathrm{diag}[\boldsymbol{p}]$ and $\sigma_S = \mathrm{diag}[\boldsymbol{q}]$ be two quantum states with dimension d_S, Hamiltonian H_S, and a corresponding thermal state $\tau_S = \mathrm{diag}[\boldsymbol{g}]$ such that

$$F_\alpha(\boldsymbol{p}, \boldsymbol{g}) \geq F_\alpha(\boldsymbol{q}, \boldsymbol{g}) \quad \forall\, \alpha \geq 0. \tag{40}$$

Then, for sufficiently large k, the following holds:

$$\boldsymbol{p}^{\otimes k} \succ_{\mathrm{T}} \boldsymbol{q}^{\otimes k}. \tag{41}$$

The Lemma ensures that a k-copy transformation between ρ_S and σ_S is possible for a finite k if the second laws are satisfied for all $\alpha \geq 0$. The second ingredient that we use is a special catalyst state that can "simulate" any k-copy state transformation. It turns out that if k copies of the state ρ_S can be transformed into k copies of another state σ_S, then there exists a special state that can be used as a catalyst when transforming only a single copy of ρ_S into a single copy of σ_S. With this in mind, let us introduce the Duan state $\omega_k^{\mathrm{D}}(\rho, \sigma)$ [74,75], which is of the form

$$\omega_k^{\mathrm{D}}(\rho, \sigma) := \frac{1}{k} \sum_{i=1}^{k} \sigma^{\otimes k-i} \otimes \rho^{\otimes i-1} \otimes |i\rangle\langle i|. \tag{42}$$

Then, as shown in Ref. [74], the Duan state $\omega_k^{\mathrm{D}}(\rho, \sigma)$ can be used as a catalyst that "simulates" the k-copy transformation between ρ_S and σ_S. This transformation is exact, in the sense that if $\rho_S^{\otimes k} \to \sigma_S^{\otimes k}$, then

$$\rho_S \otimes \omega_k^{\mathrm{D}}(\rho, \sigma) \to \sigma_S \otimes \omega_k^{\mathrm{D}}(\rho, \sigma). \tag{43}$$

The above can be easily verified (see Appendix C for details). The dimension of the Duan state is a function of both k and d_S, that is, $\dim[\omega_k^{\mathrm{D}}(\rho, \sigma)] = k d_S^{k-1}$; hence, for a given ρ_S and σ_S, it is constant and does not scale with n.

In this way, once the second laws are satisfied, there is always a large enough (and finite) integer k such that k copies of ρ_S can be converted into k copies of σ_S. On the other hand, this means that there is always a special catalyst (the Duan state) that can catalyze the transformation from ρ_S to σ_S *without* any disturbance on the catalyst. We formalize this case in the following theorem:

Theorem 3. Let $\rho_S = \mathrm{diag}[\boldsymbol{p}]$ and $\sigma_S = \mathrm{diag}[\boldsymbol{q}]$ be two quantum states with dimension d_S, Hamiltonian H_S, and a corresponding thermal state $\tau_S = \mathrm{diag}[\boldsymbol{g}]$ such that

$$\forall\, \alpha \geq 0 \quad F_\alpha(\boldsymbol{p}, \boldsymbol{g}) \geq F_\alpha(\boldsymbol{q}, \boldsymbol{g}). \tag{44}$$

Then, for sufficiently large k, the following holds:

$$\rho_S \otimes \omega_k^{\mathrm{D}}(\rho, \sigma) \xrightarrow{\mathrm{TO}} \sigma_S \otimes \omega_k^{\mathrm{D}}(\rho, \sigma), \tag{45}$$

where $\omega_k^{\mathrm{D}}(\rho, \sigma)$ is the Duan state defined in Eq. (42).

Notice that the above theorem tells us explicitly how to find a good catalyst when the second laws hold. Indeed, once the conditions in Eq. (44) are satisfied, we have a method for choosing the catalyst state that can facilitate a given transformation.

Let us now return to our main protocol and choose the intermediate state η_C to be precisely the Duan state corresponding to ρ_S and σ_S, that is,

$$\eta_C = \omega_k^{\mathrm{D}}(\rho, \sigma). \tag{46}$$

In fact, we only need one copy of the state η_C to transform ρ_S into σ_S on the system S, so any $m \geq 1$ will lead to a valid transformation. However, now we have to ensure that our preprocessing step applied to the initial catalyst state produces at least one copy of the respective Duan state. If we recall that $m = n \cdot r_n$, then $m \geq 1$ can be guaranteed if

$$n \geq r_n^{-1} \approx \frac{\log D - H(\omega_k^{\mathrm{D}}(\rho, \sigma))}{\log d_C - H(\omega_C)}, \tag{47}$$

where $H(\rho) := -\mathrm{Tr}[\rho \log \rho]$ is the von Neuman entropy and $D = k \cdot d_S^{k-1}$ is the dimension of the corresponding Duan state.

Now, from Theorem 3, we know that there exists a TO that transforms ρ_S into σ_S using the Duan state as in Eq. (45). This transformation is exact, so it does not introduce any additional error in the main protocol. In this way, the only disturbance of the catalyst is applied by the preprocessing and postprocessing steps. In this way, any n-copy catalyst state ω can be used to catalyze any allowed state transformation, i.e., any transformation that obeys the family of the second laws, Eq. (13). This concludes the proof of Theorem 2.

From a practical point of view, it is interesting to see what the typical value of k is such that catalytic universality holds. Indeed, by Lemma 3, we know that the second laws imply the existence of a finite k and a thermal operation such that $\rho_S^{\otimes k} \to \sigma_S^{\otimes k}$. It turns out that for many pairs of states, a multicopy transformation exists even for small values of k, which implies that the dimension of the associated Duan state $\omega_k^{\mathrm{D}}(\rho, \sigma)$ is often not too large. In such situations, the main protocol does not require one to have control over an asymptotically large Hilbert space, as might be expected *a priori*. This claim can be seen by looking at Fig. 2, which estimates the fraction of all transitions that can be realized by having only a small number of copies k. We will return to the discussion of the problem of the amount of control required by the main protocol in Sec. III E.
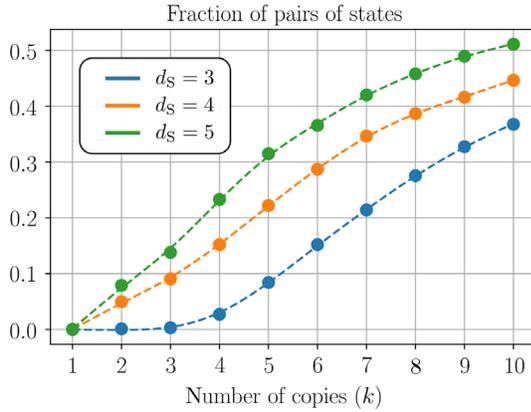
FIG. 2. An estimate of the volume of all block-diagonal pairs of states (ρ_S, σ_S) with $H_S \propto \mathbb{1}_S$ for which there is a transformation taking $\rho_S^{\otimes i}$ into $\sigma_S^{\otimes i}$ for some $i \leq k$, divided by the volume of all block-diagonal pairs that can be catalytically activated. Catalytically activated pairs are such that (i) they satisfy the respective second laws and (ii) ρ_S cannot be directly converted into σ_S.

E. Practical aspects of the main protocol

We have described a general protocol that allows for the use of multiple copies of any nonequilibrium state to catalyze any state transformation that is allowed by the second laws, Eq. (5). Still, in order to show that catalytic universality is a relevant feature of single-shot quantum thermodynamics, a similar behavior must also appear outside of the idealized assumptions of our framework. In other words, the catalytic universality should not be merely an artifact of the idealized model, but it should be robust to its reasonable relaxations.

One might raise two natural and fair objections about the methods we use to demonstrate catalytic universality. First, one might be worried that the set of transformations that we consider here (thermal operations) is too large because, at least in principle, it contains all possible energy-preserving unitaries—among them, also those that might be impossible to implement in practice. Such unitaries might require the experimenter to accurately manipulate all of the particles contained in a typical heat bath, which is clearly beyond the scope of even the most passionate experimenter. Second, our protocol essentially requires that the number of catalyst particles n is large enough so that the preprocessing step can prepare a sufficiently large Duan state. Again, one might be worried that for practically relevant situations, this number will be unrealistically large, making any reasonable implementation of the protocol infeasible. These two problems must be resolved before catalytic universality can be seen as a practical and relevant feature of single-shot quantum thermodynamics. In the remaining part of this section, we address these two important issues separately.

1. How much control is needed by thermal operations?

The framework of thermal operations proved to be a useful approach in deriving fundamental limitations for general thermodynamic processes. In parallel, the practical applicability of the framework was criticized for its requirement of accessing a huge number of degrees of freedom involved in the dynamics, even for small quantum systems (see, e.g., Ref. [76] for a discussion). Indeed, the unitaries from Eq. (1) are required to be energy conserving but are otherwise arbitrary. Such unitaries may, in principle, act on a large number of energy levels of the heat bath at once, which is beyond the scope of any realistic scenario since realizing such unitaries might require the experimenter to access and manipulate an overwhelming number of different parameters.

Since thermal operations allow for such unitaries, we cannot ensure *a priori* that the results derived within this formalism are also relevant beyond the paradigm of infinite control. Thankfully, this important problem was recently mitigated in Ref. [49], where it was shown that any transformation of the form (1) can be realized using a much simpler class of operations called crude thermal operations. These thermodynamic transformations require much less control and consist of three types of operations:

(1) Partial-level thermalizations, which selectively thermalize any two energy levels of the system. This type of operation can be implemented either by performing a partial SWAP between the system and the bath or by selectively putting the system's energy levels in contact with the bath, preceded by filtering out irrelevant frequencies.

(2) Level transformations, which either raise or lower any two energy levels of the system's Hamiltonian. This is a standard type of transformation considered within thermodynamics, whose implementation generally requires performing work. Interestingly, it is enough to consider only those level transformations that do not require work.

(3) Subspace rotations, which involve energy-conserving unitaries acting upon the system only. For example, when the system has degenerate energy levels, one may apply such unitaries within the degenerate subspace to rotate the state into a state diagonal in a specific basis.

The main result of Ref. [49] states that, for block-diagonal states in the energy eigenbasis, any transformation of the form (1) can be implemented using the above three types of operations applied to the system and a single thermal qubit. In other words, even though the framework of thermal operations allows for unitaries with arbitrary complexity and level of control, such unitaries cannot provide any thermodynamic advantage over their much simpler counterparts. However, let us also remember that although Ref. [49] shows that thermal operations can be decomposed into a sequence of simpler unitaries, even this might not be easy to implement in practice. First, the actual sequence of crude thermal operations may be very long and thus experimentally infeasible; second, the three basic types

of crude operations (1)–(3) might still be difficult to realize in a practical scenario. This difficulty is mainly because realizing partial-level thermalizations (1) and level transformations (2) requires, in general, a considerable amount of effort. Finally, the approach presented in Ref. [49] does not seem to be easily scalable, and therefore, it might still be necessary to search for alternative solutions that could bring thermal operations closer to their experimental implementations.

Let us now return to our main problem. Translating the result of Ref. [49], for our purposes, means that the unitaries U_{CB} and V_{SCB}, which we apply in the main protocol (see Fig. 1), require only a coarse-grained control over the joint state of the system and the catalyst (SC) and the heat bath (B).

2. How large must the catalyst be?

Unfortunately, the argument from the previous section only partially solves the problem of control in the main protocol. Although the transformation can be realized using simple interactions with a small region of the heat bath, it may still be necessary to manipulate a large number of particles composing the multicopy catalyst.

Let us study this problem in more detail. Notice that before the unitary V_{SCB} from the main protocol can be applied, the associated Duan state $\omega_k^D(\rho, \sigma)$ must be determined, which requires finding a number k such that k copies of ρ_S can be converted into k copies of σ_S [see Eq. (41)]. Because of Lemma 2, we know that, for states satisfying respective second laws, such a k (however large) always exists, which ensures that the unitary V_{SCB} can realize the catalytic transformation. However, it might still be difficult to apply this unitary since the required number of copies k can be large, and hence also the dimension of the associated Duan state. Consequently, both unitaries U_{CB} and V_{SCB} might need to act on a large number of energy levels of the joint state of the system and the catalyst.

Let us explain the origin of this problem. The second laws of thermodynamics provide a mathematically clean and succinct characterization of allowed transformations in the resource theory of quantum thermodynamics. However, the generality of this characterization also leads to certain drawbacks. In particular, there are transformations that are allowed by the second laws, but at the same time, the catalyst they require has to be infinitely large (see Proposition 2 from Ref. [77]). This situation is far from being physical, and it demonstrates that certain transformations, although technically allowed by the second laws, can never be realized using practical catalysts. Thus, in such instances, our main protocol may also require asymptotically large catalysts.

This problem can be circumvented if we sacrifice the elegant mathematical description in terms of the second laws for a more operational characterization. In particular,

instead of using α-generalized free energies, we can describe the partial order of states using the concept of k-copy transformations. This approach amounts to considering only those pairs of states (ρ_S, σ_S) for which there is a transformation that takes $\rho_S^{\otimes i}$ into $\sigma_S^{\otimes i}$ for some $i \leq k$. Interestingly, the partial orders described by the second laws and k-copy transformations (for all k) are exactly the same, which can be seen as a direct consequence of Theorem 1 from Ref. [74] and our Lemma 3. For a fixed k, this characterization involves checking at most $d_S^2(d_S^{k-1} - 1)/(d_S - 1)$ conditions, which can be done, e.g., by looking at the elbows of the thermo-majorization curves. We emphasize that the price to pay for considering a *fixed k* is that we limit the set of all possible transformations, as compared to those allowed by the second laws. At the same time, a large fraction of all transformations allowed by the second laws can be k-copy transformed for a relatively small k (see Fig. 2). Using the concept of k-copy transformations gives rise to the following alternative version of Theorem 2:

Theorem 2 (alternative). Let ρ_S and σ_S be two states for which there exists a k-copy transformation such that

$$\rho_S^{\otimes k} \rightarrow \sigma_S^{\otimes k}. \tag{48}$$

Then, for any catalyst state ω_C and for a sufficiently large n satisfying,

$$n \geq \frac{\log D - H(\omega_k^D(\rho, \sigma))}{\log d_C - H(\omega_C)}, \tag{49}$$

there is a thermal operation $\mathcal{T}_{SC}$ such that

$$\mathcal{T}_{SC}[\rho_S \otimes \omega_C^{\otimes n}] = \sigma'_{SC}, \tag{50}$$

and $\mathrm{Tr}_C[\sigma'_{SC}] = \sigma_S$ with the following disturbance of the catalyst:

$$\epsilon_C := \|\mathrm{Tr}_S[\sigma'_{SC}] - \omega_C^{\otimes n}\|_1 \leq \mathcal{O}(e^{-n^\kappa}), \tag{51}$$

where $\kappa \in (0, 1)$ can be chosen arbitrarily. The explicit constants are provided in Appendix B.

