Efficient quantum work reservoirs at the nanoscale

Jinghao Lyu,[1,*] Alexander B. Boyd,[2,†] and James P. Crutchfield[1,‡]

[1]*Complexity Sciences Center and Department of Physics and Astronomy,*
University of California, Davis, 1 Shields Avenue, Davis, California 95616, USA
[2]*School of Physics, Trinity College Dublin, College Green, Dublin 2, Ireland*

When reformulated as a resource theory, thermodynamics can analyze system behaviors in the single-shot regime. In this, the work required to implement state transitions is bounded by α-Rényi divergences and so differs in identifying efficient operations compared to stochastic thermodynamics. Thus, a detailed understanding of the difference between stochastic and resource-theoretic thermodynamics is needed. To this end, we explore reversibility in the single-shot regime, generalizing the two-level work reservoirs used there to multilevel work reservoirs. This achieves reversibility in any transition in the single-shot regime. Building on this, we systematically develop multilevel work reservoirs in the nondissipation regime with and without catalysts. The resource-theoretic results show that two-level work reservoirs undershoot Landauer's bound, misleadingly implying energy dissipation during computation. In contrast, we demonstrate that multilevel work reservoirs achieve Landauer's bound while producing arbitrarily low entropy.

I. INTRODUCTION

The second law of thermodynamics states that the total entropy of a system and its surrounding environment increases when undergoing a transformation—the entropy production of any thermodynamic transformation is nonnegative [1]. This places strong resource bounds on computations performed by a Hamiltonian system coupled to a single thermal bath at temperature T. Specifically, the work that can be extracted in transforming a system between potentially nonequilibrium states (from ρ to ρ') is bounded above by the reduction in nonequilibrium free energy [2–4]:

$$\langle W \rangle_{\max} = F(\rho) - F(\rho')$$
$$= k_B T [D_1(\rho||\tau) - D_1(\rho'||\tau)]. \tag{1}$$

Here, k_B is Boltzmann's constant, $F(\rho) = \text{Tr}(\rho H) - TS(\rho)$ is the nonequilibrium free energy with $S(\rho) \equiv -\text{Tr}[\rho \log \rho]$ the von Neumann entropy, $D_1(\rho||\tau) \equiv \text{Tr}[\rho \log \rho - \rho \log \tau]$ is the relative entropy between ρ and τ, and τ is the Gibbs state with Hamiltonian H. Throughout this work, log represents the natural logarithm. This result is a general expression of Landauer's principle, which relates information processing to the energy requirements for a computation [5].

From the perspective of thermodynamic control, we can achieve Landauer's bound on work [6] by evolving the system under a time-dependent Hamiltonian $H_S(t)$, while maintaining weak coupling to a thermal reservoir [7]. However, the resulting unitary operator from this Hamiltonian control does not necessarily preserve the total energy of the thermal bath and

the system. Rather, the extracted work is the negative total-energy difference of the system and bath together [8]. Stochastic thermodynamics addresses work production as the result of external control, without explicitly describing the battery that stores the harvested work energy. This begs the question: What are the thermodynamic limits when accounting for the dynamics of the battery that drives a state transition forward? This requires a more detailed accounting of resources.

Recently, thermodynamics was reformulated as a resource theory—alternately called single-shot thermodynamics, resource theory of athermality, or simply nanoscale thermodynamics [9–13]. In resource theory, work must be stored in specific subsystems that we refer to as *work reservoirs* and that function as batteries to power state transitions. In parallel to thermal reservoirs, a work reservoir is defined by a specific relationship between its energy and entropy: a change in energy corresponds to zero entropy change. External control cannot violate energy conservation. That is, the unitary evolution of bath, system, and work reservoir together must commute with the joint free Hamiltonian.

Typically, a work reservoir is a two-level quantum system and the corresponding work is called *deterministic work* [12]. The work reservoir starts in one pure state at the beginning and ends in another pure state. The work is defined as the energy gap between those two levels. The deterministic work that can be extracted from the state transition $\rho \to \tau$ is [12]

$$W_{\text{one-shot}}^{\text{ext}} = k_B T D_0(\rho||\tau), \tag{2}$$

where $D_\alpha(\rho||\tau) \equiv \frac{1}{\alpha-1} \log \text{Tr}[\rho^\alpha \tau^{1-\alpha}]$ is the Rényi α divergence between state ρ and τ [14].

This work extraction result differs from the bound set by the second law of thermodynamics in Eq. (1), which would yield the result $D_1(\rho||\tau)$. Recall that $\alpha = 0$ Rényi divergence vanishes when both ρ and σ have full rank. So in the

*Contact author: jolyu@ucdavis.edu
†Contact author: alboyd@tcd.ie
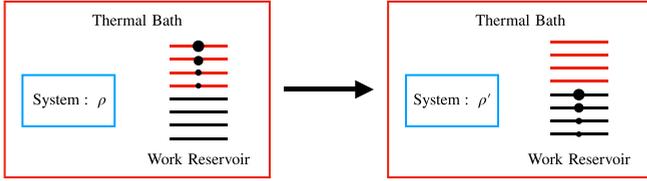‡Contact author: chaos@ucdavis.edu

FIG. 1. State transitions with multilevel work reservoirs rather than two-level work reservoirs. We show that for any transition $\rho \rightarrow \rho'$, there is a multilevel work reservoir such that the dissipation can be arbitrarily small

deterministic work setup, if we have a full rank state ρ, there is no work we can extract from it.

However, there is a connection between these two work values. The thermodynamic bound is recovered by considering many copies of ρ and tolerating error ϵ. If we loosen the requirement such that the final state can be ϵ close to the copies of thermal states, the work can be described by the smoothed version of $\alpha = 0$ Rényi divergence [12,15]:

$$\lim_{\epsilon \to 0} \lim_{n \to \infty} \frac{1}{n} D_0^{(\epsilon)}(\rho^{\otimes n} || \tau^{\otimes n}) = D_1(\rho || \tau). \quad (3)$$

We expect this since the classical thermodynamic result is supposed to be correct for a large ensemble of identical systems. Since the Rényi divergence is nondecreasing as a function of order α [16], we have

$$\begin{aligned} W_{\text{one-shot}}^{\text{ext}} &= k_B T D_0(\rho \| \tau) \\ &\leqslant k_B T D_1(\rho \| \tau). \end{aligned} \quad (4)$$

That is, the resource-theoretic bound on work extractable from state ρ is tighter than Landauer's bound of stochastic thermodynamics.

The two-level constraint also leads to tighter bounds in state formation. The deterministic work to form system state ρ in single-shot thermodynamics is [12]

$$W_{\text{one-shot}}^{\text{form}} = -k_B T D_\infty(\rho || \tau). \quad (5)$$

Here, the minus sign indicates that work must be supplied to form the state ρ. Similar to extraction, one-shot analysis puts a tighter bound on state formation than Landauer's bound:

$$\begin{aligned} W_{\text{one-shot}}^{\text{form}} &= -k_B T D_\infty(\rho || \tau) \\ &\leqslant -k_B T D_1(\rho || \tau). \end{aligned} \quad (6)$$

In some cases, $W_{\text{one-shot}}^{\text{form}}$ and $W_{\text{one-shot}}^{\text{ext}}$ equal the average results from thermodynamics. Landauer's bound on erasure [5] and the energy that can be stored in a work reservoir by randomizing a pure bit are both $k_B T \log 2$ [17]. However, resource-theoretic results, such as in Eqs. (2) and (5) with two-level work reservoirs, usually undershoot Landauer's bound [18]. Energy must be dissipated during state transitions [19–24].

The following establishes that the disparity arises from assuming that work is stored in a two-level system. We show how to approach the thermodynamic limit of Landauer's bound in nanoscale thermodynamics by abandoning two-level work reservoirs. When using multilevel work reservoirs as shown in Fig. 1, thermodynamically efficient state transformations are directly implementable.

Our development is organized as follows. Section II sets up the basic framework. Section III reviews the definition of entropy production at both the macroscopic scale and the nanoscale and gives an equivalent condition of approaching zero dissipation at the nanoscale. Section IV generalizes the two-level work reservoirs typically employed in nanoscale thermodynamics. It gives an explicit construction for a multilevel work reservoir that can be used to approach zero entropy production for any state transition. Section V goes on to study efficient work reservoirs in the presence of catalysts and introduces an alternative way to describe almost-nondissipation scenarios.

II. FRAMEWORK

The total system consists of system S, work reservoir W, and thermal bath B with Hamiltonians H_S, H_W, and H_B, respectively. Initially, they are uncorrelated. The initial state is $\rho_{SWB} = \rho_S \otimes \rho_W \otimes \tau_B$, where τ_B is the Gibbs state of the thermal bath at temperature T. The three subsystems interact via Hamiltonian H_{int}. They evolve by the unitary operator $U = \text{T} \exp(-\frac{i}{\hbar} \int H dt)$, where T is the time-ordering operator and H is the total Hamiltonian $H = H_S + H_B + H_W + H_{\text{int}}$. In thermodynamics, there is often no need to include a work reservoir and U does not preserve total energy in general. In resource theory, though, we specify that $[U, H_S + H_B + H_W] = 0$—strict energy conservation. The final state is given by $\rho'_{SWB} = U \rho_{SWB} U^\dagger$.

Here, we focus on states that are incoherent in energy. Since incoherent states are diagonal in the energy eigenstates, we identify a quantum state ρ with the vector $\boldsymbol{p}$ of its eigenvalues, a Hamiltonian H with its energy levels $\boldsymbol{E}$, and the eigenstates of Hamiltonian H with a classical set $\mathcal{S} = \{1, 2, \dots\}$. Throughout, greek letter ρ denotes a state, bold $\boldsymbol{p}$ denotes a probability distribution, and $p_i/(\boldsymbol{p})_i$ denotes the ith component in the latter. τ denotes the Gibbs state and $\boldsymbol{\tau}$ denotes the corresponding distribution. Subscripted notation $(\cdot)_S$ or $(\cdot)_B$ refers to the system or the thermal bath, respectively, while $(\cdot)_{SW}$ denotes the joint distribution of the system and the work reservoir. Notation without subscripts refers to a general state. Primed notation $(\cdot)'$ refers to a final state.