Let us summarize the reasoning presented in this section. First, by replacing the partial order of second laws with a mathematically equivalent partial order characterized by k-copy transformations, one can formulate an alternative version of Theorem 2. This version allows the phenomenon of catalytic universality to be demonstrated using multicopy catalysts composed of a moderate number of particles. Although, in that case, the multicopy catalyst will no longer be useful for all transformations (unless more copies are supplied), it will be useful for all of the transformations in which the participating states are k-copy convertible.

F. Extension to general majorization-based resource theories

As a final note, we emphasize that although we have focused our presentation on quantum thermodynamics, catalysis can be easily introduced into any QRT. Arguably, the most well-studied class of resource theories are those that are governed by majorization. In such theories, transitions between states are governed by pure majorization or its generalized version, **_d_**-majorization [8]. In this work, we focus mainly on quantum thermodynamics, which can be thought of as a particular resource theory whose transitions are governed by a variant of majorization called thermo-majorization. In fact, each theory that can be described using majorization has its own collection of "second laws" that can be expressed using α-Renyi entropies. Although the physical settings and interpretation of such laws differ among resource theories, the mathematical framework governing state transitions in such theories remains the same. Thanks to this wide applicability of majorization, the results presented in this work can be interpreted as well in the context of other majorization-based QRTs, like the theory of pure-state entanglement or pure-state coherence. In this way, the phenomenon of catalytic universality naturally transcends into other physical settings and can be viewed as a general feature of all majorization-based QRTs.

IV. GENERIC CATALYSTS

We have shown that multicopy states are universal catalysts. It is interesting to ask if, and to what extent, these results may be generalized even further. As a first step, one might ask whether any high-dimension state is a catalyst, i.e., whether the crucial property is just high dimensionality or whether the multicopy form is essential since, in that case, we have much stronger typicality properties emerging. This extension is relevant from an experimental point of view, where experimenters' ability to manipulate the system is often limited by the number of degrees of freedom that can be effectively controlled. In this section, we present numerical evidence that indicates that the catalytic universality phenomenon is more general and, in fact, concerns almost all large-dimensional catalysts. We leave the proof of this conjecture for future research. The code used to run the numerics presented in this section was developed using MATLAB and is freely available in Ref. [78].

Throughout this section, the Hamiltonians of the system S and the catalyst C are fully degenerate, meaning that $H_S \propto H_C \propto \mathbb{1}$. This case will allow us to simplify both the presentation and numerical computation since checking majorization is computationally easier than checking thermo-majorization. It should be noted that this approach does not reduce the generality of our findings, as thermo-majorization criteria can always be expressed in terms of

standard majorization using the embedding map [11]. Moreover, for the purpose of visualization, we focus here on the case when $d_S = 3$, which allows us to describe the numerical findings in a more natural and visually appealing way. In Appendix D, we report further numerical evidence, which indicates that these conclusions naturally extend to larger-dimensional systems.

A. Fixed initial and final states

Let us consider two states ρ_S and σ_S such that $\boldsymbol{p} = \mathrm{diag}[\rho_S]$ and $\boldsymbol{q} = \mathrm{diag}[\sigma_S]$, which are chosen such that (i) they satisfy the corresponding second laws in Eq. (5), meaning that $H_\alpha(\boldsymbol{p}) \leq H_\alpha(\boldsymbol{q})$ for all $\alpha \geq 0$, and such that (ii) the probability vector $\boldsymbol{p}$ does *not* majorize $\boldsymbol{q}$ and vice versa. In this way, we know that neither ρ_S nor σ_S can be transformed into each other, but there exists a catalyst ω_C that can be used to facilitate the transformation from ρ_S to σ_S. For illustrative purposes, let us choose the following two representative states:

$$\boldsymbol{p}^\star = (0.65, 0.2, 0.15), \qquad \boldsymbol{q}^\star = (0.5, 0.4, 0.1). \quad (52)$$

It is easy to check that $\boldsymbol{p}^\star$ and $\boldsymbol{q}^\star$ are incomparable using, e.g., the concept of Lorenz curves [22]. Here, we focus exclusively on these particular states.

Suppose now that we choose a probability distribution $\mathcal{P}_{\mathrm{dist}}$ and draw d_C positive numbers according to this distribution. We organize them in a vector and then normalize, obtaining a valid probability vector. In this way, we have a simple method of drawing random catalysts, which, for a large dimension d_C, well approximates drawing from the probability simplex. Let us denote with $\boldsymbol{c}^{(i)} = (c_1^{(i)}, c_2^{(i)}, \ldots, c_{d_C}^{(i)})$ an ith probability vector obtained via this method. Each $\boldsymbol{c}^{(i)}$ will model a random catalyst drawn according to a respective probability distribution. In this way, the elements of each such random catalyst are given by

$$c_k^{(i)} = \frac{X_{\mathrm{dist}}^k}{\sum_{k=1}^{d_C} X_{\mathrm{dist}}^k}, \quad (53)$$

where X_{dist}^k is a random variable drawn according to the probability distribution $\mathcal{P}_{\mathrm{dist}}$. In what follows, we consider three different distributions:

$$\mathcal{P}_{\mathrm{ray}} \rightarrow \mathsf{Prob}(X_{\mathrm{ray}}^k = x) \sim x e^{-x^2/2}, \quad (54)$$

$$\mathcal{P}_{\mathrm{uni}} \rightarrow \mathsf{Prob}(X_{\mathrm{uni}}^k = x) \sim \mathrm{const}, \quad (55)$$

$$\mathcal{P}_{\mathrm{exp}} \rightarrow \mathsf{Prob}(X_{\mathrm{exp}}^k = x) \sim e^{-x}. \quad (56)$$

Next, we fix the error that we can tolerate on the catalyst ϵ_C and repeat the process of sampling catalysts many times. Having done so, we can now ask the following question:

How frequently does a randomly chosen catalyst catalyze a given state transformation for a fixed error? Counting the frequency of cases in which the following transformation is possible,

$$p^\star \otimes c^{(i)} \to q^\star \otimes \tilde{c}^{(i)}, \tag{57}$$

with $\tilde{c}^{(i)}$ chosen such that $\|\tilde{c}^{(i)} - c^{(i)}\|_1 \leq \epsilon_C$, leads to the success probability $p_{\text{succ}}(p^\star, q^\star, \epsilon_C)$. This quantity is an estimate of the probability that a randomly chosen catalyst can help facilitate a given state transformation, with the disturbance on the catalyst being at most ϵ_C. Moreover, using the results of Ref. [79], we can readily determine the final state of the catalyst $\tilde{c}^{(i)}$ to be the so-called ϵ-flattest state (see Ref. [79] for the method of constructing these states). To summarize, the success probability $p_{\text{succ}}(p^\star, q^\star, \epsilon_C)$ is computed using the following set of steps:

Algorithm 1. Estimating $p_{\text{succ}}(p, q, \epsilon_C)$ by sampling.

Input: $p, q, d_C, \epsilon_C, \mathcal{P}_{\text{dist}}$
Output: Estimate of $p_{\text{succ}}(p, q, \epsilon_C)$
Parameters: N_C //precision of estimation
$\text{pos} = 0$
for each $i \in \{1, \ldots, N_C\}$ **do**
$\quad | \quad c^{(i)} \leftarrow$ random catalyst sampled using $\mathcal{P}_{\text{dist}}$
$\quad | \quad$ **if** there exists $\tilde{c}^{(i)}$s.t. $p \otimes c^{(i)} \to q \otimes \tilde{c}^{(i)}$ and
$\quad | \quad \|\tilde{c}^{(i)} - c^{(i)}\|_1 \leq \epsilon_C$ **then**
$\quad |\_\_\ |\_\_ \text{pos} \leftarrow \text{pos} + 1$
$p_{\text{succ}}(p, q, \epsilon_C) \leftarrow \text{pos}/N_C$

The results of this numerical experiment are summarized in Fig. 3. As we can see, when we increase the dimension d_C, the probability that a randomly chosen catalyst can catalyze a given transformation increases and very rapidly approaches a fixed value. This value, as well as the rate at which it is approached, depends on the specific distribution $\mathcal{P}_{\text{dist}}$ we choose, which indicates that the success probability $p_{\text{succ}}(p^\star, q^\star, \epsilon_C)$ depends on both the dimension of the catalyst and the distribution of its eigenvalues. This numerical experiment allows us to conclude that there are state transformations for which random states act as catalysts with high probability.

B. Fixed initial state and arbitrary final state

In the previous section, we studied how useful random catalysts are for a fixed-state transformation. We now go one step further and generalize this investigation to arbitrary final states while still keeping the initial state fixed. Let us then consider again the state $p^\star$ given by Eq. (52) as the input state, and let q be an arbitrary state. Since $p^\star$ and q are d_S-dimensional probability vectors, it is useful to think of them as points in the space of all d_S-dimensional
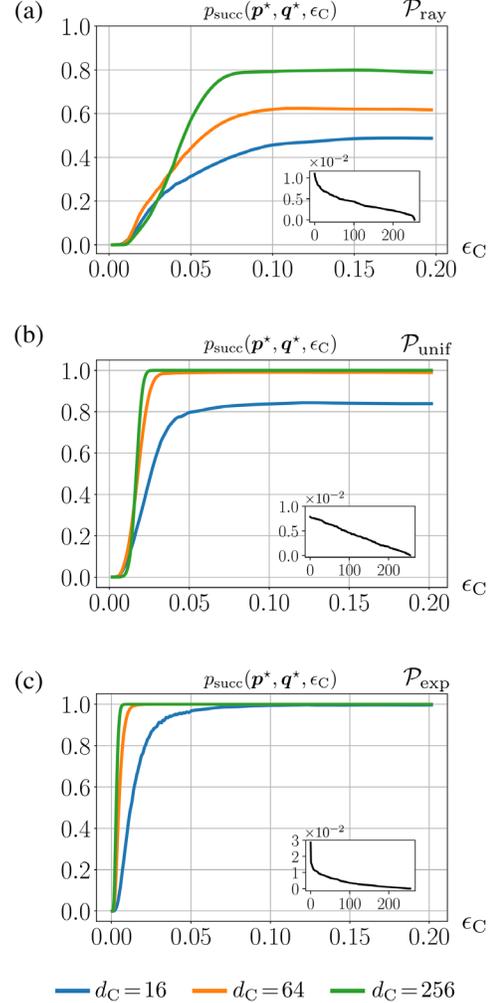

FIG. 3. Probability $p_{\text{succ}}(p^\star, q^\star, \epsilon_C)$ that a random state of dimension d_C drawn from probability distribution $\mathcal{P}_{\text{dist}}$ can catalyze a fixed-state transformation $p^\star \to q^\star$. Each panel corresponds to a different distribution: (a) Rayleigh $\mathcal{P}_{\text{ray}}$, (b) uniform $\mathcal{P}_{\text{unif}}$, and (c) exponential $\mathcal{P}_{\text{exp}}$. The insets illustrate an exemplary distribution of eigenvalues $c_k^{(i)}$ of a random catalyst $c^{(i)}$ drawn according to a respective distribution and then normalized.

probability vectors, the so-called probability simplex Δ_{d_S} defined as

$$\Delta_N := \left\{ x = (x_1, \ldots, x_N) | x_i \geq 0 \quad \text{and} \quad \sum_{i=1}^{N} x_i = 1 \right\}. \tag{58}$$

Let us now define two sets of states inside Δ_{d_S}:

$$\mathsf{S}(p) = \{q | p \to q \text{ and } q \in \Delta_{d_S}\}, \tag{59}$$

$$\mathsf{T}(p) = \{q | p \otimes c \to q \otimes c, q \in \Delta_{d_S} \text{ and } c \in \Delta\}, \tag{60}$$

where Δ is the set of all N-dimensional probability simplices Δ_N for all natural N. The set $\mathsf{S}(p)$ contains all

states q that are (thermo-) majorized by p, that is, all states that can be reached via thermal operations when starting from a state described by p. The set $\mathsf{T}(p)$ contains all states q that can be reached via thermal operations with the help of some (unspecified) catalyst. We refer to these sets as the thermal and the catalytic-thermal set, respectively. It can be readily verified that $\mathsf{S}(p) \subseteq \mathsf{T}(p)$ for all p. In this language, the main result of Ref. [13] shows that $\mathsf{S}(p) \subset \mathsf{T}(p)$ for some p. Moreover, because of the results of Refs. [11,80,81], a complete characterization of the set $\mathsf{T}(p)$ is known, and whether $q \in \mathsf{T}(q)$ is determined by the second laws in Eq. (5).

Let us now perform our second numerical experiment. In the previous section, we saw that for a fixed transformation, catalysts sampled from the exponential distribution in Eq. (56) achieve a high probability of success $p_{\mathrm{succ}}(p^\star, q^\star, \epsilon_{\mathrm{C}})$, even for moderate dimensions of catalysts. Let us now use the exponential distribution to sample random catalysts and compute the associated success probability. Furthermore, to ensure that we do not work in the embezzlement regime, we also fix the allowable error on the catalyst to be $\epsilon_{\mathrm{C}} = \mu \epsilon_{\mathrm{C}}^{\mathrm{bnd}}$, where $\epsilon_{\mathrm{C}}^{\mathrm{bnd}}$ is the embezzlement bound from Eq. (9) and $0 \leq \mu < 1$. For arbitrary points $q \in \Delta_{d_{\mathrm{S}}}$, we then estimate $p_{\mathrm{succ}}(p^\star, q, \epsilon_{\mathrm{C}})$, the probability that a random catalyst can be used to transform $p^\star$ into q using the method described in Algorithm 1.

The results of this numerical experiment are summarized in Fig. 4. For the purpose of illustration, we also draw the sets $\mathsf{S}(p^\star)$ and $\mathsf{T}(p^\star)$. The numerics demonstrate that the probability $p_{\mathrm{succ}}(p^\star, q, \epsilon_{\mathrm{C}})$ is large for most q in the region $\mathsf{D}(p^\star) := \mathsf{T}(p^\star) \backslash \mathsf{S}(p^\star)$ even for small dimensions of the catalyst (e.g., when $d_{\mathrm{C}} = 2^4$). Interestingly, the success probability increases significantly with the dimension of the catalyst, so for $d_{\mathrm{C}} = 2^8$, the value of $p_{\mathrm{succ}}(p^\star, q, \epsilon_{\mathrm{C}}) \approx 1$ for almost all points q inside $\mathsf{D}(p^\star)$. As a consequence, we can infer that there are (input) states for which random states act as catalysts with high probability *for all* possible output states.

C. Arbitrary initial and final states

In the previous section, we saw that a random catalyst can catalyze most of the possible state transformations for a fixed state p, even for catalysts with a moderate dimension. In this section, we extend our analysis and show that this behavior is a generic feature valid for arbitrary initial states.

Before going into the details, let us emphasize that not all initial states p lead to an interesting catalytic advantage. For example, when the system starts in a thermal state, $p = g$, there is no catalyst that can enhance the system's transformation potential. In that case, the thermal and catalytic-thermal sets coincide, i.e., $\mathsf{S}(g) = \mathsf{T}(g)$. A similar situation happens when the initial state of the system is a pure state.

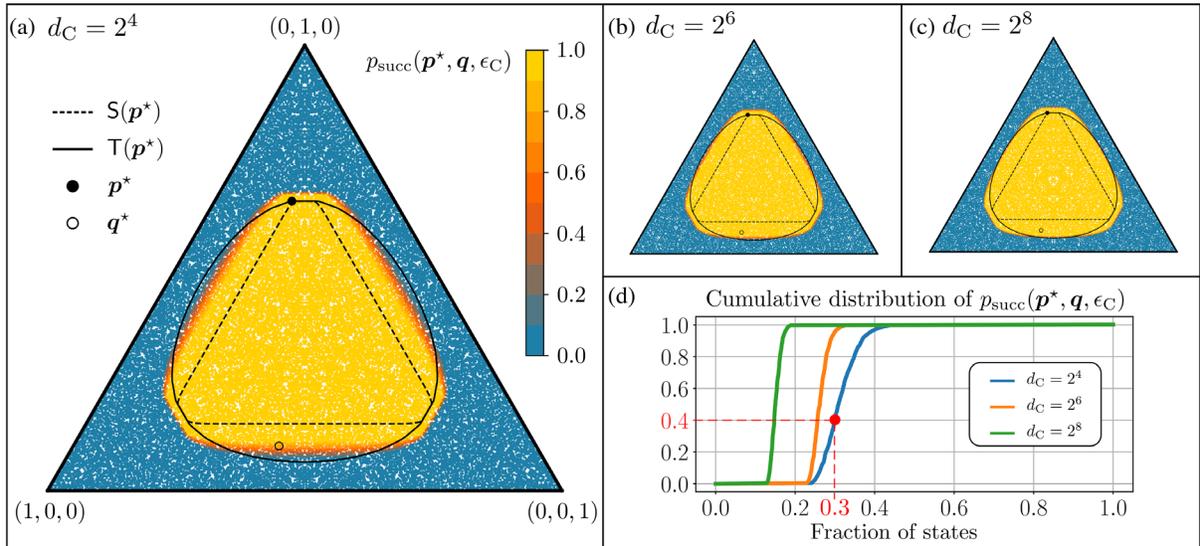FIG. 4. Probability $p_{\mathrm{succ}}(p^\star, q, \epsilon_{\mathrm{C}})$ that a random state can be used to enable the transformation from $p^\star$ to q approximately catalytically, i.e., with an error $\epsilon_{\mathrm{C}} = \mu \epsilon_{\mathrm{C}}^{\mathrm{bnd}}$ and $\mu = 0.1$. Plots (a)–(c) correspond to different dimensions of the random catalyst ($d_{\mathrm{C}} = 2^4$, 2^6, and 2^8, respectively). States inside the region bounded by dashed lines define the thermal set $\mathsf{S}(p^\star)$, consisting of all states that can be reached from $p^\star$ using thermal operations. The solid line corresponds to the catalytic-thermal set $\mathsf{T}(p^\star)$, consisting of all states that can be reached from $p^\star$ with the help of some (potentially finely tuned) catalyst. Note that the probability of success $p_{\mathrm{succ}}(p^\star, q, \epsilon_{\mathrm{C}})$ is generally very close to 1 for most final states q inside $\mathsf{D}(p^\star) := \mathsf{T}(p^\star) \backslash \mathsf{S}(p^\star)$, even when the dimension of the catalyst is relatively small. Plot (d) illustrates the cumulative distribution of $p_{\mathrm{succ}}(p^\star, q, \epsilon_{\mathrm{C}})$. To simplify the interpretation, an exemplary point is drawn in red. It corresponds to the case when 30% of all states $q \in \mathsf{D}(p^\star)$ can be reached using random catalysts of dimension $d_{\mathrm{C}} = 2^4$, with probability less than 0.4. In other words, 70% of all possible catalytic transformations can be realized using random catalysts with probability 0.4 or higher.

One natural way to quantify the potential for a catalytic improvement is to estimate the volume of a set defined as the difference between the thermal and the catalytic-thermal set. In what follows, we refer to such a set of states $D(p) := T(p) \backslash S(p)$ as the catalytic activation set (CAS). Naturally, the volume of this region in the space of distributions largely varies between different initial states p.

The aim of the next numerical experiment is to extend the results from the previous section to arbitrary initial states. We again fix a small error on the catalyst, $\epsilon_C = \mu \epsilon_C^{bnd}$, to ensure that we do not work in the embezzlement regime. We then uniformly sample the initial state p and compute the associated CAS, denoted $D(p)$. For each point $q \in D(p)$, we estimate the probability that a random catalyst can be used to transform p into q using the methods described in Algorithm 1. Finally, we calculate the number of states inside $D(p)$ for which the probability of catalyzing using random catalysts, $p_{succ}(\epsilon_C)$, is larger than a fixed threshold value γ_{thd} [82]. This process allows us to estimate, for each p, the fraction $f(p)$ of all possible transformations that can be catalyzed using random catalysts with probability of at least γ_{thd}, i.e.,

$$f(p) := \frac{|\tilde{D}(p)|}{|D(p)|}, \qquad (61)$$

where $\tilde{D}(p) \subseteq D(p)$ and $q \in \tilde{D}(p)$ if and only if $p_{succ}(p, q, \epsilon_C) \geq \gamma_{thd}$. The quantity $f(p)$ can be estimated using the following simple algorithm:

Algorithm 2. Estimating $f(p)$ by sampling.

Input: $p, d_C, \epsilon_C, \gamma_{thd}, \mathcal{P}_{dist}$
Output: Estimate of $f(p)$
Parameters: N_S

$A(p) \leftarrow$ initialize uniformly N_S states of dimension d_S
$S(p) \leftarrow$ all states in $A(p)$ satisfying Eq. (59)
$T(p) \leftarrow$ all states in $A(p)$ satisfying Eq. (60)
$D(p) \leftarrow T(p) \backslash S(p)$

$pos = 0$
for each $q \in D(p)$ **do**
  | $p_{succ}(p, q, \epsilon_C) \leftarrow$ compute using Algorithm 1
  | **if** $p_{succ}(p, q, \epsilon_C) \geq \gamma_{thd}$ **then**
  |__ |__ pos $\leftarrow$ pos + 1
$f(p) \leftarrow$ pos$/|D(p)|$

The results of this numerical experiment are summarized in Fig. 5. Interestingly, even for relatively small catalyst dimensions (e.g., $d_C = 16$), there is a modest fraction of possible transformations that, with high probability, can be catalyzed with a random catalyst. Furthermore, by increasing the dimension of the catalyst, this fraction improves significantly; thus, already for moderate-sized catalysts ($d_C = 256$), most of the possible transformations can be

catalyzed using random catalysts with a large probability. As a consequence, this numerical investigation allows us to infer that most of the possible transformations can be catalytically activated with high probability using random states as catalysts. In Appendix D, we give analogous plots for a different choice of the relative error μ, the threshold value γ_{thld}, and system dimension d_S, to demonstrate that this behavior is generic; i.e., it does not depend on our particular choice of parameters.

D. Comparison with multicopy states

In the previous sections, we studied how useful random states are in catalyzing thermodynamic transformations. In the final numerical experiment, we compare these insights with the analytical results presented in this paper. In particular, we compute the quantity $f(p)$ defined in Eq. (61) using multiple copies of a fixed state as a catalyst. This method allows us to examine some of the practical aspects of our construction, i.e., when the catalysts consist of a moderate number of particles.

We again fix the error on the catalyst to be $\epsilon_C = \mu \epsilon_C^{bnd}$ and compute the quantity $f(p)$ using Algorithm 2, with the only difference that now $p_{succ}(p, q, \epsilon_C)$ is computed using a fixed multicopy catalyst. Hence, it can be either 0 (the multicopy catalyst does not allow us to transform p into q within the allowed error on the catalyst) or 1 (when p can be transformed into q within the allowed error). The single-copy catalyst is chosen to be a qubit in a state $\omega_C = \text{diag}(1 - r, r)$ with $0 \leq r < 1/2$. The results of this numerical experiment are summarized in Fig. 6. Comparing these results with Fig. 5 illustrates that multicopy catalysts generally achieve a larger fraction $f(p)$ for the same dimension of the catalyst. However, in the multicopy case, the improvement in $f(p)$ obtained by increasing the catalyst's dimension is generally smaller than in the case of random catalysts, which indicates that catalytic universality using only a few copies might generally be possible when the catalyst is sufficiently mixed. Finally, Fig. 6 demonstrates that some marks of catalytic universality can be observed for a relatively modest number of particles comprising the catalyst.

E. Further directions

Although still somewhat preliminary in nature, these numerical findings strongly suggest that high-dimensional states, with high probability, will act as catalysts. This result indicates that the universality phenomenon we uncovered here may be even more general than we can yet prove analytically. It seems reasonable to expect that a potential route to further analytic results will be to look for statements that hold with high probability. We leave this tantalizing extension of our results for future work.

Finally, in Appendix D, we provide further numerical evidence that the catalytic universality phenomenon is a generic feature of sufficiently high-dimensional catalysts.
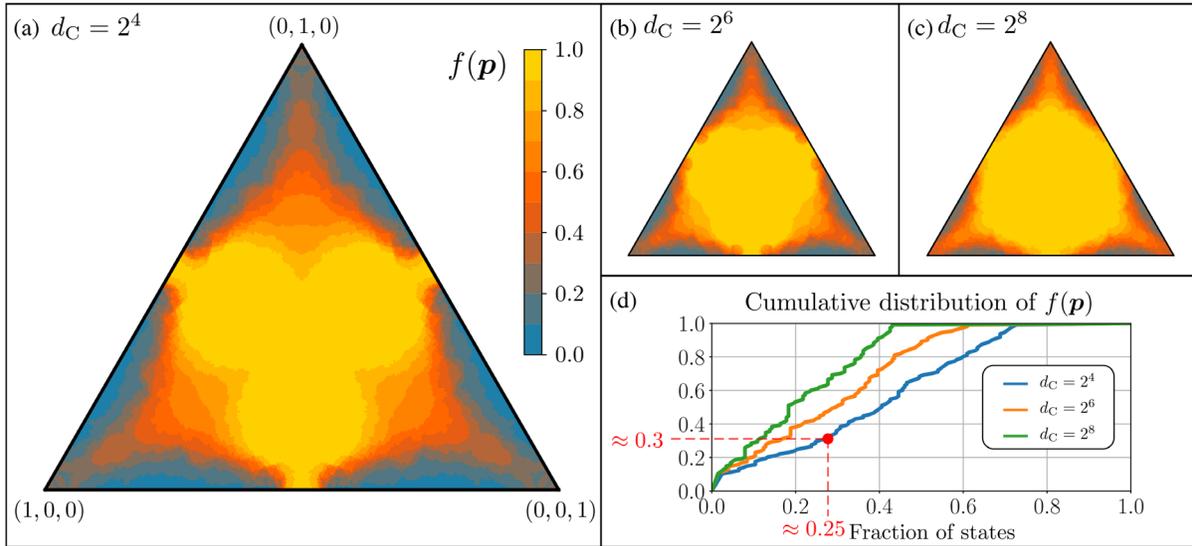
FIG. 5. Fraction $f(\boldsymbol{p})$ of all states inside the catalytic activation set $\mathsf{D}(\boldsymbol{p})$ (CAS) for which the probability $p_{\text{succ}}(\boldsymbol{p}, \boldsymbol{q}, \epsilon_\text{C})$ that a random state can be used as a catalyst is larger than the threshold value $\gamma_{\text{thd}} = 0.9$. Plots (a)–(c) correspond to random catalysts of dimensions 2^4, 2^6, and 2^8, respectively. Plot (d) illustrates the cumulative distribution of $f(\boldsymbol{p})$. As an example, the red point corresponds to the situation where random states of dimension $d_\text{C} = 2^4$ are used to catalyze possible transformations. These random catalysts are not useful for roughly 25% of all possible initial states $\boldsymbol{p}$; i.e., for each such state, they allow, at most, approximately 30% of all output states $\boldsymbol{q}$ in CAS to be reached with probability equal to or greater than γ_{thld}. In other words, such random catalysts can be used to reach more than 30% of all possible output states $\boldsymbol{q} \in \mathsf{D}(\boldsymbol{p})$, with probability at least γ_{thld}, for at least 75% of all initial states $\boldsymbol{p}$.
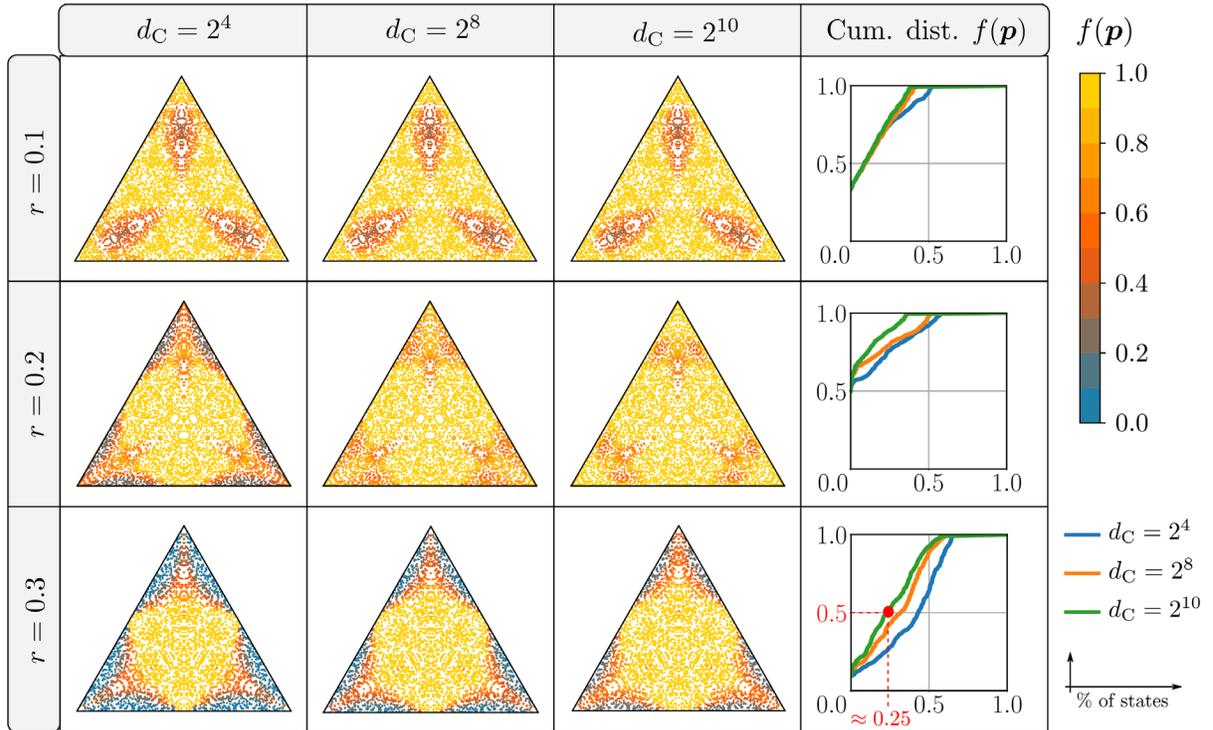

FIG. 6. Fraction $f(\boldsymbol{p})$ of all states inside the catalytic activation set of $\boldsymbol{p}$ that can be catalyzed using a multicopy catalyst composed of $n \in \{4, 8, 10\}$ qubits $\omega_\text{C} = \text{diag}(1 - r, r)$, for different values of parameter r. Column 4 shows a cumulative distribution of $f(\boldsymbol{p})$; i.e., it illustrates the fraction of catalytic transformations that can be activated using a multicopy catalyst. For example, the red exemplary point indicates that for around 0.25 of all possible input states $\boldsymbol{p}$, a quantum system composed of $n = 10$ qubits in a state with $r = 0.3$ acts as a catalyst for less than 0.5 of all possible output states $\boldsymbol{q}$ in CAS. Equivalently, for this choice of parameters, the multicopy catalyst can activate more than 0.5 of all possible transformations for approximately 0.75 of all possible input states.