III. APPROACH TO ZERO ENTROPY PRODUCTION AND WORK BOUNDS

This section reviews the bounds mentioned above and entropy production in single-shot thermodynamics.

Thermodynamic entropy production Σ is defined as [25,26]

$$\Sigma = \Delta S_S + \frac{Q}{T}, \quad (7)$$

where ΔS_S is the system's entropy change and Q is the amount of heat transferred from the system to the thermal bath.

We assume that the system and bath are initially uncorrelated and the bath is in equilibrium, such that $\rho_{SB} = \rho_S \otimes \tau_B$. The global unitary operator U acts on the system and bath to extract work. Using Klein's inequality—$\text{Tr}(\rho \log \rho) \geqslant \text{Tr}(\rho \log \sigma)$—we can show that the entropy production Σ is nonnegative [27]. Define the missing energy of the total
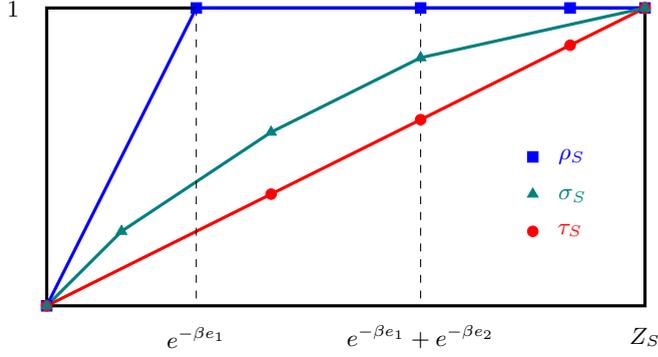
FIG. 2. Thermomajorization curves of states: We show thermo-majorization curves of three states ρ_S, σ_S, and τ_S. ρ_S is a pure state, σ_S a general state, and τ_S the Gibbs state. Applying the criterion, we can have transitions $\rho_S \to \sigma_S/\tau_S$ and $\sigma_S \to \tau_S$ under thermal operations.

system as work production $W = -Q - \Delta U_S$, where ΔU_S is the system's energy change, and rewrite Eq. (7) as

$$\Sigma = \frac{1}{T}(T\Delta S_S - \Delta U_S - W) \geqslant 0. \qquad (8)$$

This gives the familiar thermodynamic bound $W \leqslant -\Delta F_S$, where $\Delta F_S = \Delta U_S - T\Delta S_S$. The equal sign holds if and only if the entropy production vanishes.

Resource theory limits thermodynamic evolution to unitary operators U that commute with the total free Hamiltonian. So, there can be no "missing energy": $-Q - \Delta U_S = 0$. Such operations on the system are called *thermal operations*.

Without work input, the constraint on state transitions is *thermomajorization* [12,28]. That is, to transition from ρ_S to ρ_S', ρ_S must *thermomajorize* ρ_S'. There is a geometric way to determine this condition: thermomajorization *curves* reveal whether a state ρ_S thermomajorizes ρ_S' [12].

For any state ρ, the thermomajorization curve is constructed as follows. Suppose the eigenvalues of ρ are $\boldsymbol{p} = \{p_i\}_{i \in \mathcal{S}}$ and the corresponding energy levels are $\boldsymbol{E} = \{e_i\}_{i \in \mathcal{S}}$. We first rank $\{p_i\}_{i=1}^n$ in descending order of $p_i e^{\beta e_i}$. This is called β *order*. The thermomajorization curve of state ρ is formed by connecting points

$$(0,0) \text{ and } \left(\sum_{i=1}^{k} e^{-\beta e_i^\downarrow}, \sum_{i=1}^{k} p_i^\downarrow \right)_{k=1}^{n} \qquad (9)$$

piecewise linearly where $\downarrow$ means that p_i and e_i have been β ordered. The thermomajorization curve of state ρ is a monotonic concave-down curve $f_{\boldsymbol{p}, \boldsymbol{E}}(x)$ that interpolates between $(x, f(x)) = (0,0)$ and $(x, f(x)) = (Z_S, 1)$, where $Z_S = \sum_{i \in \mathcal{S}} \exp(-e_i/k_B T)$ is the system's partition function. Geometrically, to have a transition $\rho_S \to \rho_S'$ under a thermal operation, the ρ_S thermomajorization curve must lie above or on the curve of ρ_S'. (See Fig. 2.)

Now, we are ready to study work extraction bounds in the single-shot regime. Consider a two-level work reservoir with Hamiltonian $H_W = W_0|W_0\rangle\langle W_0| + W_1|W_1\rangle\langle W_1|$. For a work extraction transition $(\rho_S \otimes |W_0\rangle\langle W_0|, H_S + H_W) \to (\tau_S \otimes |W_1\rangle\langle W_1|, H_S + H_W)$ to occur in single-shot thermodynamics, $\rho_S \otimes |W_0\rangle\langle W_0|$ must thermomajorize $\tau_S \otimes |W_1\rangle\langle W_1|$

and we have

$$W = W_1 - W_0 \leqslant D_0(\rho_S \| \tau_S). \qquad (10)$$

(See Appendix B for details.)

In this case, the maximum work extractable from a state (ρ_S, H_S) cannot achieve the upper bound $-\Delta F_S$, because a two-level nanoscale work reservoir cannot approach zero entropy production for every work extraction. By contrast, stochastic thermodynamics approaches zero entropy production by employing a quasistatic process connecting the initial and final states [29].

Next, let us address how to compute the entropy production in the single-shot regime. The entropy production is still defined as in Eq. (7). Consider an energy preserving unitary operation such that $Q = -\Delta U_S$, where

$$\Delta U_S = k_B T(-\text{Tr}(\rho_S' \log \tau_S) + \text{Tr}(\rho_S \log \tau_S)). \qquad (11)$$

(Here, we assume there is no work reservoir. But if we wish to include one, we treat the work reservoir as part of the system.) Then we can write the entropy production of Eq. (7) in an information-theoretic form [30,31]:

$$\Sigma = -\Delta U_S/T + \Delta S_S \qquad (12)$$

$$= D(\rho_S \| \tau_S) - D(\rho_S' \| \tau_S). \qquad (13)$$

This represents the entropy produced when the system undergoes a Gibbs-preserving thermal operation, whose steady state τ_S produces zero entropy. In essence, when there is no work reservoir to guide the transformation, any relaxation towards equilibrium corresponds to irreversibility.

Let thermal operation $\mathcal{E}$ transform ρ_S to ρ_S': $\mathcal{E}(\rho_S) = \rho_S'$. This thermal operation preserves the Gibbs state, such that $\mathcal{E}(\tau_S) = \tau_S$, and from the data processing inequality [32], we have

$$D(\rho_S \| \tau_S) \geqslant D(\mathcal{E}(\rho_S) \| \mathcal{E}(\tau_S)) \qquad (14)$$

$$= D(\rho_S' \| \tau_S). \qquad (15)$$

Entropy production is always nonnegative in single-shot thermodynamics. Now, we are ready to state a theorem on approaching zero entropy production at the nanoscale.

Theorem 1. Consider a d-dimensional system with Hamiltonian H. Given two states ρ and σ, the following are equivalent.

(a) The thermomajorization curves of states ρ and σ coincide.

(b) There exists a thermal operation $\mathcal{E}$ such that $\mathcal{E}(\rho)$ can be arbitrarily close to σ and the corresponding entropy production can be arbitrarily small.

Theorem 1 is one of our main results. Appendix C gives the proof. Note that for two different states to have exactly the same thermomajorization curve, there must be energy degeneracy in H [33,34]. Theorem 1 illustrates geometrically why the familiar thermodynamics bounds are not the same as the bounds at the nanoscale. To approach the latter bounds, the entropy production needs to be arbitrarily small. Here, the work reservoir entropy change must be included:

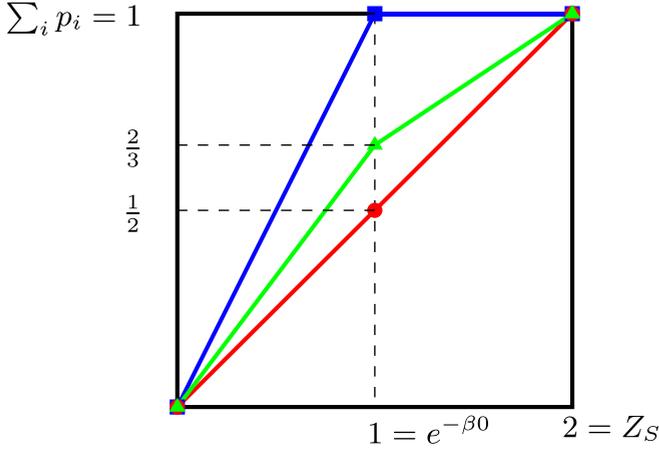$$\Sigma = \Delta S_S + \Delta S_W + \frac{Q}{T}. \qquad (16)$$

FIG. 3. Thermodynamics' bound cannot be achieved at the nanoscale: Consider a two-level system spanned by $\{|0\rangle, |1\rangle\}$ with $H_S = 0$. The red circle is the thermomajorization curve of $\rho_S = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|)$. The blue square is the curve for $\rho'_S = |0\rangle\langle 0|$. The green triangle is that of $\sigma_S = (\frac{1}{3}|0\rangle\langle 0| + \frac{2}{3}|1\rangle\langle 1|)$. The red circle and blue square curves coincide with a two-level work reservoir. The corresponding transition $(\rho_S, H_S) \rightarrow (\rho'_S, H_S)$ is the well-known Landauer's erasure. We can approach this bound arbitrarily closely. However, this cannot be done for the green triangle and blue square curves.

Under deterministic work extraction, $\Delta S_W = 0$ and the work reservoirs' initial and final states are pure states. They can only contract the system's thermomajorization curves along the x axis by a factor. And so, to approach zero entropy production, the system's initial thermomajorization curve must coincide with its final thermomajorization curve up to a contraction factor. This is not always possible. Figure 3 depicts the situation.

IV. BEYOND DETERMINISTIC WORK

This section generalizes two-level work reservoirs in such a way that initial and final thermomajorization curves coincide. This achieves arbitrarily small entropy production for a transition. Before the general case, though, we first review an elementary example to give a simple picture.

A. Example

Consider Landauer's erasure with the initial distribution $\boldsymbol{p}_S = (\frac{1}{3}, \frac{2}{3})$ stored in a two-level system with trivial Hamiltonian $H = 0$ and a four-level work reservoir with energy levels $\{W_0, W_1, W_2, W_3\}$. We set the work reservoir's initial distribution to $\boldsymbol{p}_W = (r_1, r_2, 0, 0)$ and the final to $\boldsymbol{p}'_W = (0, 0, r_1, r_2)$. Initially, the nonzero populations of the work reservoir are with the first half of energy levels and the final nonzero populations of the work reservoir are with the second set of energy levels. The work reservoir's entropy does not change overall. The total initial state is

$$\rho_{SW} = \left(\tfrac{1}{3}|0\rangle\langle 0| + \tfrac{2}{3}|1\rangle\langle 1|\right) \otimes \tag{17}$$

$$(r_1|W_0\rangle\langle W_0| + r_2|W_1\rangle\langle W_1|) \tag{18}$$

and the final is

$$\rho'_{SW} = |0\rangle\langle 0| \otimes (r_1|W_2\rangle\langle W_2| + r_2|W_3\rangle\langle W_3|). \tag{19}$$

First, consider the final state's thermomajorization curve. At most, it has two distinct slopes. For the two curves to coincide, the initial curve can contain at most two distinct slopes. One possibility is that the initial work reservoir's thermomajorization curve has one distinct slope. This leads to

$$\tfrac{1}{3}r_1 e^{\beta W_0} = \tfrac{1}{3}r_2 e^{\beta W_1} = r_1 e^{\beta W_2}, \tag{20}$$

$$\tfrac{2}{3}r_1 e^{\beta W_0} = \tfrac{2}{3}r_2 e^{\beta W_1} = r_2 e^{\beta W_3}, \tag{21}$$

$$\tfrac{1}{3}r_1 + \tfrac{1}{3}r_2 = r_1, \tag{22}$$

$$\tfrac{2}{3}r_1 + \tfrac{2}{3}r_2 = r_2. \tag{23}$$

The first two equations come from requiring the initial curve to have only two distinct slopes and the same slopes as the final curve's. And, the last two equations come from requiring the same y-coordinate change. Solving those equations gives

$$r_1 = \tfrac{1}{3}, \quad r_2 = \tfrac{2}{3}, \tag{24}$$

$$e^{-\beta W_0} = a, \quad e^{-\beta W_1} = 2a, \quad e^{-\beta W_2} = 3a, \quad \text{and} \quad e^{-\beta W_3} = 3a, \tag{25}$$

where a is an arbitrary positive number.

Table I demonstrates that the initial and final curves coincide. The expected energy change in the work reservoir is

$$\langle W \rangle = r_1(W_2 - W_0) + r_2(W_3 - W_1) \tag{26}$$

$$= k_{\text{B}}T\left(\tfrac{1}{3}\log\tfrac{1}{3} + \tfrac{2}{3}\log\tfrac{2}{3}\right). \tag{27}$$

This is the system entropy change as expected. This demonstrates that energy levels $\boldsymbol{E}_W = \{W_0, W_1, W_2, W_3\}$ with probability distributions $\boldsymbol{p}_W = (\frac{1}{3}, \frac{2}{3}, 0, 0)$ and $\boldsymbol{p}'_W = (0, 0, \frac{1}{3}, \frac{2}{3})$ form an efficient work reservoir for Landauer erasure with the initial distribution $\boldsymbol{p}_S = (\frac{1}{3}, \frac{2}{3})$.

One subtlety to highlight is that, although the total curves coincide, with thermal operations we can only make the final state arbitrarily close to the desired state ρ'_{SW}. So, we cannot use exactly $\langle W \rangle$ to erase $\boldsymbol{p}_S$. Instead, we can use the amount of work arbitrarily close to $\langle W \rangle$ to erase $\boldsymbol{p}_S$ and then the corresponding entropy production will be arbitrarily small.

For simplicity, from now on we treat thermomajorization curves coinciding as the same as zero entropy production. Corresponding bounds on work can be computed by setting entropy production to be zero. However, we should keep in mind that the precise statement is that the entropy production can be arbitrarily small and the corresponding work can be arbitrarily close to the bounds.

A key observation from this example is that for the two total thermomajorization curves to coincide, the nonzero slope part of the final work reservoir's curve must coincide with the nonzero slope part of the initial system's curve up to a scale constant. In the above example, the scale constant is $3a$. We further require that the nonzero slope part of the initial work reservoir's curve coincide with the nonzero slope part of the final system's curve up to the same scale constant. Thus, the key step in constructing an efficient work reservoir for a state transformation is to find a suitable probability distribution for the work reservoir. And then we can fine tune energy levels such that the work reservoir's thermomajorization curve can coincide with both the initial and final state's curves.

TABLE I. Efficient work reservoir for Landauer erasure: The first row shows thermomajorization curves of the initial system state $\rho_S = \frac{1}{3}|0\rangle\langle 0| + \frac{2}{3}|1\rangle\langle 1|$, the initial work state $\rho_W = \frac{1}{3}|W_0\rangle\langle W_0| + \frac{2}{3}|W_1\rangle\langle W_1|$, and the initial total state $\rho_{SW} = \rho_S \otimes \rho_W$. The second row shows thermomajorization curves of the final system state $\rho_S' = |0\rangle\langle 0|$, the final work state $\rho_W' = \frac{1}{3}|W_2\rangle\langle W_2| + \frac{2}{3}|W_3\rangle\langle W_3|$, and the final total state $\rho_{SW}' = \rho_S' \otimes \rho_W'$.
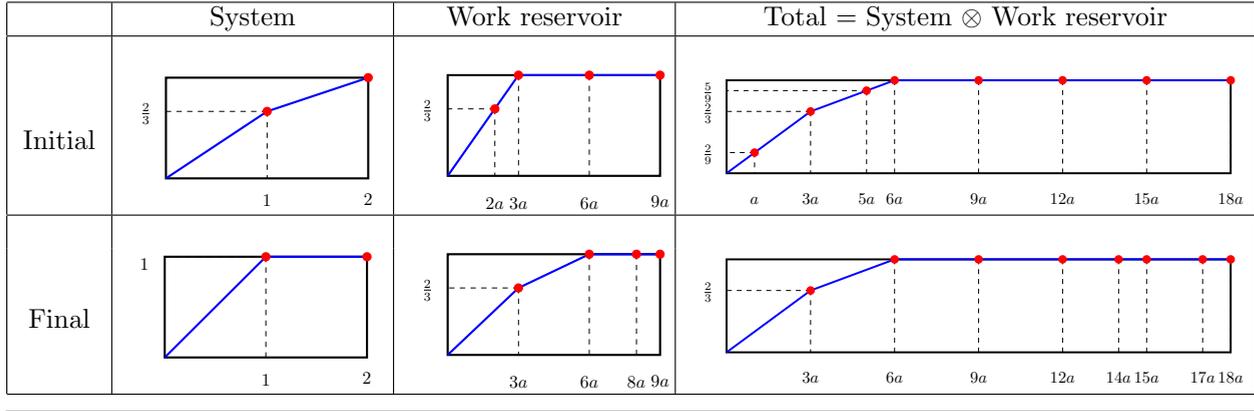
In the first example, the probability distribution we chose was $(\frac{1}{3}, \frac{2}{3})$. We set the initial energy levels to be $W_0 = -k_B T \log a$ and $W_1 = -k_B T \log 2a$ and the final's to be $W_2 = -k_B T \log 3a$ and $W_3 = -k_B T \log 3a$. Under those parameters, the erasure is efficient; i.e., the entropy production vanishes.

B. General efficient work reservoirs

Now, we turn to develop efficient work reservoirs for arbitrary state transitions. First, we introduce a notation using tuples to aid in describing thermomajorization curves. Then, we present the definition of efficient work reservoirs and briefly discuss how to construct them. Recall that the thermomajorization curve $f_{p,E}$ of a distribution $p = \{p_i\}_{i\in\mathcal{S}}$ over the energy levels $E = \{\epsilon_i\}_{i\in\mathcal{S}}$ can be derived from the collection of segments $\{(e^{-\beta\epsilon_i}, p_i)\}_{i\in\mathcal{S}}$. The thermomajorization curve orders the segments from highest slope—the slope of the ith element is $p_i e^{\beta\epsilon_i}$—to lowest and then concatenates them end to end.

Consider a coarse-graining function $\lambda : \mathcal{S} \to \mathcal{S}'$ that defines a new distribution and energy landscape: $p' = \lambda(p) = \{p_j'\}_{j\in\mathcal{S}'}$ and energy landscape $E' = \lambda(E) = \{\epsilon_j'\}_{j\in\mathcal{S}'}$ via

$$p_j' = \sum_{i\in\lambda^{-1}(j)} p_i, \tag{28}$$

$$e^{-\beta\epsilon_j'} = \sum_{i\in\lambda^{-1}(j)} e^{-\beta\epsilon_i}, \tag{29}$$

where

$$\lambda^{-1}(j) \equiv \{i | i \in \mathcal{S}, \lambda(i) = j\}. \tag{30}$$

If λ only coarse grains elements of (p, E) whose segments have the same slope—meaning $\lambda(i) = \lambda(i')$ implies $p_i e^{\beta\epsilon_i} = p_{i'} e^{\beta\epsilon_{i'}}$—then the coarse-grained distribution and energies $(\lambda(p), \lambda(E))$ have the same thermomajorization curve $f_{\lambda(p),\lambda(E)} = f_{p,E}$. The segments $(e^{-\beta\epsilon_i}, p_i)$ and $(e^{-\beta\epsilon_{i'}}, p_{i'})$ of elements i and i' with the same slope in the thermomajorization curve comprise a long line segment with (width, height) $= (e^{-\beta\epsilon_i} + e^{-\beta\epsilon_{i'}}, p_i + p_{i'})$.

Suppose λ coarse grains all segments with the same slopes. After the coarse graining, the thermomajorization curve has n distinct slopes, excluding the segments with slope zero. Let $\#f_{p,E} = n$ denote the number of distinct slopes in $f_{p,E}$ and n tuples $f_{p,E} = \{(y_i, k_i)\}_{i=1}^n$ represent f where k_i is the ith distinct slope and y_i is the corresponding y-coordinate change. In some cases, we allow repeating slopes in $f_{p,E}$.