In particular, we (i) perform numerical calculations for larger-dimensional systems S, (ii) change the sampling of catalysts to other distributions, and (iii) choose different thresholds for the catalyst error ϵ_C and δ.

V. SUMMARY

In this work, we have studied the problem of catalysis in quantum thermodynamics. We have shown that any state can act as a (universal) catalyst for all transformations allowed by the laws of thermodynamics, provided that enough copies of the catalyst are available. In particular, in the case of genuine catalysis, we have shown that all states can be used as catalysts in transforming ρ into σ, as long as the two states satisfy the second laws of thermodynamics. In this case, the error on the catalyst decreases subexponentially with the number of particles. Furthermore, in the embezzlement regime, which appears when the second laws completely vanish, we found an analogous behavior. In that case, the error on the catalyst scales with the number of particles n much worse than in the regime of genuine catalysis; however, it still approaches zero as $n \to \infty$.

We have also emphasized that this surprising property of catalysis is a genuine feature arising in any majorization-based resource theory. In this way, the results can be applied in a wide range of other contexts, ranging from the theory of pure entanglement to the theory of purity or coherence.

Finally, we conjectured that this phenomenon is a genuine feature of large-dimensional catalysts, and we provided simple numerical evidence to support this conjecture.

VI. DISCUSSION AND OPEN PROBLEMS

In this work, we have presented and proved a surprising property of multicopy catalyst states: that every state, given sufficiently many copies, can act as a universal catalyst. We believe that this new realization is a substantial step forward in our understanding of catalysis and that it provides new insights in both the field of quantum thermodynamics and resource theories. What is more, our work opens the door for new avenues of exploration, which will be of independent interest. In the following subsections, we briefly sketch the most promising directions, in our opinion, of extending the results presented in this work.

A. Mechanism of catalysis

Since the seminal paper of Jonathan and Plenio [13], our understanding of catalysis has grown significantly. However, we still do not fully understand the real mechanism behind catalysis and how it allows for lifting some of the restrictions imposed by allowable operations.

Here, we made a step forward in explaining this mechanism. However, before a satisfactory understanding can be reached, several important challenges still need to be tackled. In particular, a long-standing open problem is determining which physical properties of states are important for catalysis. Moreover, we do not know how the set of states reachable via catalytic transformations is modified when additional constraints on the catalyst are made—e.g., in terms of energy, entropy, or the distribution of its eigenvalues. What is the main property or "resource" relevant for catalysis? Our analytic results and preliminary numerics strongly suggest that the dimension of the catalyst and distribution of its eigenvalues are both important properties of a good catalyst. This also indicates a trade-off relation between the catalyst dimension and its ability to catalyze transformations. Quantifying and understanding this potential trade-off will significantly advance our understanding of catalysis.

B. Catalytic universality for generic states

In Sec. IV, we presented simple numerical evidence that indicates that the catalytic universality might appear for arbitrary large-dimensional catalysts. We believe that solving this problem will shed more light on the fundamental problem of what the catalyst really does to facilitate the transformation. In particular, should we expect to find only specific catalysts if we modify some of our initial assumptions?

Another interesting way to proceed would be to study how important the correlations are, for the catalytic universality, between the subsystems that form the catalyst. Looking more closely at the proofs presented here, we can see that, both in the embezzlement and genuine catalysis regimes, the main catalytic transformation $\mathcal{E}_{SC}$ does not build such correlations. In this respect, the only time when correlations can increase is during the preprocessing and postprocessing steps. However, since this potential increase in correlations is only due to the transformation error, we conjecture that it is not a necessary requirement for our results to hold.

In this respect, it would also be interesting to revisit the results from Ref. [56] and check whether, in the regime where only correlations are allowed to build up (that is, when the reduced state of the catalyst subsystems remain undisturbed), multicopy catalysts can still be viewed as universal catalysts.

C. Improving the error scaling

Another interesting direction of extending the results presented in this paper would be to reduce the disturbance induced on the catalyst during the main protocol.

In particular, in the embezzlement regime, this would involve choosing a different intermediate state η_C and choosing a more specialized transformation $\mathcal{E}_{SC}$. It seems plausible that using a more elaborate mixing transformation would allow one to further reduce the error scaling and, potentially, approach the threshold specified by Eq. (9).

On the other hand, in the regime of genuine catalysis, we expect that the scaling of the catalyst disturbance can be further improved using the tools of large-deviation theory. The primary sources of error in this regime are the preprocessing and postprocessing steps, which both incur a subexponential disturbance on the catalyst. Indeed, the results of Ref. [66] were obtained in the regime when the error term $\delta(n)$ scales no better than $\mathcal{O}(e^{-n^\kappa})$, where $\kappa \in (0, 1)$. In the large-deviation regime, the error is exponentially vanishing at the cost of a constant gap between the effective (r_n) and asymptotic (r_∞) conversion rates. Since the presence of such a gap would not alter our main protocol, we believe that working in the large-deviation regime would effectively allow the error scaling to be improved to an exponential one.

Finally, in our work, we assumed that the catalyst system has a fully degenerate energetic spectrum. Because of the result from Ref. [11], we know that it is sufficient to consider only such catalysts. However, what we do not know is whether these catalysts are optimal with respect to either the dimension or entropy. It would be interesting to study in what way considering a nontrivial Hamiltonian of the catalyst allows the error scaling or the minimal number of necessary copies to be improved. In particular, one can ask if it is possible to achieve a faster error scaling or, equivalently, to require smaller catalysts for the same error, by using more energetic catalysts.

D. Quantification of catalysis regimes

In this work, we divided catalysis into two different regimes. We explored the embezzlement regime in which the partial order between states completely vanishes and the genuine catalysis regime in which we are guaranteed that at least some of the second laws remain.

It would be interesting to pursue this idea more carefully and examine which of the second laws remain as valid monotones when allowing for a certain type of error scaling on the catalyst. We know from Ref. [11] that when one allows for an error scaling that is linear in the number of particles, that is, $\epsilon_C \sim \mathcal{O}(n^{-1})$, then the nonequilibrium Helmholtz free energy remains as the only necessary and sufficient second law. What we do not know is how many and when we allow other types of error scaling. Solving this problem would certainly increase our understanding of catalysis and its physical importance for quantum thermodynamics and other resource theories.

E. Catalytic universality and second laws for coherence

In our work we have not explored catalysis in the regime where states ρ_S and σ_S contain coherences between energy levels. It is known that, in this case, the second laws in Eq. (5) provide only necessary but not sufficient conditions for state transformations. When considering fully general states with coherences, one has to additionally satisfy a completely new set of conditions resulting from the time-symmetry constraints [83]. Loosely speaking, these new laws tell us that coherences between energy levels must decrease during thermodynamic transformation. In that case, it would be interesting to see if the catalytic universality phenomenon can also appear for fully general coherent states.

F. Other potential directions

Consequences of the resonance phenomenon. One of the main tools that we used in our protocol was the multicopy state conversion in the moderate-deviation regime [66]. In a recent article [84], it was shown that moderate-deviation analysis exhibits an interesting phenomenon of resource resonance, which arises during nonasymptotic state conversions in the resource theories of entanglement, coherence, and thermodynamics. This resource resonance implies that certain pairs of resource states can be interconverted at the asymptotically optimal rate with negligible error, even in the regime of finite n. In the context of our results, this means that, for certain states, catalytic transformations can be achieved by using much fewer copies of the catalyst state. We believe that understanding the role of the resonance behavior in catalysis can lead to novel insights not only for quantum thermodynamics but also for the resource theories of entanglement, purity, and coherence.

Extending catalytic universality to arbitrary QRTs. A natural question that arises when studying catalysis in the context of majorization-based QRTs is whether the catalysis phenomenon can be properly defined and studied for general resource theories as well. Interestingly, there are examples of QRTs for which catalysis does not enlarge the set of states that can be reached using free operations [85], which leads to an interesting question: What are the necessary properties of a general QRT that allow it to have a nontrivial catalysis? Consequently, one can further ask if the catalytic universality phenomenon can also emerge for such theories. If not, then it would mean that catalytic universality is a unique feature of majorization-based QRTs, and it would be interesting to see which special aspects of such theories allow for the catalytic universality.

APPENDIX A: NOTATION

For a discrete probability distribution $\boldsymbol{p} = (p_1, p_2, \ldots, p_{d_S})$, the Shannon entropy $H(\boldsymbol{p})$ and entropy variance $V(\boldsymbol{p})$ are defined as

$$H(\boldsymbol{p}) := -\sum_i p_i \log p_i, \qquad V(\boldsymbol{p}) := \sum_i p_i [-\log p_i - H(\boldsymbol{p})]^2. \tag{A1}$$

Similarly, we define the relative entropy $D(\boldsymbol{p}\|\boldsymbol{q})$ and the relative entropy variance $V(\boldsymbol{p}\|\boldsymbol{q})$ as

$$D(\boldsymbol{p}\|\boldsymbol{q}) := \sum_i p_i \log\left(\frac{p_i}{q_i}\right), \qquad V(\boldsymbol{p}\|\boldsymbol{q}) := \sum_i p_i \left[\log\left(\frac{p_i}{q_i}\right) - D(\boldsymbol{p}\|\boldsymbol{q})\right]^2. \tag{A2}$$

Renyi entropies H_α and the corresponding Renyi relative entropies $D_\alpha(\boldsymbol{p}\|\boldsymbol{q})$ for all $\alpha \in \mathbb{R}$ are defined by

$$H_\alpha(\boldsymbol{p}) := \frac{\mathrm{sgn}(\alpha)}{1-\alpha} \log\left[\sum_i p_i^\alpha\right], \qquad D_\alpha(\boldsymbol{p}\|\boldsymbol{q}) := \frac{\mathrm{sgn}(\alpha)}{1-\alpha} \log\left[\sum_i p_i^\alpha q_i^{1-\alpha}\right]. \tag{A3}$$

The generalized free energies for a block-diagonal state in the energy eigenbasis ρ, such that $\boldsymbol{p} = \mathrm{diag}[\rho]$, with Hamiltonian H and in contact with the environment at inverse temperature β, are defined as

$$F_\alpha(\boldsymbol{p}) = D_\alpha(\boldsymbol{p}\|\boldsymbol{g}) - \log Z, \tag{A4}$$

where $Z = \mathrm{Tr}[e^{-\beta H}]$ is the partition function, $\boldsymbol{g} = \mathrm{diag}[\tau]$, and $\tau = e^{-\beta H}/Z$ is the thermal state.

APPENDIX B: PRELIMINARY LEMMAS

Here, we present two lemmas that are essential for proving our results. We start with a simple realization that for any thermal operation that maps the system's state into another state with some error, we can always find a "gentle" unitary that achieves the same error, as measured by the trace distance, on the system and its environment.

Lemma 4. Let $\mathcal{T}$ be a thermal operation satisfying

$$\|\mathcal{T}[\rho_S] - \sigma_S\|_1 \leq \epsilon \tag{B1}$$

for block-diagonal states ρ_S and σ_S. Then, there exists a unitary U_{SB} and an environment system B with Hamiltonian H_B such that

$$\|U_{SB}(\rho_S \otimes \tau_B)U_{SB}^\dagger - \sigma_S \otimes \tau_B\|_1 \leq \epsilon, \tag{B2}$$

where $\tau_B := e^{-\beta H_B}/Z_B$ with $Z_B := \mathrm{Tr}[e^{-\beta H_B}]$ is the thermal state of the environment and $[U_{SB}, H_S + H_B] = 0$.

Proof.—Let us write the states ρ_S and σ_S in their energy eigenbasis as

$$\rho_S = \sum_i p_i |i\rangle\langle i|_S, \qquad \sigma_S = \sum_i q_i |i\rangle\langle i|_S. \tag{B3}$$

Let $\{r(j|i)\}$ denote the transition probabilities of the map $\mathcal{T}$, i.e., $\mathcal{T}[\rho_S] = \sum_{i,j} p_i r(j|i)|j\rangle\langle j|_S$. Then, Eq. (B1) implies

$$\|\mathcal{T}[\rho_S] - \sigma_S\|_1 = \frac{1}{2}\sum_j \left|q_j - \sum_i p_i r(j|i)\right| \leq \epsilon. \tag{B4}$$

We now represent our total state $\rho_S \otimes \gamma_B$ in blocks of constant energy. This standard approach is described in more detail, e.g., in Refs. [22,61]. To do so, we first write the Hamiltonian of the bath as

$$H_B = \sum_j \sum_g^{g(E_j^B)} E_j^B |E_j^B\rangle\langle E_j^B|_B, \tag{B5}$$

where $g(E)$ is the degeneracy of the energy level E. In what follows, we make two assumptions about the spectrum of the heat bath: (i) All energy gaps are present; i.e., for any two energy levels of the system, E_i^S and E_j^S, there exist E_k^B and E_l^B such that $E_i^S - E_j^S = E_k^B - E_l^B$. (ii) Degeneracies scale exponentially; that is, $g(E + \epsilon) = g(E)e^{\beta\epsilon}$. Both of these are standard assumptions in thermodynamics. The first condition is valid for heat baths with continuous energy spectra and can be approached arbitrarily well by discrete heat baths. The second condition is naturally satisfied when the average energy of the heat bath is much larger than that of the system.

With Eq. (B5) in mind, we can write the initial state of the environment as

$$\tau_B = \sum_j \sum_g^{g(E_j^B)} \frac{e^{-\beta E_j^B}}{Z_B} |E_j^B, g\rangle\langle E_j^B, g|_B. \tag{B6}$$

The joint state of the system S and the environment B can be written as

$$\rho_S \otimes \tau_B = \sum_{i,j} \sum_g^{g(E_j^B)} p_i \frac{e^{-\beta E_j^B}}{Z_B} |i\rangle\langle i|_S \otimes |E_j^B, g\rangle\langle E_j^B, g|_B \tag{B7}$$

$$= \sum_E \sum_i \sum_g^{g(E-E_i^S)} p_i \frac{e^{-\beta E}}{Z_B} e^{\beta E_i^S} |i\rangle\langle i|_S \otimes |E - E_i^S, g\rangle\langle E - E_i^S, g|_B, \tag{B8}$$

where, in the second line, we replace the summation over the heat bath energies with a summation over the total energies $E := E_i^S + E_j^B$. Using assumption (ii) and denoting $d_i(E) = g(E)e^{-\beta E_i^S}$ leads to

$$\rho_S \otimes \tau_B = \sum_E \sum_i \sum_g^{d_i(E)} C(E) \frac{p_i}{d_i(E)} |E - E_i^S, i, g\rangle\langle E - E_i^S, i, g|_{SB}, \tag{B9}$$

where we labeled $C(E) := g(E)e^{-\beta E}/Z_B$. Now, the assumption that $[U_{SB}, H_S + H_B] = 0$ implies that the unitary U_{SB} is block diagonal in the basis of H_{SB}. Writing $U_{SB} = \bigoplus_E U_{SB}^{(E)}$, we can choose each $U_{SB}^{(E)}$ to be a permutation of eigenvalues within a fixed energy shell determined by E. Such a permutation can be described by providing a collection of numbers $\{n_{j|i}(E)\}$ that denote the number of eigenvalues moved from block i to block j in energy shell E. Unitarity of U_{SB} and the fact that it is energy preserving implies that these numbers for all E have to satisfy the constraints $\sum_i n_{j|i}(E) = d_j(E)$ and $n_{j|i}(E) = d_i(E)$. For our purposes, we choose these numbers to be

$$\forall E \quad n_{j|i}(E) = d_i(E)r(j|i). \tag{B10}$$

It can be easily checked that this is a feasible choice as long as the channel probabilities $\{r(j|i)\}$ preserve the thermal state (which is always the case). The final state of the system and the environment after application of the unitary U_{SB} becomes

$$U_{SB}[\rho_S \otimes \tau_B]U_{SB}^\dagger = \sum_E \sum_{i,j} \sum_g^{d_i(E)} C(E) \frac{p_i}{d_i(E)} \frac{n_{j|i}(E)}{d_j(E)} |E, j, g\rangle\langle E, j, g|_{SB} \tag{B11}$$

$$= \sum_E \sum_{i,j} C(E) \frac{p_i}{d_j(E)} r(j|i) |E, j, g\rangle\langle E, j, g|_{SB} \tag{B12}$$

$$= \sum_E \sum_j C(E) \frac{q_j'}{d_j(E)} |E, j, g\rangle\langle E, j, g|_{SB}, \tag{B13}$$

where, in the third line, we labeled $q_j' = \sum_i p_i r(j|i)$. The total error on the system and the bath then reads

$$\|U_{SB}[\rho_S \otimes \tau_B]U_{SB}^\dagger - \sigma_S \otimes \tau_B\|_1 = \left\|\sum_{j,E}\sum_g^{d_j(E)}\frac{C(E)}{d_j(E)}(q_j' - q_j)|E,j,g\rangle\langle E,j,g|_{SB}\right\|_1 \tag{B14}$$

$$= \sum_{j,E}\sum_g^{d_j(E)}\frac{C(E)}{d_j(E)}\cdot\frac{1}{2}|q_j' - q_j| \tag{B15}$$

$$= \frac{1}{2}\sum_j|q_j' - q_j| \tag{B16}$$

$$\leq \epsilon, \tag{B17}$$

where the inequality follows from Eq. (B4).

The second lemma was proven in Ref. [66], and it provides an estimate of the transformation error when converting between multiple copies of states.

Lemma 5. For any $\kappa \in (0,1)$ and any states diagonal in the energy basis $\rho = \mathrm{diag}[p]$ and $\sigma = \mathrm{diag}[q]$, there exists a thermal operation $\mathcal{T}$ such that

$$\|\mathcal{T}[\rho^{\otimes n} \otimes \tau^{\otimes n r_n}] - \sigma^{\otimes n r_n} \otimes \tau^{\otimes n}\|_1 \leq \epsilon_n, \tag{B18}$$

where the error ϵ_n and the conversion rate r_n are given by

$$\epsilon_n = e^{-n^\kappa}, \tag{B19}$$

$$r_n = \frac{D(\rho\|\tau)}{D(\sigma\|\tau)}\left(1 - \sqrt{\frac{2V(\rho\|\tau)}{D(\rho\|\tau)}}\left|1 - \frac{1}{\sqrt{v}}\right|\cdot\frac{1}{\sqrt{n^{1-\kappa}}}\right) = \frac{D(\rho\|\tau)}{D(\sigma\|\tau)} - \mathcal{O}\left(\frac{1}{\sqrt{n^{1-\kappa}}}\right), \tag{B20}$$

and where the parameter v is given by

$$v := \frac{V(p\|g)/D(p\|g)}{V(q\|g)/D(q\|g)}. \tag{B21}$$

APPENDIX C: DETAILS OF THE MAIN PROTOCOL

1. Setting up the scene

We begin by describing our main protocol of catalytic state conversion in full detail. Let S label the system, C the catalyst, and let $B = B_1 B_2$ denote the ambient heat bath, which we decompose into two parts for reasons that will become clear later. Let U_{CB_1} be the unitary that is applied in the first step of the protocol. Similarly, we define the unitary V_{SCB_2}, which is applied in the second step and which acts on SC and the second part of the heat bath B_2. To simplify notation, we denote the channels generated by these unitaries by

$$\mathcal{U}_{CB_1}[\cdot] := U_{CB_1}(\cdot)U_{CB_1}^\dagger, \qquad \mathcal{U}_{CB_1}^\dagger[\cdot] := U_{CB_1}^\dagger(\cdot)U_{CB_1}, \qquad \mathcal{V}_{SCB_2} := V_{SCB_2}(\cdot)V_{SCB_2}^\dagger. \tag{C1}$$

Our protocol starts with a product state $\rho_{SCB}^{(0)} = \rho_S \otimes \omega_C^{\otimes n} \otimes \tau_{B_1} \otimes \tau_{B_2}$. The full state of the joint system at each step of the protocol can be written as

$$\rho_{SCB_1B_2}^{(1)} = (\mathcal{I}_S \otimes \mathcal{U}_{CB_1} \otimes \mathcal{I}_{B_2})[\rho_{SCB}^{(0)}], \qquad \rho_{SCB_1B_2}^{(2)} = (\mathcal{V}_{SCB_2} \otimes \mathcal{I}_{B_1})[\rho_{SCB_1B_2}^{(1)}], \tag{C2}$$

$$\rho_{SCB_1B_2}^{(3)} = (\mathcal{I}_{SB_2} \otimes \mathcal{U}_{CB_1}^\dagger)[\rho_{SCB_1B_2}^{(2)}]. \tag{C3}$$

Notice that if the unitaries U_{CB_1} and V_{SCB_2} both commute with the total Hamiltonian H_{SCB}, then their composition commutes as well. Hence, tracing out the degrees of freedom associated with the bath leads to a valid thermal operation.

The final state of the system and the catalyst after this procedure can be expressed as

$$\rho'_{SC} = \text{Tr}_{B_1 B_2}[\rho^{(3)}_{SCB_1 B_2}] = \text{Tr}_{B_1 B_2}[(\mathcal{I}_S \otimes \mathcal{U}^\dagger_{CB_1} \otimes \mathcal{I}_{B_2})(\mathcal{V}_{SCB_2} \otimes \mathcal{I}_{B_1})(\mathcal{I}_{SB_2} \otimes \mathcal{U}_{CB_1})[\rho_S \otimes \omega_C^{\otimes n} \otimes \tau_{B_1} \otimes \tau_{B_2}]] \quad (\text{C4})$$

$$=: \mathcal{T}_{SC}[\rho_S \otimes \omega_C^{\otimes n}], \quad (\text{C5})$$

where we implicitly defined the effective thermal operation $\mathcal{T}_{SC}$ acting on the system and the catalyst. In what follows, we argue that by an appropriate choice of unitaries U_{CB_1} and V_{SCB_2}, we can obtain the approximate catalytic state conversion for a pair of states ρ_S and σ_S, i.e.,

$$\mathcal{T}_{SC}[\rho_S \otimes \omega_C^{\otimes n}] \approx \sigma_S \otimes \omega_C^{\otimes n}. \quad (\text{C6})$$

Before we get into the details of how to choose these unitaries, let us first find a general expression for the errors on the system and the catalyst.

2. Error analysis

We define the errors on the system and the catalyst in the following way:

$$\epsilon_S := \|\text{Tr}_C[\mathcal{T}_{SC}[\rho_S \otimes \omega_C^{\otimes n}]] - \sigma_S\|_1, \qquad \epsilon_C := \|\text{Tr}_S[\mathcal{T}_{SC}[\rho_S \otimes \omega_C^{\otimes n}]] - \omega_C^{\otimes n}\|_1. \quad (\text{C7})$$

Let us start by explicitly writing the error on the catalyst. To keep the notation compact, we define the following effective channel acting on the catalyst:

$$\mathcal{E}_C[\omega] := \text{Tr}_{SB_2}[V_{SCB_2}(\rho_S \otimes \omega_C \otimes \tau_{B_2})V^\dagger_{SCB_2}]. \quad (\text{C8})$$

Using this definition, we can write the final error on the catalyst as

$$\epsilon_C = \|\text{Tr}_{SB_1 B_2}[(\mathcal{I}_S \otimes \mathcal{U}^\dagger_{CB_1} \otimes \mathcal{I}_{B_2})(\mathcal{V}_{SCB_2} \otimes \mathcal{I}_{B_1})(\mathcal{I}_{SB_2} \otimes \mathcal{U}_{CB_1})[\rho_S \otimes \omega_C^{\otimes n} \otimes \tau_{B_1} \otimes \tau_{B_2}]] - \omega_C^{\otimes n}\|_1 \quad (\text{C9})$$

$$= \|\text{Tr}_{B_1}[\mathcal{U}^\dagger_{CB_1}(\mathcal{E}_C \otimes \mathcal{I}_{B_1})\mathcal{U}_{CB_1}[\omega_C^{\otimes n} \otimes \tau_{B_1}]] - \omega_C^{\otimes n}\|_1 \quad (\text{C10})$$

$$= \|\text{Tr}_{B_1}[\mathcal{U}^\dagger_{CB_1}(\mathcal{E}_C \otimes \mathcal{I}_{B_1})(\mathcal{U}_{CB_1}[\omega_C^{\otimes n} \otimes \tau_{B_1}] - \omega'_{CB_1})] + \text{Tr}_{B_1}[\mathcal{U}^\dagger_{CB_1}(\mathcal{E}_C \otimes \mathcal{I}_{B_1})[\omega'_{CB_1}]] - \omega_C^{\otimes n}\|_1 \quad (\text{C11})$$

$$\leq \|\text{Tr}_{B_1}[\mathcal{U}^\dagger_{CB_1}(\mathcal{E}_C \otimes \mathcal{I}_{B_1})(\mathcal{U}_{CB_1}[\omega_C^{\otimes n} \otimes \tau_{B_1}] - \omega'_{CB_1})]\|_1 + \|\text{Tr}_{B_1}[\mathcal{U}^\dagger_{CB_1}(\mathcal{E}_C \otimes \mathcal{I}_{B_1})[\omega'_{CB_1}]] - \omega_C^{\otimes n}\|_1 \quad (\text{C12})$$

$$\leq \|\mathcal{U}_{CB_1}[\omega_C^{\otimes n} \otimes \tau_{B_1}] - \omega'_{CB_1}\|_1 + \|\text{Tr}_{B_1}[\mathcal{U}^\dagger_{CB_1}(\mathcal{E}_C \otimes \mathcal{I}_{B_1})[\omega'_{CB_1}]] - \omega_C^{\otimes n}\|_1. \quad (\text{C13})$$

Let us label the first term above with $\delta(n)$, i.e., $\delta(n) := \|\mathcal{U}_{CB_1}[\omega_C^{\otimes n} \otimes \tau_{B_1}] - \omega'_{CB_1}\|_1$. With this in mind and after subtracting and adding ω'_{CB_1} in the second term, we can further write

$$\epsilon_C \leq \delta(n) + \|\text{Tr}_{B_1}[\mathcal{U}^\dagger_{CB_1}((\mathcal{E}_C \otimes \mathcal{I}_{B_1})[\omega'_{CB_1}] - \omega'_{CB_1})] + \text{Tr}_{B_1}[\mathcal{U}^\dagger_{CB_1}[\omega'_{CB_1}]] - \omega_C^{\otimes n}\|_1 \quad (\text{C14})$$

$$\leq \delta(n) + \|(\mathcal{E}_C \otimes \mathcal{I}_{B_1})[\omega'_{CB_1}] - \omega'_{CB_1}\|_1 + \|\text{Tr}_{B_1}[\mathcal{U}^\dagger_{CB_1}[\omega'_{CB_1}] - \omega_C^{\otimes n} \otimes \tau_{B_1}]\|_1. \quad (\text{C15})$$

We now label the second term with $\nu(n) := \|(\mathcal{E}_C \otimes \mathcal{I}_{B_1})[\omega'_{CB_1}] - \omega'_{CB_1}\|_1$ and again use the fact that the trace distance decreases under a partial trace and is invariant under unitaries. This approach leads to the following upper bound:

$$\epsilon_C \leq 2\delta(n) + \nu(n). \quad (\text{C16})$$

This upper bound decomposes the total error on the catalyst into two contributions, $\delta(n)$ and $\nu(n)$. The first of these terms accounts for the error due to producing a state that is different from ω'_{CB_1} in the preprocesssing step, as well as the failure in recovering the initial state $\omega_C^{\otimes n} \otimes \tau_{B_1}$ after applying channel $\mathcal{E}_C$ in the postprocessing step. The second term, $\nu(n)$, is

responsible for the disturbance applied to the catalyst and the heat bath B_1 in the catalytic step via channel $\mathcal{E}_C$ and changes depending on which regime of catalysis one is currently interested in.