For a composite system, the joint thermomajorization curve is constructed as follows. Given one distribution $p_S = \{p_i\}_{i\in\mathcal{S}}$ over energy levels $E_S = \{e_i\}_{i\in\mathcal{S}}$ with thermomajorization curve $f_{p_S,E_S} = \{(x_i, k_i)\}_{i\in\mathcal{S}}$ and another distribution $p_{S'} = \{q_i\}_{i\in\mathcal{S}'}$ over energy levels $E_{S'} = \{h_i\}_{i\in\mathcal{S}'}$ with thermomajorization curve $f_{q_{S'},H_{S'}} = \{(y_i, m_i)\}_{i\in\mathcal{S}'}$, then the composite configuration is the probability distribution $p_{SS'}$ over energy levels $E_{SS'}$ where

$$p_{SS'} = \{p_i q_j\}_{i\in\mathcal{S},j\in\mathcal{S}'}, \tag{31}$$

$$E_{SS'} = \{e_i + h_j\}_{i\in\mathcal{S},j\in\mathcal{S}'}, \tag{32}$$

and

$$f_{p_{SS'},E_{SS'}} = \{(x_i y_j, k_i m_j)\}_{i\in\mathcal{S},j\in\mathcal{S}'}. \tag{33}$$

Slopes may repeat in $f_{p_{SS'},E_{SS'}}$.

With this enhanced notation, we now define multilevel work reservoirs.

Definition 1: Multilevel work reservoirs. A $2d$-level work reservoir (p_W, p_W', E_W) for a state transition $p_S \to p_S'$ in a system with energy levels $E_S = \{e_s\}_{s\in\mathcal{S}}$ has initial distribution $p_W = \{q_w\}_{w\in\mathcal{W}}$, final distribution $p_W' = \{q_w'\}_{w\in\mathcal{W}}$, and energy eigenstates $E_W = \{\epsilon_w\}_{w\in\mathcal{W}}$. Here, p_W and p_W' have the form of $p_W = (r, 0)$ and $p_W' = (0, r)$, where r is a d-dimensional probability distribution. The initial configuration of the system with the reservoir is (p_{SW}, E_{SW}), where

$$p_{SW} = \{p_s q_w\}_{s\in\mathcal{S},w\in\mathcal{W}}, \tag{34}$$

$$E_{SW} = \{e_s + \epsilon_w\}_{s\in\mathcal{S},w\in\mathcal{W}}. \tag{35}$$

The final configuration is (p_{SW}', E_{SW}), where

$$p_{SW}' = \{p_s' q_w'\}_{s\in\mathcal{S},w\in\mathcal{W}}, \tag{36}$$

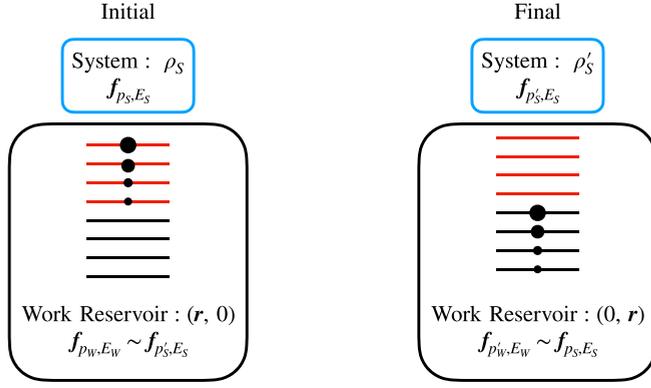$$E_{SW} = \{e_s + \epsilon_w\}_{s\in\mathcal{S},w\in\mathcal{W}}. \tag{37}$$

FIG. 4. One way for two total thermomajorization curves to coincide is to find a probability distribution r and energy levels E_W such that when r occupies the first half energy levels—i.e., $p_W = (r, 0)$—the thermomajorization curve f_{p_W, E_W} coincides with the final system state's curve $f_{p'_S, E_S}$ up to a contraction factor—denoted $f_{p_W, E_W} \sim f_{p'_S, E_S}$. When the probability distribution occupies the second half energy levels—i.e., $p'_W = (0, r)$—the thermomajorization curve $f_{p'_W, E_W}$ coincides with the initial system state's curve f_{p_S, E_S} up to the same contraction factor. With this, the two total curves coincide: $f_{p_{SW}, E_{SW}} = f_{p'_{SW}, E_{SW}}$.

This requires p_W and p'_W to have the forms $p_W = (r, 0)$ and $p'_W = (0, r)$ so that the overall work reservoir's entropy change vanishes. This satisfies the stochastic thermodynamics' entropyless assumption for work reservoirs [35]. Furthermore, from our definition the initial nonzero distribution in the work reservoir occupies the first half of energy levels and the final occupies the second half of the energy levels. This leads immediately to the following definition.

Definition 2: Efficient work reservoirs. A work reservoir (p_W, p'_W, E_W) is efficient for a state transition $p_S \to p'_S$ in a system with energy levels E_S if the thermomajorization curves of (p_{SW}, E_{SW}) and (p'_{SW}, E_{SW}) coincide.

The previous example showed that the key to constructing an efficient work reservoir is to find a probability distribution r and energy levels E_W for work reservoirs such that its curve coincides with the final state's curve with the distribution $(r, 0)$ and with the initial state's curve with the distribution $(0, r)$ up to the same constant. Then the efficient work reservoir's initial and final thermomajorization curves mimic the system's final and initial thermomajorization curves as shown in Fig. 4.

C. Work extraction and state formation reservoirs

We first study how to construct efficient work reservoirs for two kinds of state transitions: work extractions and state formations. For work extraction $(p_S, E_S) \to (\tau_S, E_S)$, suppose there are m distinct slopes in the thermomajorization curve f_{p_S, E_S} and $f_{p_S, E_S} = \{(r_i, a_i)\}_{i=1}^m$, where m is the number of distinct slopes in the thermomajorization curve of the system. We now show that a work reservoir must have a dimension greater than $2(m-1)$ to achieve efficient work extraction.

TABLE II. Initial and final thermomajorization curves for the efficient work extraction reservoir, ignoring the zero-slope parts.

To see this, assume that an efficient work reservoir has dimension $2d \leqslant 2(m-1)$. Now, let the initial work reservoir probability distribution be $p_W = (r, 0)$, the corresponding thermomajorization curve have a distinct slopes, the final work reservoir probability distribution be $p'_W = (0, r)$, and the corresponding thermomajorization curve have b distinct slopes. Since the dimension of r is d, then, we have $a, b \leqslant d \leqslant (m-1)$.

The final total probability distribution is $p'_{SW} = \tau_S \otimes p'_W$. We have $\#f_{p'_S, E_S} = 1$ and $\#f_{p'_W, E_W} = b$. The number of distinct slopes of the thermomajorization curve $f_{p'_{SW}, E_{SW}}$ is b. The initial total probability distribution is $p_{SW} = p_S \otimes p_W$. Since the number of distinct slopes in p_S's thermomajorization is m, we have $\#f_{p_{SW}, E_{SW}} \geqslant m$. The equality holds if and only if the number of the segments of p_W's thermomajorization is 1. Since we have $b \leqslant m - 1 < m$, it is impossible for curve $f_{p_{SW}, E_{SW}}$ to coincide with curve $f_{p'_{SW}, E_{SW}}$. Hence, the dimension of the efficient work reservoir is at least $2m$.

With a $2m$-dimensional work reservoir, we choose the probability distribution to be $r = (r_1, \ldots, r_m)$. We fine tune the first half energy levels such that the initial work reservoir's curve only contains one slope which coincides with the final thermal state of the system's curve up to a constant. For the second half energy levels, they are fine tuned such that the final work reservoir's curve coincides with f_{p_S, E_S} up to the same constant. (See Table II.)

The detailed calculation follows. Suppose the energy levels of the work reservoir are $E_W = \{\epsilon_1, \ldots, \epsilon_m, \epsilon'_1, \ldots, \epsilon'_m\}$. For the energy levels $\{\epsilon_1, \ldots, \epsilon_m\}$, we require

$$e^{\beta \epsilon_i} = \frac{c}{r_i}, \tag{38}$$

where c can be an arbitrary positive number. For the energy levels $\{\epsilon'_1, \ldots, \epsilon'_m\}$, we stipulate

$$e^{\beta \epsilon'_i} = c Z_S \frac{a_i}{r_i}. \tag{39}$$

With our notation, we can verify that the two final curves coincide. For the initial setup,

$$f_{p_S, E_S} = \{(r_i, a_i)\}_{i=1}^{m}, \tag{40}$$

$$f_{p_W, E_W} = \{(1, c)\}. \tag{41}$$

And for the final setup,

$$f_{p'_S, E_S} = \{(1, 1/Z_S)\}, \tag{42}$$

$$f_{p'_W, E_W} = \{(r_i, c Z_S a_i)\}_{i=1}^{m}. \tag{43}$$

From Eq. (33) we have

$$f_{p_{SW}, E_{SW}} = f_{p'_{SW}, E_{SW}} \tag{44}$$

$$= \{(r_i, c a_i)\}_{i=1}^{m}, \tag{45}$$

which means the two final total curves indeed coincide. The energy change in this work reservoir is

$$W = \sum_{i=1}^{m} r_i (\epsilon'_i - \epsilon_i) \tag{46}$$

$$= k_B T D_1(p_S || \tau_S). \tag{47}$$

It is not hard to prove that this is the unique $2m$-dimensional efficient work reservoir for ρ_S work extraction.

Since entropy production vanishes, we can use the same work reservoir to form the state $\tau_S \to p_S$. Hence, the minimal dimension of the efficient work reservoir for both work extraction and state formation is equal to $2 \cdot \# f_{p_S, E_S}$. Appendix H goes on to construct thermomajorization curves of all possible efficient work reservoirs for state formation and work extraction from the minimal efficient work reservoirs.

D. Efficient reservoirs exist

We will not develop all possible efficient work reservoirs for general state transitions here, though. Nonetheless, the next theorem establishes the existence of efficient work reservoirs for them—our second main result.