Note that, so far, the state ω'_{CB_1} is arbitrary and appears in both contributions $\delta(n)$ and $\nu(n)$ to the total error on the catalyst. Let us now decompose the bath B_1 into two parts B'_1 and B''_1 and choose the following state:

$$\omega'_{CB_1} := \eta_C^{\otimes nr_n} \otimes \tau_{B'_1}^{\otimes n} \otimes \tau_{B''_1}, \tag{C17}$$

where $0 \leq r_n \leq 1$ is some real number that potentially depends on n, and η_C is an arbitrary state that we will choose later.

We now invoke Lemma 5, which ensures that there is a thermal operation $\mathcal{T}_{CB'_1}$ that transforms n copies of the initial catalyst state $\omega_C^{\otimes n}$ into another state $\eta_C^{\otimes nr_n}$ (potentially with different dimensions). Here, r_n is the conversion rate, which, up to the leading order, depends on nonequilibrium Helmholtz free energies of ω and η. Formally, thermal operation $\mathcal{T}_{CB'_1}$ satisfies

$$\left\| \mathcal{T}_{CB'_1}[\omega_C^{\otimes n} \otimes \tau_{B'_1}^{\otimes nr_n}] - \eta_C^{\otimes nr_n} \otimes \tau_{B'_1}^{\otimes n} \right\|_1 \leq \epsilon_n, \tag{C18}$$

where the conversion rate r_n and the transformation error ϵ_n are given in Eq. (B19). Now, we use Lemma 4, which states that every thermal operation can be written in a "Stinespring form" by using a global unitary $U_{CB'_1 B''_1}$ acting on the system CB'_1 and the heat bath B''_1, i.e.,

$$\mathcal{T}_{CB'_1}[\rho_{CB'_1}] = \mathrm{Tr}_{B''_1}[U_{CB'_1 B''_1}(\rho_{CB'_1} \otimes \tau_{B''_1})U^\dagger_{CB'_1 B''_1}]. \tag{C19}$$

Importantly, this unitary does not increase the transformation error ϵ_n when enlarged to the bigger system $CB'_1 B''_1$, that is,

$$\left\| U_{CB'_1 B''_1}(\omega_C^{\otimes n} \otimes \tau_{B'_1}^{\otimes nr_n} \otimes \tau_{B''_1})U^\dagger_{CB'_1 B''_1} - \eta_C^{\otimes nr_n} \otimes \tau_{B'_1}^{\otimes n} \otimes \tau_{B''_1} \right\|_1 \leq \epsilon_n. \tag{C20}$$

This result implies that the transformation error induced by the unitary channel $\mathcal{U}_{CB_1}$ is upper bounded as

$$\delta(n) \leq \epsilon_n = e^{-n^\kappa}. \tag{C21}$$

Up to this point, we have the freedom to choose the operation $\mathcal{E}_C$ and the state η, both of which can be thought of as parameters of our protocol. We now discuss two different choices, which both lead to quantitatively different results.

a. Embezzlement regime

In this section, we apply a recent result from the theory of quantum communication called "convex-split lemma" to show that any state, given that enough copies of it are available, can act as an embezzler for any state transformation.

Recall that our main goal is to carry out the transformation $\rho \to \sigma$ on the system S, at the same time keeping the error on the catalyst small. To simplify notation, let us denote the number of copies of the state η obtained after applying the unitary U_{CB_1} with $m = nr_n$. In order to specify the channel $\mathcal{E}_C$ defined in Eq. (C8), let us first recall the process from the main text:

$$\mathcal{T}^{(\mathrm{mix})}[\cdot] = \frac{1}{m}\sum_{i=0}^{m} S_{(0,i)}(\cdot)S^\dagger_{(0,i)}, \tag{C22}$$

where $S_{(i,j)}$ is a unitary that swaps subsystems i and j leaving all the remaining systems untouched, i.e.,

$$S_{(i,j)}|a_0, a_1, a_2, \ldots a_i, \ldots a_j, \ldots\rangle = |a_0, a_1, a_2, \ldots a_j, \ldots a_i, \ldots\rangle. \tag{C23}$$

We apply this transformation to the state of the system ρ_S (which is treated as the zeroth subsystem) and m copies of the catalyst state $\eta_C^{\otimes m}$ (which are treated as the remaining m subsystems). Because of Lemma 4, we can always find a unitary V_{SCB_2}, which acts on SC and the corresponding part of the heat bath B_2 such that, after tracing out the bath, the action on SC is fully described by the channel in Eq. (32). With this in mind, we can write the error term $\nu(n)$ as

$$\nu(n) = \|(\mathcal{E}_C \otimes \mathcal{I}_{B_1})[\omega'_{CB_1}] - \omega'_{CB_1}\|_1 \tag{C24}$$

$$= \|(\mathcal{E}_C \otimes \mathcal{I}_{B_1})[\eta_C^{\otimes m} \otimes \tau_{B'_1}^{\otimes n} \otimes \tau_{B''_1}] - \eta_C^{\otimes m} \otimes \tau_{B'_1}^{\otimes n} \otimes \tau_{B''_1}\|_1 \tag{C25}$$

$$= \|\mathcal{E}_C[\eta_C^{\otimes m}] - \eta_C^{\otimes m}\|_1 \tag{C26}$$

$$= \|\mathrm{Tr}_{SB_2}[V_{SCB_2}(\rho_S \otimes \eta_C^{\otimes m} \otimes \tau_{B_2})V_{SCB_2}^\dagger] - \eta_C^{\otimes m}\|_1 \tag{C27}$$

$$= \|\mathrm{Tr}_S[\mathcal{T}_{SC}^{(\mathrm{mix})}[\rho_S \otimes \eta_C^{\otimes m}]] - \eta_C^{\otimes m}\|_1 \tag{C28}$$

$$\leq \|\mathcal{T}_{SC}^{(\mathrm{mix})}[\rho_S \otimes \eta_C^{\otimes m}] - \sigma_S \otimes \eta_C^{\otimes m}\|_1, \tag{C29}$$

where, in the second line, we used the explicit form of the state ω'_{CB_1} given in Eq. (C17) and, in the fourth line, we used the definition of the channel $\mathcal{E}_C$ from Eq. (C8). In the fifth line, we labeled the mixing channel induced by the unitary V_{SCB_2} with $\mathcal{T}_{SC}^{(\mathrm{mix})}$, i.e., $\mathcal{T}_{SC}^{(\mathrm{mix})}[\cdot] := \mathrm{Tr}_{B_2}[V_{SCB_2}((\cdot)_{SC} \otimes \tau_{B_2})V_{SCB_2}^\dagger]$. The last inequality follows from the fact that the trace distance is contractive when tracing out subsystems. Notice that, so far, we have not made the choice for the state η. As we will soon see, a good choice is to pick the state η to be precisely our target state on S, i.e., $\eta = \sigma$. In this way, the error term $\nu(n)$ becomes

$$\nu(n) \leq \|\mathcal{T}_{SC}^{(\mathrm{mix})}[\rho_S \otimes \sigma_C^{\otimes m}] - \sigma_S \otimes \sigma_C^{\otimes m}\|_1. \tag{C30}$$

In what follows, we label the subsystems that comprise the catalyst C with C_i for $i \in [1, m]$, i.e., $C = C_1 C_2 \ldots C_m$. To further upper bound $\nu(n)$, we need the following result adapted from Ref. [72]. Actually, we write the lemma in a more specialized form that better demonstrates its applicability to our particular problem.

Lemma 6. (Convex split, Ref. [72]). Let ρ and σ be two quantum states satisfying $\mathrm{supp}(\rho) \subseteq \mathrm{supp}(\sigma)$. Then, the following state,

$$\mathcal{T}_{SC}^{(\mathrm{mix})}[\rho_S \otimes \sigma_C^{\otimes m}] = \frac{1}{m}[\rho_S \otimes \sigma_{C_1} \otimes \ldots \otimes \sigma_{C_m} + \sigma_S \otimes \rho_{C_1} \otimes \ldots \otimes \sigma_{C_m} + \cdots + \sigma_S \otimes \sigma_{C_1} \otimes \ldots \otimes \rho_{C_m}], \tag{C31}$$

for large m is close to the state $\sigma_S \otimes \sigma_C^{\otimes m}$; that is, for all $m \geq 1$, the following holds:

$$\|\mathcal{T}_{SC}^{(\mathrm{mix})}[\rho_S \otimes \sigma_C^{\otimes m}] - \sigma_S \otimes \sigma_C^{\otimes m}\|_1 \leq \frac{1}{\sqrt{m}} \cdot 2^{\frac{1}{2}D_{\mathrm{max}}(\rho\|\sigma)}, \tag{C32}$$

where $D_{\mathrm{max}}(\rho\|\sigma) := \log \min\{\lambda | \rho \leq \lambda\sigma\}$ is the max-relative entropy.

Using the above lemma, we can readily bound the error term from Eq. (C30) as

$$\nu(n) \leq \frac{1}{\sqrt{m}} \cdot 2^{\frac{1}{2}D_{\mathrm{max}}(\rho\|\sigma)} \tag{C33}$$

$$= \sqrt{\frac{2^{D_{\mathrm{max}}(\rho\|\sigma)}}{r_n}} \cdot \frac{1}{\sqrt{n}} \tag{C34}$$

$$= c_n \cdot \frac{1}{\sqrt{n}}, \tag{C35}$$

where we used $m = n r_n$ and r_n is given in Eq. (B20). Notice that for fixed input and output states ρ and σ and for large n, the factor c_n is effectively constant. Hence, the error term $\nu(n)$, up to the leading order in n, scales with n as

$$\nu(n) \sim \frac{1}{\sqrt{n}}. \tag{C36}$$

Importantly, notice that we have not assumed anything special about the states ρ and σ [in fact, our only technical assumption is that $\mathrm{supp}(\rho) \subseteq \mathrm{supp}(\sigma)$, which can always be satisfied by considering arbitrarily small perturbations of the states]. Consequently, the two states are arbitrary, which is an embodiment of the fact that, in the embezzlement regime, partial order between states fully vanishes.

b. Genuine catalysis regime

We now move to the case when the partial order between states is fully retained, i.e., when the second laws of thermodynamics are satisfied by a pair of states ρ and σ. Recall that we are working with block-diagonal states, and hence, any such state can be expressed as a probability vector. Let us denote

$$\boldsymbol{p} := \mathrm{diag}[\rho_S], \qquad \boldsymbol{q} := \mathrm{diag}[\sigma_S], \qquad \boldsymbol{c} := \mathrm{diag}[\eta_C], \qquad \boldsymbol{g} := \mathrm{diag}[\tau_S]. \tag{C37}$$

By definition, $\boldsymbol{p}$, $\boldsymbol{q}$, and $\boldsymbol{g}$ are d_S-dimensional vectors, and $\boldsymbol{c}$ is a d_C-dimensional vector. Our only assumption in this section is that the states described by probability vectors $\boldsymbol{p}$ and $\boldsymbol{q}$ satisfy the second laws of thermodynamics, i.e.,

$$\forall \alpha \geq 0 \quad F_\alpha(\boldsymbol{p}, \boldsymbol{g}) \geq F_\alpha(\boldsymbol{q}, \boldsymbol{g}), \tag{C38}$$

where the generalized free energies are defined in Eq. (A4). Before we specify the state η_C and the channel $\mathcal{E}_C$, let us rephrase the conditions (C38) in a form that relates them with Renyi entropies.

The generalized free energies F_α can be connected with Renyi entropies H_α using the so-called embedding map introduced in Ref. [11]. Intuitively, the embedding map is an operation that allows us to translate between the microcanonical and macrocanonical descriptions of a thermodynamic system (see, e.g., Ref. [86]). For clarity, we also define it here.

Definition 1. [Embedding map]. The embedding map $\Gamma_{\boldsymbol{d}} : \mathbb{R}^n \to \mathbb{R}^D$ is a transformation between vectors such that for $\boldsymbol{x} = (x_1, x_2, \ldots, x_n)$, we have

$$\Gamma_{\boldsymbol{d}}(\boldsymbol{x}) := \left(\underbrace{\frac{x_1}{d_1}, \ldots, \frac{x_1}{d_1}}_{d_1 \text{ terms}}, \underbrace{\frac{x_2}{d_2}, \ldots, \frac{x_2}{d_2}}_{d_2 \text{ terms}}, \ldots, \underbrace{\frac{x_n}{d_n}, \ldots, \frac{x_n}{d_n}}_{d_n \text{ terms}} \right) = \bigoplus_{i=1}^n [x_i \cdot \boldsymbol{u}_i], \tag{C39}$$

where $\boldsymbol{d} = (d_1, d_2, \ldots, d_n)$ is a vector of natural numbers that sum to $D = \sum_{i=1}^n d_i$ and $\boldsymbol{u}_i := (1/i)(1, 1, \ldots, 1)$ is an i-dimensional uniform distribution.

We assume that the thermal state $\boldsymbol{g}$ is a vector with rational entries; i.e., there exists a collection of natural numbers $\{d_1, d_2, \ldots, d_{d_S}\}$ such that $D = \sum_{i=1}^{d_S} d_i$ and

$$\boldsymbol{g} := \left(\frac{d_1}{D}, \frac{d_2}{D}, \ldots, \frac{d_{d_S}}{D} \right). \tag{C40}$$

Taking the thermal state as in Eq. (C40) and applying the embedding map with $\boldsymbol{d} = (d_1, d_2, \ldots, d_{d_S})$ leads to

$$\Gamma_{\boldsymbol{d}}(\boldsymbol{g}) = \boldsymbol{u}_D, \tag{C41}$$

where $\boldsymbol{u}_D$ is the uniform distribution of dimension $D = \sum_{i=1}^{d_S} d_i$. As described in Ref. [11], the embedding map leads to the following relationship between the generalized free energies F_α and Renyi entropies H_α:

$$\log Z_S + \beta F_\alpha(\boldsymbol{x}, \boldsymbol{g}) = \log D - H_\alpha(\Gamma_{\boldsymbol{d}}(\boldsymbol{p})). \tag{C42}$$

In this way, the embedding map also allows us to rewrite the second laws purely in terms of the Renyi entropies. Denoting $\tilde{\boldsymbol{p}} := \Gamma_{\boldsymbol{d}}(\boldsymbol{p})$ and $\tilde{\boldsymbol{q}} := \Gamma_{\boldsymbol{d}}(\boldsymbol{q})$, the conditions in Eq. (C38) become

$$H_\alpha(\tilde{\boldsymbol{p}}) \leq H_\alpha(\tilde{\boldsymbol{q}}). \tag{C43}$$

The second laws expressed using Renyi entropies not only imply the existence of a state that catalyzes a given transformation. In fact, they also determine when multiple copies of one state can be converted into multiple copies of another state asymptotically. This relationship is captured by the following result from majorization theory adapted from Ref. [73] (Proposition 3.2.7):

Lemma 7. Let $\tilde{p}$ and $\tilde{q}$ be two probability distributions of dimension D such that

$$H_\alpha(\tilde{p}) < H_\alpha(\tilde{q}) \quad \forall \, \alpha \geq 0. \tag{C44}$$

Then, for sufficiently large k, the following holds:

$$\tilde{p}^{\otimes k} \succ \tilde{q}^{\otimes k}. \tag{C45}$$

Let us note that using the properties of the embedding map, it can be easily verified that Eq. (C45) can be equivalently written as

$$p^{\otimes k} \succ_{\mathrm{T}} q^{\otimes k}. \tag{C46}$$

Let us begin by showing that we can replace strict inequalities in the above Lemma with nonstrict ones. The argument proceeds similarly as in Ref. [11] (Appendix B, Proposition 3), and we repeat it here for convenience.

It is easy to see that when Eq. (C45) holds, then the nonstrict inequalities are satisfied. In order to prove the converse, suppose that the conditions (C44) hold for all $\alpha \geq 0$ but with nonstrict inequalities. Consider $q_\epsilon := (1 - \epsilon)q + \epsilon u$, with u being a uniform distribution. Since q_ϵ is more mixed than q, we have that $q \succ q_\epsilon$. Since Renyi entropies are (strictly) Schur-concave functions for any $\alpha > 0$ [9], we have that $H_\alpha(p) < H_\alpha(q_\epsilon)$. Therefore, for a sufficiently large k, we have that $p^{\otimes k} \succ q_\epsilon^{\otimes k}$. Now, since this holds for any $\epsilon \geq 0$ and the majorization relation is continuous with respect to probability distributions, we also have that $p^{\otimes k} \succ q^{\otimes k}$.

Let us now recall the definition of the Duan state $\omega_k^{\mathrm{D}}(\rho, \sigma)$ [74]. For convenience, we denote $z_k^{\mathrm{D}}(\tilde{p}, \tilde{q}) = \mathrm{diag}[\omega_k^{\mathrm{D}}(\rho, \sigma)]$, where

$$z_k^{\mathrm{D}}(\tilde{p}, \tilde{q}) := \frac{1}{k}[\tilde{p}^{\otimes k-1} \oplus (\tilde{p}^{\otimes k-2} \otimes \tilde{q}) \oplus (\tilde{p}^{\otimes k-3} \otimes \tilde{q}^{\otimes 2}) \oplus \dots \oplus (\tilde{p} \otimes \tilde{q}^{\otimes k-2}) \oplus \tilde{q}^{\otimes k-1}]. \tag{C47}$$

Then, as was shown in Refs. [74,75], the Duan state $z_k^{\mathrm{D}}(\tilde{p}, \tilde{q})$ is an exact catalyst for a transformation between states $\tilde{p}$ and $\tilde{q}$ if k copies of $\tilde{p}$ can be converted into k copies of $\tilde{q}$. In other words, if the condition (C45) is satisfied, then the following also holds:

$$\tilde{p} \otimes z_k^{\mathrm{D}}(\tilde{p}, \tilde{q}) \succ \tilde{q} \otimes z_k^{\mathrm{D}}(\tilde{p}, \tilde{q}). \tag{C48}$$

To see that the above equation holds, note that if Eq. (C45) is satisfied for some k, then we also have

$$\tilde{p} \otimes z_k^{\mathrm{D}}(\tilde{p}, \tilde{q}) = \frac{1}{k}[\tilde{p}^{\otimes k} \oplus (\tilde{p}^{\otimes k-1} \otimes \tilde{q}) \oplus (\tilde{p}^{\otimes k-2} \otimes \tilde{q}^{\otimes 2}) \oplus \dots \oplus (\tilde{p}^{\otimes 2} \otimes \tilde{q}^{\otimes k-2}) \oplus (\tilde{p} \otimes \tilde{q}^{\otimes k-1})] \tag{C49}$$

$$\succ \frac{1}{k}[\tilde{q}^{\otimes k} \oplus (\tilde{p}^{\otimes k-1} \otimes \tilde{q}) \oplus (\tilde{p}^{\otimes k-2} \otimes \tilde{q}^{\otimes 2}) \oplus \dots \oplus (\tilde{p}^{\otimes 2} \otimes \tilde{q}^{\otimes k-2}) \oplus (\tilde{p} \otimes \tilde{q}^{\otimes k-1})] \tag{C50}$$

$$= \tilde{q} \otimes z_k^{\mathrm{D}}(\tilde{p}, \tilde{q}). \tag{C51}$$

Hence, if the second laws are satisfied, there exists large enough k such that k copies of $\tilde{p}$ can be converted into k copies of $\tilde{q}$. On the other hand, this means that there exists a special catalyst (the Duan state) that can catalyze the transformation from $\tilde{p}$ to $\tilde{q}$ *without* any disturbance. In this way, we obtain the following theorem:

Theorem 4. Let p and q be two probability distributions of dimension d_S such that

$$F_\alpha(p,g) \geq F_\alpha(q,g) \quad \forall\ \alpha \geq 0. \tag{C52}$$

Then, for sufficiently large k, the following holds:

$$p \otimes z_k^D(p,q) \succ_T q \otimes z_k^D(p,q), \tag{C53}$$

where $z_k^D(p,q)$ is the Duan state defined in Eq. (C47).

We can now return to our main protocol. We choose the Duan state corresponding to p and q as the intermediate state, i.e.,

$$\eta_C = \omega_k^D(\rho,\sigma). \tag{C54}$$

In fact, we only need one copy of the state η_C to transform ρ_S into σ_S, so we choose $m = 1$. In order to specify the intermediate transformation $\mathcal{E}_C$, let us recall that it is fully specified by the unitary V_{SCB_2} and defined as

$$\mathcal{E}_C := \mathrm{Tr}_{SB_2}[V_{SCB_2}(\rho_S \otimes \eta_C^{\otimes m} \otimes \tau_{B_2})V_{SCB_2}^\dagger] \tag{C55}$$

$$= \mathcal{T}_{SC}^{(\mathrm{cat})}[\rho_S \otimes \eta_C^{\otimes m}], \tag{C56}$$

where we labeled the thermal operation induced by the unitary V_{SCB_2} with

$$\mathcal{T}_{SC}^{(\mathrm{cat})}[\cdot] := \mathrm{Tr}_{B_2}[V_{SCB_2}((\cdot)_{SC} \otimes \tau_{B_2})V_{SCB_2}^\dagger]. \tag{C57}$$

Theorem 4 ensures us that for η as chosen in Eq. (C54) and $m \geq 1$, the state $\rho_S \otimes \eta_C$ thermo-majorizes the state $\sigma_S \otimes \eta_C$. Because of the fundamental result of Ref. [22], this also means that there exists a thermal operation connecting these two states; hence, we choose $\mathcal{T}_{SC}^{(\mathrm{cat})}$ to be precisely this transformation. As as a result, we have

$$\mathcal{T}_{SC}^{(\mathrm{cat})}[\rho_S \otimes \omega_k^D(\rho_S,\sigma_S)] = \sigma_S \otimes \omega_k^D(\rho,\sigma). \tag{C58}$$

Notice that even though we chose the transformation $\mathcal{T}_{SC}^{(\mathrm{cat})}$ implicitly, it can still be constructed using the methods described, e.g., in Ref. [87] (p. 29, below Lemma 7; see also the references therein), i.e., by finding an appropriate Gibbs-stochastic matrix and then using the methods described in the proof of Lemma 4 to construct a permutation unitary that leads to the desired thermal operation.

Importantly, the catalytic transformation from Eq. (C58) is exact; i.e., it does not induce any new error on the system nor on the catalyst. As a result, the error term $\nu(n)$ vanishes:

$$\nu(n) \leq \|\mathcal{T}_{SC}^{(\mathrm{cat})}[\rho_S \otimes \omega_k^D(\rho,\sigma)] - \sigma_S \otimes \omega_k^D(\rho,\sigma)\|_1 \tag{C59}$$

$$= 0, \tag{C60}$$

so the only error on the catalyst system is due to the preprocessing and postprocessing steps of the main protocol (C16).

APPENDIX D: NUMERICAL ANALYSIS FOR HIGHER-DIMENSIONAL SYSTEMS

In this section, we present the results of a supplementary numerical computation that provides further evidence that catalytic universality is a generic phenomenon. In particular, we compute the fraction $f(p)$ from Sec. IV C for different dimensions of the system d_S and different choices of the error parameter μ and threshold value γ_{thld}. The results are presented in Fig. 7.
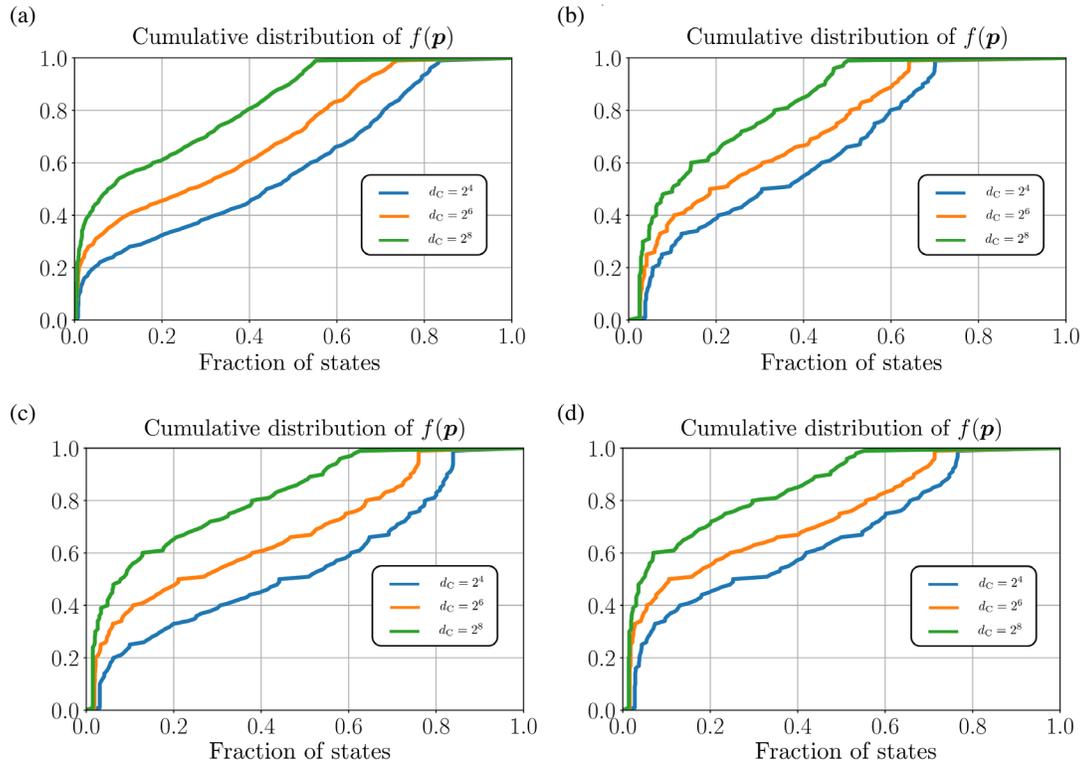
FIG. 7. Cumulative distribution of $f(\boldsymbol{p})$ for different choices of parameters: (a) $[d_S = 4, \mu = 0.05, \gamma_{\text{thld}} = 0.9]$, (b) $[d_S = 5, \mu = 0.05, \gamma_{\text{thld}} = 0.9]$, (c) $[d_S = 4, \mu = 0.1, \gamma_{\text{thld}} = 0.8]$, and (d) $[d_S = 5, \mu = 0.1, \gamma_{\text{thld}} = 0.8]$.

[1] J. V. Koski, V. F. Maisi, T. Sagawa, and J. P. Pekola, *Experimental Observation of the Role of Mutual Information in the Nonequilibrium Dynamics of a Maxwell Demon*, Phys. Rev. Lett. **113**, 030601 (2014).

[2] J. V. Koski, A. Kutvonen, I. M. Khaymovich, T. Ala-Nissila, and J. P. Pekola, *On-Chip Maxwell's Demon as an Information-Powered Refrigerator*, Phys. Rev. Lett. **115**, 260602 (2015).

[3] K. Chida, S. Desai, K. Nishiguchi, and A. Fujiwara, *Power Generator Driven by Maxwell's Demon*, Nat. Commun. **8**, 15310 (2017).

[4] P. A. Camati, J. P. S. Peterson, T. B. Batalhão, K. Micadei, A. M. Souza, R. S. Sarthour, I. S. Oliveira, and R. M. Serra, *Experimental Rectification of Entropy Production by Maxwell's Demon in a Quantum System*, Phys. Rev. Lett. **117**, 240502 (2016).

[5] J. P. S. Peterson, R. S. Sarthour, A. M. Souza, I. S. Oliveira, J. Goold, K. Modi, D. O. Soares-Pinto and L. C. Céleri, *Experimental Demonstration of Information to Energy Conversion in a Quantum System at the Landauer Limit*, Proc. R. Soc. A **472**, 20150813 (2016).

[6] G. L. Zanin, T. Häffner, M. A. A. Talarico, E. I. Duzzioni, P. H. S. Ribeiro, G. T. Landi, and L. C. Céleri, *Experimental Quantum Thermodynamics with Linear Optics*, arXiv:1905.02829.

[7] C. E. Shannon, *A Mathematical Theory of Communication*, Bell Syst. Tech. J. **27**, 379 (1948).

[8] E. Ruch and A. Mead, *The Principle of Increasing Mixing Character and Some of Its Consequences*, Theor. Chim. Acta **41**, 95 (1976).

[9] A. W. Marshall, I. Olkin, and B. C. Arnold, *Inequalities: Theory of Majorization and Its Applications*, 2nd ed. (Springer, New York, 2011), Vol. 143.

[10] D. Janzing, P. Wocjan, R. Zeier, R. Geiss, and T. Beth, *Thermodynamic Cost of Reliability and Low Temperatures: Tightening Landauer's Principle and the Second Law*, Int. J. Theor. Phys. **39**, 2717 (2000).

[11] F. Brandão, M. Horodecki, N. Ng, J. Oppenheim, and S. Wehner, *The Second Laws of Quantum Thermodynamics*, Proc. Natl. Acad. Sci. U.S.A. **112**, 3275 (2015).