Theorem 2. For two general n-dimensional states p_S and p'_S over energy levels E_S, there exists a work reservoir (p_W, p'_W, E_W) such that the thermomajorization curves of (p_{SW}, E_{SW}) and (p'_{SW}, E_{SW}) coincide.

Appendix D gives the details on how to construct the probability distribution and energy levels for efficient work reservoirs.

Here, we discuss several properties and applications of efficient work reservoirs. If $E_W = \{\epsilon_1, \dots, \epsilon_N, \epsilon'_1, \dots, \epsilon'_N\}$ determines the energy levels for an efficient work reservoir with probability transition $(r, 0) \to (0, r)$, then $E'_W = \{\epsilon_1 + c, \dots, \epsilon_N + c, \epsilon'_1 + c, \dots, \epsilon'_N + c\}$ gives the energy levels of an efficient work reservoir with the same probability distribution, where c is a constant. This shows that efficient work reservoirs have translational symmetry. That is, only gaps between energy levels in efficient work reservoirs matter.

Since our efficient work reservoirs have more than two levels, the work fluctuates. The entropy production with efficient work reservoirs could be arbitrarily small. The variance of the work, however, could be greater than noneffient work reservoirs. This can be seen by noting that the work variance is zero in two-level work reservoirs since the work is deterministic,
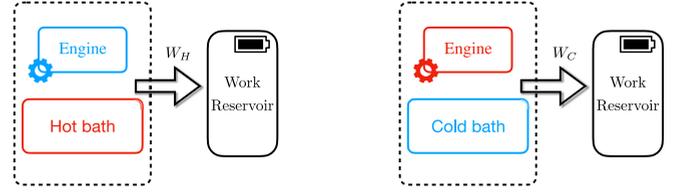

FIG. 5. Work stored into the reservoir during the engine and work reservoir interacting with the hot bath and the cold bath. First, the engine and reservoir interact with the hot bath. The engine begins with the cold Gibbs state and ends with the hot Gibbs state. The amount of work $W_H = k_B T_H D_1(\tau_C || \tau_H)$ is stored in the work reservoir. Then the engine and reservoir are brought to the cold bath. Similarly, the amount of work $W_C = k_B T_C D_1(\tau_H || \tau_C)$ is stored in the work reservoir during the interaction with the cold bath.

while the work variance in efficient work reservoirs is greater than zero.

Consider an example. Suppose the system is three dimensional with trivial Hamiltonian $H = 0$ and the initial distribution is $(\frac{1}{3}, \frac{2}{3}, 0)$. Using a two-level work reservoir to harness work from this system, the extractable work is $W_{2\text{-level}} = k_B T \log 3/2$ and the work variance is zero. The zero variance is due to the fact that the work is deterministic in a two-level work reservoir. If we use an efficient work reservoir to harness work from this system, though, the average work is $W_{\text{efficient}} = k_B T (\log 3 - H(1/3))$, where $H(\cdot)$ is the binary entropy function. The work variance, however, is nonzero. We have $W_{\text{efficient}} > W_{2\text{-level}}$. This example shows us that for a protocol with nonzero entropy production, the work variance might be less compared to a protocol with zero entropy production.

For transitions under time-dependent Hamiltonians, we introduce a clock system [12]. Suppose the initial and final Hamiltonians are H_S and H'_S, respectively. The total Hamiltonian including the clock system is

$$H = H_S \otimes |0\rangle\langle 0| + H'_S \otimes |1\rangle\langle 1|. \tag{48}$$

With the clock system, we require any transition to be $\rho_S \otimes |0\rangle\langle 0| \to \rho'_S \otimes |1\rangle\langle 1|$. In this, the Hamiltonian changes from H_S to H'_S. Appendix G presents two examples of efficient work reservoirs for nontrivial Hamiltonians and for time-dependent Hamiltonian state transitions.

One of the applications of efficient work reservoirs is to build a quantum engine that approaches Carnot efficiency. Suppose we pick a two-dimensional system spanned by $\{|0\rangle, |1\rangle\}$ with Hamiltonian $H_{\text{eng}} = \epsilon |1\rangle\langle 1|$. The engine functions with a hot bath at temperature T_H and a cold bath at temperature T_C. Initially, the work reservoir is in its Gibbs state at temperature T_C. Fig. 5 presents a sketch of the qubit engine. First, it is brought to the hot bath, interacts with the hot bath to extract work, and ends up in the Gibbs state at temperature T_H. Then, it is brought to the cold bath, interacts with it to extract work, and ends up in the Gibbs state at temperature T_C finishing the cycle. If we use efficient work reservoirs to extract work, then the entropy production is arbitrarily close to zero. Then the engine's efficiency approaches Carnot efficiency $1 - T_C/T_H$. Appendix I gives the details for

constructing the work reservoir's probability distribution and energy levels.

V. CATALYZED WORK RESERVOIRS

The development to this point was limited to noncatalytic scenarios. The following explores efficient work extraction with the aid of catalysts. Here, the intention is not to surpass the bound set by free-energy differences. Rather, we ask whether we can extract work without dissipation by using a smaller work reservoir with catalysts.

The main result in catalytic thermal operations is that the transition from state ρ_S to ρ_S' is possible through a *catalytic thermal operation*—denoted $\rho_S \xrightarrow{\text{CTO}} \rho_S'$—if and only if $D_\alpha(\rho_S \| \tau_S) \geqslant D_\alpha(\rho_S' \| \tau_S)$, for all $\alpha \in \mathbb{R}$ [13]. The next theorem shows that catalysts do not help reach zero entropy production.

Theorem 3. Consider a system with Hamiltonian H and a catalyst state c with Hamiltonian H_c. If state ρ can be converted into a state that is arbitrarily close to state σ through a thermal operation with the catalyst c under arbitrarily small entropy production, then the transition can be achieved through a noncatalytic thermal operation.

Appendix C gives the proof. This shows that close to the zero dissipation regime, thermal operations and catalytic thermal operations are equivalent. Theorem 3 provides yet another criterion for checking if two thermomajorization curves coincide.

Theorem 4. Given a system with Hamiltonian H and states ρ and σ, the following are equivalent.

(a) Thermomajorization curves of ρ and σ coincide.

(b) $D_\alpha(\rho \| \tau) = D_\alpha(\sigma \| \tau)$, for all $\alpha \in \mathbb{R}$.

Again, we place the proof in Appendix C. It seems the catalysts are useless if we require the entropy production to be arbitrarily small. However, we find that if catalysts are allowed to correlate states in a trivial Hamiltonian, every state transition's entropy production can be reduced to zero; see Appendix K.

VI. DISCUSSION

In stochastic thermodynamics, it is well known that the maximal extractable work from a state transition $\rho_S \to \rho_S'$ is the (negative) nonequilibrium free-energy difference. The maximum is approached when the dissipation is arbitrarily small. However, as we showed, zero dissipation with two-level work reservoirs cannot always be approached in single-shot thermodynamics. This is due to the fact that, with two-level work reservoirs, we can only contract a thermomajorization curve by a factor. Two-level work reservoirs are not powerful enough to approach zero dissipation for every state transition.

To remove this restriction, we generalized two-level work reservoirs to multilevel work reservoirs. The extractable work is then defined as the difference in the expectation values of work reservoir energies: $W = \sum_i r_i(\epsilon_i' - \epsilon_i)$. Naturally, a two-level work reservoir can be treated as a special case where $W = \epsilon' - \epsilon$. Our work value definition is similar to that in stochastic thermodynamics: $dw = \sum_i p_i d\epsilon_i$, where the work is defined as the system energy change while keeping the system probability distribution unchanged [36].

Here, though, the probability distribution components of the work reservoirs do not change overall. For each nonzero component, there is a corresponding energy-level change in the work reservoir. Our results show that we can achieve reversibility in single-shot thermodynamics with multilevel work reservoirs. The price paid, however, is that the size of the thermal baths must be infinite. The dissipation can be written as

$$\Sigma = I(\rho_S'; \rho_B') + D_1(\rho_B' \| \tau_B), \tag{49}$$

where $I(\cdot; \cdot)$ is the mutual information [31,37]. Since the heat Q transferred to the bath is nonzero, if we only have thermal baths of finite size, the dissipation is strictly positive. Appendix J gives an example where we construct the joint unitary operator explicitly. We show that to approach zero dissipation, the bath size must be infinite.

References [38–40] develop the general framework of work extraction in single-shot thermodynamics. Rather than considering strict energy conservation, work extraction can be monitored via average energy conservation [41]. There, work extraction uses a series of transformations, arriving at the same bound when the number of transformations diverges. Reference [19] considers a weighted Hamiltonian $H_W = \int dx \, x |x\rangle\langle x|$ as a work reservoir. With translational invariance, it derives several compact fluctuation theorems. This allows changes in work reservoir probability distribution, but assumes the work reservoir energy levels are unbounded. References [42,43] consider the work extraction of systems that exchange both energy and particles with the environment with multilevel batteries.

In contrast, our development here keeps the work reservoir probability distribution unchanged. This follows from the entropyless assumption of work reservoirs. Reference [44] considers a work reservoir with lower-bounded energy levels. Reference [45] systematically explores quantum fluctuation theorems. Recently, in single-shot thermodynamics, there are other setups that extract work equal to the (negative) free-energy difference [46–48]. In this, correlations build up between catalysts and so stochastic independence of catalysts allows extracting more work from given states.

Generalizing to multilevel work reservoirs offers several new directions in nanoscale thermodynamics. Since work is no longer deterministic, it is natural to ask how to compute higher moments $\langle W^n \rangle$ ($n > 1$) and to construct a fluctuation theorem for the work probability distribution. With two-level work reservoirs, the characteristic functions of work extraction and state formation are the Rényi $\alpha = 0$ and ∞ divergences, respectively. What are the characteristic functions of work extraction and state formation with multilevel work reservoirs? Our development focused on single-copy state transitions. The structure of the efficient work reservoirs for more complicated state transitions—for example, mapping an input information tape to output tape [49]—must wait for the future.