[12] A. Rényi, *On Measures of Entropy and Information*, in *Proceedings of the Fourth Berkeley Symposium on Mathematical Statistics and Probability, Volume 1: Contributions to the Theory of Statistics* (University of California Press, Berkeley, California, 1961), pp. 547–561.

[13] D. Jonathan and M. B. Plenio, *Entanglement-Assisted Local Manipulation of Pure Quantum States*, Phys. Rev. Lett. **83**, 3566 (1999).

[14] M. Horodecki and J. Oppenheim, *(Quantumness in the context of) resource theories*, Int. J. Mod. Phys. B **27**, 1345019 (2013).

[15] E. Chitambar and G. Gour, *Quantum Resource Theories*, Rev. Mod. Phys. **91**, 025001 (2019).

[16] M. A. Nielsen, *Conditions for a Class of Entanglement Transformations*, Phys. Rev. Lett. **83,** 436 (1999).

[17] G. Vidal and R. Tarrach, *Robustness of Entanglement*, Phys. Rev. A **59,** 141 (1999).

[18] S. Du, Z. Bai, and Y. Guo, *Conditions for Coherence Transformations under Incoherent Operations*, Phys. Rev. A **91,** 052120 (2015).

[19] M. Horodecki, P. W. Shor, and M. B. Ruskai, *Entanglement Breaking Channels*, Rev. Math. Phys. **15,** 629 (2003).

[20] A. Streltsov, H. Kampermann, S. Wölk, M. Gessner, and D. Bruß, *Maximal Coherence and the Resource Theory of Purity*, New J. Phys. **20,** 053058 (2018).

[21] F. G. S. L. Brandão, M. Horodecki, J. Oppenheim, J. M. Renes, and R. W. Spekkens, *Resource Theory of Quantum States out of Thermal Equilibrium*, Phys. Rev. Lett. **111,** 250404 (2013).

[22] M. Horodecki and J. Oppenheim, *Fundamental Limitations for Quantum and Nanoscale Thermodynamics*, Nat. Commun. **4,** 2059 (2013).

[23] N. H. Y. Ng and M. P. Woods, *Resource Theory of Quantum Thermodynamics: Thermal Operations and Second Laws*, Thermodynamics in the Quantum Regime: Fundamental Aspects and New Directions, edited by F. Binder, L. A. Correa, C. Gogolin, J. Anders, and G. Adesso (Springer International Publishing, Cham, 2018), pp. 625–650, https://doi.org/10.1007/978-3-319-99046-0_26.

[24] K. Horodecki, A. Grudka, P. Joshi, W. Kłobus, and J. Łodyga, *Axiomatic Approach to Contextuality and Non-locality*, Phys. Rev. A **92,** 032104 (2015).

[25] D. Cavalcanti and P. Skrzypczyk, *Quantitative Relations between Measurement Incompatibility, Quantum Steering, and Nonlocality*, Phys. Rev. A **93,** 052112 (2016).

[26] M. Piani, M. Cianciaruso, T. R. Bromley, C. Napoli, N. Johnston, and G. Adesso, *Robustness of Asymmetry and Coherence of Quantum States*, Phys. Rev. A **93,** 042107 (2016).

[27] F. Buscemi, E. Chitambar, and W. Zhou, *Complete Resource Theory of Quantum Incompatibility as Quantum Programmability*, Phys. Rev. Lett. **124,** 120401 (2020).

[28] I. Šupić, P. Skrzypczyk, and D. Cavalcanti, *Methods to Estimate Entanglement in Teleportation Experiments*, Phys. Rev. A **99,** 032334 (2019).

[29] D. Cavalcanti, P. Skrzypczyk, and I. Šupić, *All Entangled States Can Demonstrate Nonclassical Teleportation*, Phys. Rev. Lett. **119,** 110501 (2017).

[30] M. Howard and E. Campbell, *Application of a Resource Theory for Magic States to Fault-Tolerant Quantum Computing*, Phys. Rev. Lett. **118,** 090501 (2017).

[31] S. Bhattacharya, B. Bhattacharya, and A. S. Majumdar, *Convex Resource Theory of Non-Markovianity*, J. Phys. A **54,** 035302 (2021).

[32] E. Wakakuwa, *Operational Resource Theory of Non-Markovianity*, arXiv:1709.07248.

[33] C. H. Bennett, H. J. Bernstein, S. Popescu, and B. Schumacher, *Concentrating Partial Entanglement by Local Operations*, Phys. Rev. A **53,** 2046 (1996).

[34] W. Kumagai and M. Hayashi, *Second-Order Asymptotics of Conversions of Distributions and Entangled States Based on Rayleigh-Normal Probability Distributions*, IEEE Trans. Inf. Theory **63,** 1829 (2016).

[35] C. Napoli, T. R. Bromley, M. Cianciaruso, M. Piani, N. Johnston, and G. Adesso, *Robustness of Coherence: An Operational and Observable Measure of Quantum Coherence*, Phys. Rev. Lett. **116,** 150502 (2016).

[36] H. Zhu, Z. Ma, Z. Cao, S.-M. Fei, and V. Vedral, *Operational One-to-One Mapping between Coherence and Entanglement Measures*, Phys. Rev. A **96,** 032316 (2017).

[37] E. Chitambar and G. Gour, *Comparison of Incoherent Operations and Measures of Coherence*, Phys. Rev. A **94,** 052336 (2016).

[38] G. Gour, M. P. Müller, V. Narasimhachar, R. W. Spekkens, and N. Y. Halpern, *The Resource Theory of Informational Nonequilibrium in Thermodynamics*, Phys. Rep. **583,** 1 (2015).

[39] A. Streltsov, H. Kampermann, S. Wölk, M. Gessner, and D. Bruß, *Maximal Coherence and the Resource Theory of Purity*, New J. Phys. **20,** 053058 (2018).

[40] F. Ding, X. Hu, and H. Fan, *Amplifying Asymmetry with Correlated Catalysts*, arXiv:2007.06247.

[41] F. G. S. L. Brandão, M. Horodecki, J. Oppenheim, J. M. Renes, and R. W. Spekkens, *Resource Theory of Quantum States out of Thermal Equilibrium*, Phys. Rev. Lett. **111,** 250404 (2013).

[42] W. van Dam and P. Hayden, *Universal Entanglement Transformations without Communication*, Phys. Rev. A **67,** 060302 (2003).

[43] N. H. Y. Ng, L. Mančinska, C. Cirstoiu, J. Eisert, and S. Wehner, *Limits to Catalysis in Quantum Thermodynamics*, New J. Phys. **17,** 085004 (2015).

[44] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information: 10th Anniversary Edition*, 10th ed. (Cambridge University Press, USA, 2011).

[45] F. G. S. L. Brandão and G. Gour, *Reversible Framework for Quantum Resource Theories*, Phys. Rev. Lett. **115,** 070503 (2015).

[46] C. Perry, P. Ćwikliński, J. Anders, M. Horodecki, and J. Oppenheim, *A Sufficient Set of Experimentally Implementable Thermal Operations for Small Systems*, Phys. Rev. X **8,** 041049 (2018).

[47] J. G. Richens, A. M. Alhambra, and L. Masanes, *Finite-Bath Corrections to the Second Law of Thermodynamics*, Phys. Rev. E **97,** 062132 (2018).

[48] M. Lostaglio, *The Resource Theory of Quantum Thermodynamics* (Imperial College London, London, 2016).

[49] C. Perry, P. Ćwikliński, J. Anders, M. Horodecki, and J. Oppenheim, *A Sufficient Set of Experimentally Implementable Thermal Operations for Small Systems*, Phys. Rev. X **8,** 041049 (2018).

[50] P. Faist, J. Oppenheim, and R. Renner, *Gibbs-Preserving Maps Outperform Thermal Operations in the Quantum Regime*, New J. Phys. **17,** 043003 (2015).

[51] L. Masanes and J. Oppenheim, *A General Derivation and Quantification of the Third Law of Thermodynamics*, Nat. Commun. **8,** 14538 (2017).

[52] M. Lostaglio, K. Korzekwa, D. Jennings, and T. Rudolph, *Quantum Coherence, Time-Translation Symmetry, and Thermodynamics*, Phys. Rev. X **5,** 021001 (2015).

[53] K. Korzekwa, M. Lostaglio, J. Oppenheim, and D. Jennings, *The Extraction of Work from Quantum Coherence*, New J. Phys. **18,** 023045 (2016).

[54] F. Brandao, M. Horodecki, N. Ng, J. Oppenheim, and S. Wehner, *The Second Laws of Quantum Thermodynamics*, Proc. Natl. Acad. Sci. U.S.A. **112**, 3275 (2015).

[55] H. Kwon, H. Jeong, D. Jennings, B. Yadin, and M. S. Kim, *Clock-Work Trade-off Relation for Coherence in Quantum Thermodynamics*, Phys. Rev. Lett. **120**, 150602 (2018).

[56] M. P. Müller, *Correlating Thermal Machines and the Second Law at the Nanoscale*, Phys. Rev. X **8**, 041051 (2018).

[57] M. Łobejko, P. Mazurek, and M. Horodecki, *Thermodynamics of Minimal Coupling Quantum Heat Engines*, Quantum **4**, 375 (2020).

[58] F. Binder, L. A. Correa, C. Gogolin, J. Anders, and G. Adesso, *Thermodynamics in the Quantum Regime*, *Fundamental Theories of Physics* (Springer, New York, 2018).

[59] J. Goold, M. Huber, A. Riera, L. del Rio, and P. Skrzypczyk, *The Role of Quantum Information in Thermodynamics—A Topical Review*, J. Phys. A **49**, 143001 (2016).

[60] S. Vinjanampathy and J. Anders, *Quantum Thermodynamics*, Contemp. Phys. **57**, 545 (2016).

[61] M. Lostaglio, *An Introductory Review of the Resource Theory Approach to Thermodynamics*, Rep. Prog. Phys. **82**, 114001 (2019).

[62] Without these two technical assumptions, the precise form of the second laws should read $\forall \alpha \in \mathbb{R} F_\alpha(\rho_S, \tau_S) > F_\alpha(\sigma_S, \tau_S)$.

[63] M. Müller-Lennert, F. Dupuis, O. Szehr, S. Fehr, and M. Tomamichel, *On Quantum Rényi Entropies: A New Generalization and Some Properties*, J. Math. Phys. (N.Y.) **54**, 122203 (2013).

[64] T. M. Cover and J. A. Thomas, *Elements of Information Theory (Wiley Series in Telecommunications and Signal Processing)* (Wiley-Interscience, New York, 2006).

[65] B. Schumacher, *Quantum Coding*, Phys. Rev. A **51**, 2738 (1995).

[66] C. T. Chubb, M. Tomamichel, and K. Korzekwa, *Moderate Deviation Analysis of Majorization-Based Resource Interconversion*, Phys. Rev. A **99**, 032332 (2019).

[67] D. Leung, B. Toner, and J. Watrous, *Coherent State Exchange in Multi-Prover Quantum Interactive Proof Systems*, arXiv:0804.4118.

[68] I. Dinur, D. Steurer, and T. Vidick, *A Parallel Repetition Theorem for Entangled Projection Games*, arXiv:1310.4113.

[69] M. Berta, M. Christandl, and R. Renner, *The Quantum Reverse Shannon Theorem Based on One-Shot Information Theory*, Commun. Math. Phys. **306**, 579 (2011).

[70] C. H. Bennett, I. Devetak, A. W. Harrow, P. W. Shor, and A. Winter, *The Quantum Reverse Shannon Theorem and Resource Tradeoffs for Simulating Quantum Channels*, IEEE Trans. Inf. Theory **60**, 2926 (2014).

[71] D. Leung and B. Wang, *Characteristics of Universal Embezzling Families*, Phys. Rev. A **90**, 042331 (2014).

[72] A. Anshu, V. K. Devabathini, and R. Jain, *Quantum Communication Using Coherent Rejection Sampling*, Phys. Rev. Lett. **119**, 120506 (2017).

[73] A. K. Jensen, *Asymptotic Majorization of Finite Probability Distributions*, IEEE Trans. Inf. Theory **65**, 8131 (2019).

[74] R. Duan, Y. Feng, X. Li, and M. Ying, *Trade-off between Multiple-Copy Transformation and Entanglement Catalysis*, Phys. Rev. A **71**, 062306 (2005).

[75] Y. Feng, R. Duan, and M. Ying, *Relation between Catalyst-Assisted Transformation and Multiple-Copy Transformation for Bipartite Pure States*, Phys. Rev. A **74**, 042312 (2006).

[76] M. Lostaglio and M. P. Mueller, *Coherence and Asymmetry Cannot Be Broadcast*, Phys. Rev. Lett. **123**, 020403 (2019).

[77] Y. R. Sanders and G. Gour, *Necessary Conditions for Entanglement Catalysts*, Phys. Rev. A **79**, 054302 (2009).

[78] MATLAB code at github.com/patryk-lb (2020).

[79] M. Horodecki, J. Oppenheim, and C. Sparaciari, *Extremal Distributions under Approximate Majorization*, J. Phys. A **51**, 305301 (2018).

[80] S. Turgut, *Catalytic Transformations for Bipartite Pure States*, J. Phys. A **40**, 12185 (2007).

[81] S. Daftuar and M. Klimesh, *Mathematical Structure of Entanglement Catalysis*, Phys. Rev. A **64**, 042314 (2001).

[82] It is worth noting that the transformations that we consider here are always deterministic, and the probability $p_{\text{succ}}(\epsilon_C)$ refers to the sampled catalysts, i.e., how probable it is to *deterministically* catalyze a given transformation using a catalyst drawn at random.

[83] M. Lostaglio, D. Jennings, and T. Rudolph, *Description of Quantum Coherence in Thermodynamic Processes Requires Constraints beyond Free Energy*, Nat. Commun. **6**, 6383 (2015).

[84] K. Korzekwa, C. T. Chubb, and M. Tomamichel, *Avoiding Irreversibility: Engineering Resonant Conversions of Quantum Resources*, Phys. Rev. Lett. **122**, 110403 (2019).

[85] D. Schmid, T. C. Fraser, R. Kunjwal, A. B. Sainz, E. Wolfe, and R. W. Spekkens, *Why Standard Entanglement Theory Is Inappropriate for the Study of Bell Scenarios*, arXiv:2004.09194.

[86] D. Egloff, O. C. O. Dahlsten, R. Renner, and V. Vedral, *A Measure of Majorization Emerging from Single-Shot Statistical Mechanics*, New J. Phys. **17**, 073001 (2015).

[87] J. M. Renes, *Relative Submajorization and Its Use in Quantum Resource Theories*, J. Math. Phys. (N.Y.) **57**, 122202 (2016).