Our development focused only on the net input-output mapping, without considering details of the stochastic map in between. The stochastic map connecting an input to an output here is not unique. If we only consider the work expectation value $\langle W \rangle$, the change in expectation value of energy in work reservoirs coincides with the expectation

value of work in the *two point measurement* (TPM) scheme commonly used in stochastic quantum thermodynamics [50]. For higher moments $\langle W^n \rangle$ ($n > 1$) in TPM, however, the values depend on the stochastic maps. Moreover, one cannot determine higher moments uniquely with only initial and final work reservoir states. We can also study the minimal cost of a stochastic map, not only a specific state transition. References [51,52] explored the minimal cost of quantum channels with two-level work reservoirs. We leave the minimal work cost with multilevel work reservoirs also to the future.

Along these lines, what if we allow coherence in both the system and the work reservoir? For example, what if $\rho_W = \sum_{ij} \rho_{ij} |W_i\rangle\langle W_j|$ and $\sum_{ij} \rho_{ij} |W_i'\rangle\langle W_j'|$? To address state transitions with coherence, α-Rényi divergences are insufficient [53,54]. Can we achieve the bounds set by free-energy difference when the states are not block diagonal in energy eigenstates with those work reservoirs? Again, we leave this open for the future efforts.

VII. CONCLUSION

We generalized two-level work reservoirs commonly used in single-shot thermodynamics to multilevel work reservoirs and systematically analyzed arbitrarily small dissipation state transitions with the latter. We derived equivalent conditions for arbitrarily small dissipation transitions in single-shot thermodynamics: thermomajorization curve coincidence and α-Rényi divergence equality. We showed that for any state transition, we can always construct a work reservoir to approach zero dissipation.

We also considered cases where the initial system Hamiltonian differs from the final Hamiltonian. The efficient work reservoir, though, for a specific state transition is not unique. For work extraction and state formation in this setting, we constructed the efficient work reservoir with minimal dimension. We showed that all thermomajorization curves at inverse temperature β form a monoid and characterized all possible efficient reservoirs for work extraction and state formation. These allowed us to analyze nanoscale engines that employ efficient work reservoirs, demonstrating that they approach Carnot efficiency.

ACKNOWLEDGMENTS

APPENDIX A: FREE-ENERGY WORK BOUND

Reference [1] establishes the second law of thermodynamics for the entropy production of a system S in contact with a heat bath B at temperature T:

$$\Sigma \equiv Q/T + \Delta S(\rho) \geqslant 0. \quad (A1)$$

Here, Q is the average heat that was dissipated in the bath, Σ is the total entropy production, and $S(\rho) \equiv -k_B \text{Tr}[\rho \log \rho]$ is the von Neumann entropy of the system S. The resulting bound on heat is

$$Q/T \geqslant -\Delta S(\rho), \quad (A2)$$

which is a quantum version of Landauer's principle [3,30,31]. We can bound the work by noting the first law of thermodynamics: the change in average energy of the system is equal to the difference between the heat flow and work produced from the system:

$$\Delta\langle E \rangle = -Q - W, \quad (A3)$$

where $\langle E \rangle = \text{Tr}(\rho H)$. Applying the entropy bound on heat to the work production, we find the work production in transforming $\rho \to \rho'$ has the upper bound

$$W \leqslant T\Delta S(\rho) - \Delta\langle E \rangle \quad (A4)$$

$$= T(S(\rho') - S(\rho)) - [\text{Tr}(\rho' H) - \text{Tr}(\rho H)]. \quad (A5)$$

With the free energy defined

$$F(\rho) \equiv \text{Tr}(\rho H) - TS(\rho), \quad (A6)$$

we have an upper bound on work via the change in free energy:

$$W \leqslant F(\rho) - F(\rho'). \quad (A7)$$

Furthermore, we have a simplification when the Hamiltonian H is the same for the initial and final state of the system. The Gibbs state τ of Hamiltonian H obeys the relationship

$$\tau = \frac{e^{-H/k_B T}}{\text{Tr}[e^{-H/k_B T}]}, \quad (A8)$$

which gives an inverse expression:

$$H = -k_B T \log \tau - k_B T \log \text{Tr}(e^{-H/k_B T}). \quad (A9)$$

Plugging this into the average energy in the bound on work production, we obtain a change in relative entropies:

$$W \leqslant [D_1(\rho||\tau) - D_1(\rho'||\tau)] \quad (A10)$$

where $D_1(\rho||\sigma) \equiv \text{Tr}(\rho \log \rho - \rho \log \sigma)$ is the quantum relative entropy.

APPENDIX B: THERMAL OPERATIONS

Our results are based on the resource theory approach to quantum thermodynamics, several results from which we briefly note here. See Refs. [55–57] for more comprehensive reviews.

The central idea is to define a set of operations—the *free operations*—and systematically analyze all possible state transitions under free operations. Suppose our state is ρ_S with Hamiltonian H_S. The set of allowed transitions then contains all joint energy-preserving unitary U operations between the
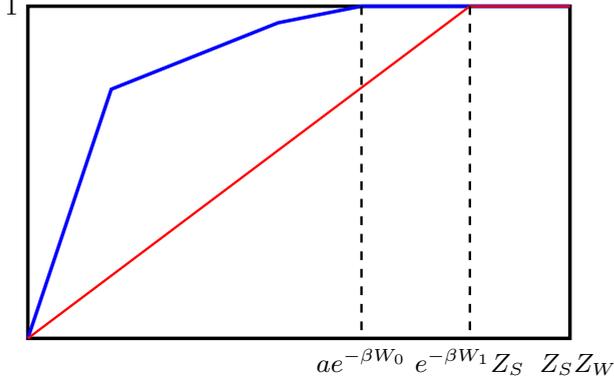
FIG. 6. Deterministic work extraction: The blue curve is the thermomajorization curve of $\rho \otimes |0\rangle\langle 0|$. $a \leqslant Z_S$ is the x coordinate of the point where the thermomajorization curve of ρ_S reaches 1. The red curve is the thermomajorization curve of $\tau_S \otimes |1\rangle\langle 1|$. Z_S and Z_W are partition functions of the system and the work reservoir, respectively.
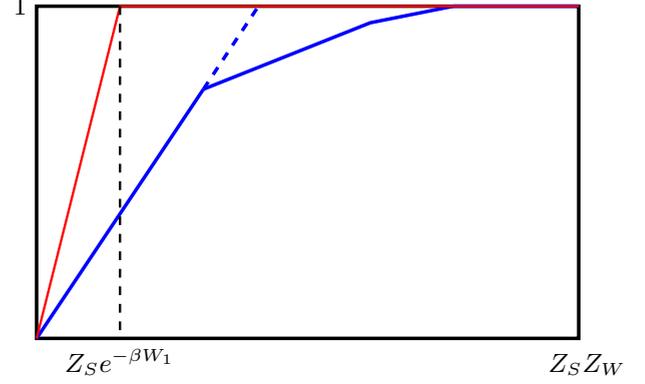

FIG. 7. Deterministic work of state formation: The blue curve is the thermomajorization curve of $\rho_S \otimes |W_0\rangle\langle W_0|$. The red curve is the thermomajorization curve of $\tau_S \otimes |W_1\rangle\langle W_1|$.

system and a thermal bath with the Hamiltonian H_B at inverse temperature β,

$$[U, H_S + H_B] = 0, \tag{B1}$$

followed by the partial trace over the thermal bath:

$$\rho'_S = \mathcal{E}(\rho_S) \tag{B2}$$

$$= \mathrm{Tr}_B[U(\rho_S \otimes \tau_B)U^\dagger], \tag{B3}$$

where $\tau_B = e^{-\beta H_B}/Z_B$ is the Gibbs state of the thermal bath. The maps $\mathcal{E}$ are called *thermal operations*.

Suppose the eigenvalues of ρ_S and ρ'_S are $\{p_i\}_{i=1}^n$ and $\{p'_i\}_{i=1}^n$ and the associated energy levels are $\{e_i\}_{i=1}^n$. Such a transition is equivalent to there being a stochastic matrix G such that $G\boldsymbol{p} = \boldsymbol{p}'$ and $G\boldsymbol{\tau} = \boldsymbol{\tau}$ [12].

We can also use a geometric method to determine whether such a transition exists. A key concept is the *thermomajorization curve* [12]. We first rank $\{p_i\}_{i=1}^n$ in descending order of $p_i e^{\beta e_i}$. This is called β *order*. The thermomajorization curve of a state ρ_S is formed by connecting points

$$\left\{ \sum_{i=1}^k e^{-\beta e_i^\downarrow}, \sum_{i=1}^k p_i^\downarrow \right\}_{k=1}^n \tag{B4}$$

piecewise linearly where $\downarrow$ means that p_i and e_i have been β ordered. If the thermomajorization curve of a state ρ_S lies above or on the thermomajorization curve of another state ρ'_S, we say ρ_S *thermomajorizes* ρ'_S. The central result is that ρ_S can be converted to ρ'_S through a thermal operation if and only if ρ_S thermomajorizes ρ'_S.

Next, we briefly review work extraction and the work of state formation. Consider a work reservoir that is a two-level system with Hamiltonian $H_W = W_0|W_0\rangle\langle W_0| + W_1|W_1\rangle\langle W_1|$. The task is to determine if the maximal work can be extracted from a state ρ_S. This is the maximal work change $W_1 - W_0$ such that $\rho_S \otimes |W_0\rangle\langle W_0| \to \tau_S \otimes |W_1\rangle\langle W_1|$ is allowed by thermal operations. This is elegantly determined from the thermomajorization curve.

For the initial curve to thermomajorize the final curve, we must have $ae^{-\beta W_0} \leqslant Z_S e^{-\beta W_1}$. See Fig. 6. Here, a is related to

Rényi divergence via $D_0(\rho_S \| \tau_S) = -\log(a/Z_S)$. We have the bound $W_1 - W_0 \leqslant k_{\mathrm{B}} T D_0(\rho_S \| \tau_S)$. The equal sign holds when two curves reach the height 1 at the same point.

Similarly, we can consider the reverse question: What is the minimal work needed to form state ρ_S? Or, in other words, what is the minimal $W_1 - W_0$ such that $(\tau_S \otimes |W_1\rangle\langle W_1|, H_S + H_W) \to (\rho_S \otimes |W_0\rangle\langle W_0|, H_S + H_W)$ is allowed by thermal operations?

For the initial curve to thermomajorize the final curve, the slope of the on-ramp part of the initial curve must not be less than the largest slope in the final curve (see Fig. 7):

$$\frac{1}{Z_S} e^{\beta W_1} \geqslant e^{\beta W_0} \max_i \frac{p_i}{e^{-\beta \epsilon_i}}, \tag{B5}$$

and

$$\max_i \left\{ \frac{p_i}{e^{-\beta \epsilon_i}} \right\} = D_\infty(\rho_S \| \tau_S), \tag{B6}$$

giving

$$W_1 - W_0 \geqslant k_{\mathrm{B}} T D_\infty(\rho_S \| \tau_S). \tag{B7}$$

If there exists an auxiliary system—a *catalyst*—with Hamiltonian H_C and state ρ_C such that the transition $(\rho_S \otimes \rho_C, H_S + H_C) \to (\rho'_S \otimes \rho_C, H_S + H_C)$ is possible, we say the transition $(\rho_S, H_S) \to (\rho'_S, H_S)$ can be achieved by a *catalytic thermal operation*.

The criterion of the catalytic thermomajorization is given in terms of Rényi α divergences. There exists a transition $(\rho_S, H_S) \xrightarrow{\mathrm{CTO}} (\rho'_S, H_S)$ if and only if [13]

$$D_\alpha(\rho_S || \tau_S) \geqslant D_\alpha(\rho'_S || \tau_S), \tag{B8}$$

for all $\alpha \in \mathbb{R}$. If we are allowed to invest an infinitesimal amount of work, only $\alpha \geqslant 0$ is needed.

We can also study work extraction and state formation in two-level work reservoirs with the help of catalysts. For work extraction,

$$(\rho_S \otimes |W_0\rangle\langle W_0|, H_S + H_W)$$
$$\to (\tau_S \otimes |W_1\rangle\langle W_1|, H_S + H_W), \tag{B9}$$

we must have

$$D_\alpha(\rho_S||\tau_S) + D_\alpha(|W_0\rangle\langle W_0|||\tau_W)$$
$$\geqslant D_\alpha(\tau_S||\tau_S) + D_\alpha(|W_1\rangle\langle W_1|||\tau_W), \quad (B10)$$

giving

$$W_1 - W_0 \leqslant k_B T D_\alpha(\rho_S||\tau_S), \quad (B11)$$

for all $\alpha \geqslant 0$. So, we have

$$W_1 - W_0 \leqslant \inf_{\alpha \geqslant 0} k_B T D_\alpha(\rho_S||\tau_S)$$
$$= k_B T D_0(\rho_S||\tau_S). \quad (B12)$$

For state formation,

$$(\tau_S \otimes |W_1\rangle\langle W_1|, H_S + H_W) \rightarrow (\rho_S \otimes |W_0\rangle\langle W_0|, H_S + H_W), \quad (B13)$$

we must have

$$D_\alpha(\tau_S||\tau_S) + D_\alpha(|W_1\rangle\langle W_1|||\tau_W)$$
$$\geqslant D_\alpha(\rho_S||\tau_S) + D_\alpha(|W_0\rangle\langle W_0|||\tau_W), \quad (B14)$$

giving

$$W_1 - W_0 \geqslant k_B T D_\alpha(\rho_S||\tau_S), \quad (B15)$$

for all $\alpha \geqslant 0$. So, we have

$$W_1 - W_0 \geqslant \sup_{\alpha \geqslant 0} k_B T D_\alpha(\rho_S||\tau_S)$$
$$= k_B T D_\infty(\rho_S||\tau_S). \quad (B16)$$

APPENDIX C: PROOFS

1. Proof of Theorem 1

We first list the precise statement on the connection between the thermomajorization curves and existence of the thermal operations and Gibbs preserving stochastic matrices and then list a theorem regarding the coinciding of thermomajorization curves. After that, we prove Theorem 1.

The distance we use is the norm-1 distance:

$$\|\rho - \sigma\|_1 = \text{Tr}(\sqrt{(\rho - \sigma)^\dagger(\rho - \sigma)}). \quad (C1)$$

Since we only consider diagonal states, the norm-1 distance is simply

$$\|\rho - \sigma\|_1 = \sum_i |(\boldsymbol{p}_\rho)_i - (\boldsymbol{p}_\sigma)_i|. \quad (C2)$$

Theorem 5: Thermal Nielsen theorem. Consider two block-diagonal states ρ and σ with Hamiltonian H and their corresponding population vectors are $\boldsymbol{p}_\rho$ and $\boldsymbol{p}_\sigma$.

(1) For any $\epsilon > 0$, there exists a thermal operation $\mathcal{E}$ such that $\mathcal{E}(\rho)$ is arbitrarily close to σ, i.e., $\|\mathcal{E}(\rho) - \sigma\|_1 < \epsilon$ if and only if the thermomajorization curve of ρ lies above or on the thermomajorization curve of σ.

(2) There exists a Gibbs preserving stochastic map G such that $G \cdot \boldsymbol{p}_\rho = \boldsymbol{p}_\sigma$ if and only if the thermomajorization curve of ρ lies above or on the thermomajorization curve of σ.

Proof. For the proof, see Theorems 6 and 7 and Remark 10 in Ref. [55].

Theorem 5 shows whether the existence of quantum thermal operations or Gibbs preserving stochastic matrices is related to thermomajorization curves. Next, we list a theorem related to thermomajorization coincidence.

Theorem 6. Consider two states ρ and σ with Hamiltonian H. If the thermomajorization curve of ρ lies above or on the thermomajorization curve of σ, then $D(\rho||\tau) \geqslant D(\sigma||\tau)$. The equality signs hold if and only if two curves coincide.

Proof. Suppose the population vectors of state ρ and σ are $\boldsymbol{p}_\rho$ and $\boldsymbol{p}_\sigma$. The thermomajorization curve of ρ lies above and on the thermomajorization curve of σ. From Theorem 5 there exists a Gibbs preserving stochastic matrix G such that $G \cdot \boldsymbol{p}_\rho = \boldsymbol{p}_\sigma$. Since ρ and σ are block diagonal, the relative entropy is the same as its classical version: $\blacksquare$

$$D(\rho||\tau) = D(\boldsymbol{p}_\rho||\boldsymbol{p}_\tau), \quad (C3)$$

$$D(\sigma||\tau) = D(\boldsymbol{p}_\sigma||\boldsymbol{p}_\tau). \quad (C4)$$

From the data processing inequality, we have

$$D(\boldsymbol{p}_\rho||\boldsymbol{p}_\tau) \geqslant D(G \cdot \boldsymbol{p}_\rho||G \cdot \boldsymbol{p}_\tau) \quad (C5)$$
$$= D(\boldsymbol{p}_\sigma||\boldsymbol{p}_\tau). \quad (C6)$$

This completes the first part of the proof.

The data processing inequality saturates if and only if there exists a recovery map R defined by $R_{ij} = G_{ji}(\boldsymbol{p}_\tau)_i/(\boldsymbol{p}_\tau)_j$ such that $R \cdot \boldsymbol{p}_\sigma = \boldsymbol{p}_\rho$, where $(\cdot)_{ij}$ is the ij component of the matrix [32]. It is straightforward to show that R preserves the Gibbs distribution: $R \cdot \boldsymbol{p}_\tau = \boldsymbol{p}_\tau$. So, $\boldsymbol{p}_\sigma$ thermomajorizes $\boldsymbol{p}_\rho$. σ's thermomajorization curve lies above or on ρ's thermomajorization. Hence, their thermomajorization curves coincide.

Now, we write down the precise version of Theorem 1.

Theorem 7. Consider two d-dimensional diagonal states ρ and σ. The following two are equivalent.

(1) The thermomajorization curves of states ρ and σ coincide.

(2) For all $\epsilon_1, \epsilon_2 > 0$, there exists a thermal operation $\mathcal{E}$ such that $\|\mathcal{E}(\rho) - \sigma\|_1 < \epsilon_1$ and the corresponding entropy production $\Sigma_{\rho \rightarrow \mathcal{E}(\rho)} < \epsilon_2$.

Proof. $1 \rightarrow 1$: Since the thermomajorization curves of state ρ and σ coincide, for any ϵ there exists a thermal operation $\mathcal{E}$ such that $\|\mathcal{E}(\rho) - \sigma\|_1 < \epsilon$. The upper bound of entropy production is given as follows. The thermomajorization curves of ρ and σ coincide. From Theorem 6, we have $D_1(\rho||\tau) = D_1(\sigma||\tau)$. By definition of the relative entropy, $D_1(\mathcal{E}(\rho)||\tau) = S(\mathcal{E}(\rho)) - \beta\text{Tr}(\mathcal{E}(\rho)H)$. $\mathcal{E}(\rho)$ and σ are ϵ close. From the Zhang-Audenaert inequality [32], we have

$$|S(\sigma) - S(\mathcal{E}(\rho))| \leqslant \tfrac{1}{2}\epsilon(\log d - 1) + H(\epsilon), \quad (C7)$$

where $H(\cdot)$ is the binary entropy function. This gives the entropy difference upper bound. The second term in relative entropy is bounded by

$$|\text{Tr}[(\sigma - \mathcal{E}(\rho))H]| \leqslant \epsilon E_{\max}, \quad (C8)$$

where $E_{\max}$ is the maximal eigenvalues in the Hamiltonian H. The relative entropy is bounded by

$$|D_1(\sigma||\tau) - D_1(\mathcal{E}(\rho)||\tau)|$$
$$\leqslant \tfrac{1}{2}\epsilon(\log d - 1) + \epsilon\beta E_{\max} + H(\epsilon). \quad (C9)$$

Since we have $D_1(\rho||\tau) = D_1(\sigma||\tau)$,

$$|D_1(\rho||\tau) - D_1(\mathcal{E}(\rho)||\tau)| \leqslant \tfrac{1}{2}\epsilon(\log d - 1) + \epsilon\beta E_{\max}$$
$$+ H(\epsilon). \tag{C10}$$

Let $f(\epsilon) = \tfrac{1}{2}\epsilon(\log d - 1) + \epsilon\beta E_{\max} + H(\epsilon)$ be an increasing function about ϵ in $[0, \tfrac{1}{2}]$ and $f(0) = 0$, $f(1/2) = \tfrac{1}{4}(\log d - 1) + \tfrac{1}{2}\beta E_{\max} + \log 2$. We denote the corresponding inverse function in $[0, f(1/2)]$ as $f^{-1}(x)$. For any $\epsilon_1, \epsilon_2 > 0$, if $\epsilon_2 < f(1/2)$, we can take $\epsilon = \tfrac{1}{2}\min\{\epsilon_1, f^{-1}(\epsilon_2)\}$. Then $||\mathcal{E}(\rho) - \sigma||_1 < \epsilon \leqslant \tfrac{1}{2}\epsilon_1 < \epsilon_1$ and $|D_1(\rho||\tau) - D_1(\mathcal{E}(\rho)||\tau)| \leqslant f(\epsilon) \leqslant f(\tfrac{1}{2}f^{-1}(\epsilon_2)) < f(f^{-1}(\epsilon_2)) = \epsilon_2$. If $\epsilon_2 \geqslant f(1/2)$, we take $\epsilon = \min\{\epsilon_1, \tfrac{1}{4}\}$. Then $||T(\rho) - \sigma||_1 < \epsilon \leqslant \epsilon_1$ and $|D_1(\rho||\tau) - D_1(T(\rho)||\tau)| \leqslant f(\epsilon) \leqslant f(1/4) < f(1/2) \leqslant \epsilon_2$.

$1 \to 1$ by contradiction: Since for all $\epsilon_1 > 0$, there exists a thermal operation $\mathcal{E}$ such that $||\mathcal{E}(\rho) - \sigma||_1 < \epsilon_1$, the thermomajorization curve ρ lies above or on the thermomajorization curve σ (Theorem 5). Assume the thermomajorization curves of ρ and σ do not coincide, then $|D_1(\rho||\tau) - D_1(\sigma||\tau)| \neq 0$ (Theorem 6). We give a bound on $|D_1(\rho||\tau) - D_1(\sigma||\tau)|$:

$$|D_1(\rho||\tau) - D_1(\sigma||\tau)|$$
$$\leqslant |D_1(\rho||\tau) - D_1(\mathcal{E}(\rho)||\tau)| + |D_1(\mathcal{E}(\rho)||\tau) - D_1(\sigma||\tau)|$$
$$< \epsilon_2 + \tfrac{1}{2}\epsilon_1(\log d - 1) + \epsilon_1\beta E_{\max} + H(\epsilon_1). \tag{C11}$$

Since ϵ_1 and ϵ_2 are arbitrary and

$$\lim_{\epsilon_1,\epsilon_2\to 0} \epsilon_2 + 2\epsilon_1(\log d - 1) + \epsilon_1\beta E_{\max} + H(\epsilon_1) = 0, \tag{C12}$$

we know that $|D_1(\rho||\tau) - D_1(\sigma||\tau)| \neq 0$ and is a finite fixed positive number. This contradicts Eq. (C12). So the two curves must coincide. ∎

2. Proof of Theorem 3

We first write down the precise version of Theorem 3.

Theorem 8. Consider two states ρ and σ with Hamiltonian H and a catalyst state c with Hamiltonian H_c. For any $\epsilon_1, \epsilon_2 > 0$, if there exists a thermal operation $\mathcal{E}$ such that $||\mathcal{E}(\rho \otimes c) - \sigma \otimes c||_1 < \epsilon_1$ and the corresponding entropy production $\Sigma_{\rho\otimes c\to\sigma\otimes c} < \epsilon_2$, then there exists another thermal operation $\mathcal{T}$ such that $||\mathcal{T}(\rho) - \sigma||_1 < \epsilon_1$ and the corresponding entropy production $\Sigma_{\rho\to\sigma} < \epsilon_2$.

Proof. From Theorem 7, the thermomajorization curves of $\rho \otimes c$ and $\sigma \otimes c$ coincide. Next, we show that the thermomajorization curves of ρ and σ coincide. Suppose $\boldsymbol{f}_{\rho,H} = \{(y_i^{(\rho)}, k_i^{(\rho)})\}_i, \boldsymbol{f}_{\sigma,H} = \{(y_i^{(\sigma)}, k_i^{(\sigma)})\}_i$, and $\boldsymbol{f}_{c,H_c} = \{(y_i^{(c)}, k_i^{(c)})\}_i$, respectively. Here, we coarse grain all segments with the same slopes and there are no repetitive slopes in $\boldsymbol{f}_{\rho,H}$, $\boldsymbol{f}_{\sigma,H}$, and $\boldsymbol{f}_{c,H_c}$. The largest slope of the $\rho \otimes c$ curve is $k_1^{(\rho)}k_1^{(c)}$ with y-coordinate change $y_1^{(\rho)}y_1^{(c)}$. And, the largest slope of the $\sigma \otimes c$ curve is $k_1^{(\sigma)}k_1^{(c)}$ with y-coordinate change $y_1^{(\sigma)}y_1^{(c)}$. Since the curves of $\rho \otimes c$ and $\sigma \otimes c$ coincide, we must have

$$k_1^{(\rho)}k_1^{(c)} = k_1^{(\sigma)}k_1^{(c)}, \tag{C13}$$

$$y_1^{(\rho)}y_1^{(c)} = y_1^{(\sigma)}y_1^{(c)}. \tag{C14}$$

This leads to $k_1^{(\rho)} = k_1^{(\sigma)}$ and $y_1^{(\rho)} = y_1^{(\sigma)}$.

We can remove the contribution of $(k_1^{(\rho)}, y_1^{(\rho)})$ and $(k_1^{(\sigma)}, y_1^{(\sigma)})$ from the curves $\rho \otimes c$ and $\sigma \otimes c$, respectively. The two new curves also coincide since we remove identical segments from two identical thermomajorization curves. With the two new curves and a similar argument, we have

$$k_2^{(\rho)}k_1^{(c)} = k_2^{(\sigma)}k_1^{(c)}, \tag{C15}$$

$$y_2^{(\rho)}y_1^{(c)} = y_2^{(\sigma)}y_1^{(c)}, \tag{C16}$$

which lead to $k_2^{(\rho)} = k_2^{(\sigma)}$ and $y_2^{(\rho)} = y_2^{(\sigma)}$. If we continue this procedure, we can show that $k_i^{(\rho)} = k_i^{(\sigma)}$ and $y_i^{(\rho)} = y_i^{(\sigma)}$ for any i. Then the ρ and σ curves coincide. So for any ϵ_1 and ϵ_2, there exists another thermal operation $\mathcal{T}$ such that $||\mathcal{T}(\rho) - \sigma||_1 < \epsilon_1$ and the corresponding entropy production $\Sigma_{\rho\to\sigma} < \epsilon_2$. ∎

3. Proof of Theorem 4

We first establish a theorem regarding the equality of α-Rényi entropy.

Theorem 9. Consider $\boldsymbol{p}$ and $\boldsymbol{q}$ two m-dimensional probability distributions. If $D_\alpha(\boldsymbol{p}||\boldsymbol{\eta}) = D_\alpha(\boldsymbol{q}||\boldsymbol{\eta})$ for any $\alpha \in \mathbf{R}$ where $\boldsymbol{\eta}$ is the m-dimensional uniform distribution, then $\boldsymbol{p}$ and $\boldsymbol{q}$ are the same up to a reorder.

Proof. The α-Rényi divergence of $\boldsymbol{p}$ from the uniform distribution $\boldsymbol{\eta}$ is

$$D_\alpha(\boldsymbol{p}||\boldsymbol{\eta}) = \frac{1}{\alpha - 1}\log(||\boldsymbol{p}||_\alpha)^\alpha + \log m, \tag{C17}$$

where $||\cdot||_\alpha$ is the α norm. And the ∞-Rényi divergence picks the maximal component in the distribution

$$D_\infty(\boldsymbol{p}||\boldsymbol{\eta}) = \max_{p_i} \log p_i + \log m. \tag{C18}$$

The equal α Rényi means $\boldsymbol{p}$ and $\boldsymbol{q}$ have the same α norm. Taking $\alpha \to \infty$ gives

$$\max_{p_i} p_i = \max_{q_i} q_i. \tag{C19}$$

$\boldsymbol{p}$ and $\boldsymbol{q}$ have the same maximal component. We can remove the corresponding maximal component from both distributions and they still have the same α norm:

$$||\boldsymbol{p} \setminus \{\max_{p_i} p_i\}||_\alpha = ||\boldsymbol{q} \setminus \{\max_{q_i} q_i\}||_\alpha. \tag{C20}$$

Again, we take $\alpha \to \infty$, which gives that the second maximal components in $\boldsymbol{p}$ and $\boldsymbol{q}$ are the same. Continuing this procedure indicates that $\boldsymbol{p}$ and $\boldsymbol{q}$ are the same up to a reorder. ∎

Now, we are ready to prove Theorem 4.

Theorem 10 (Theorem 4): Given a system with Hamiltonian H and states ρ and σ, the following are equivalent.

(1) Thermomajorization curves of ρ and σ coincide.

(2) $D_\alpha(\rho||\tau) = D_\alpha(\sigma||\tau)$, for all $\alpha \in \mathbb{R}$.

Proof. $1 \to 2$: Since the thermomajorization curves of ρ and σ coincide. There exist two Gibbs-preserving stochastic maps E and G such that $E \cdot \boldsymbol{p}_\rho = \boldsymbol{p}_\sigma$ and $G \cdot \boldsymbol{p}_\sigma = \boldsymbol{p}_\rho$. With the data processing inequality of Rényi α divergence, for all $\alpha \in \mathbb{R}$, we have [13,16]

$$D_\alpha(\boldsymbol{p}_\rho||\boldsymbol{p}_\tau) \geqslant D_\alpha(E\boldsymbol{p}_\rho||E\boldsymbol{p}_\tau) = D_\alpha(\boldsymbol{p}_\sigma||\boldsymbol{p}_\tau), \tag{C21}$$

$$D_\alpha(\boldsymbol{p}_\sigma||\boldsymbol{p}_\tau) \geqslant D_\alpha(G\boldsymbol{p}_\sigma||G\boldsymbol{p}_\tau) = D_\alpha(\boldsymbol{p}_\rho||\boldsymbol{p}_\tau). \tag{C22}$$

Then $D_\alpha(\rho||\tau) = D_\alpha(\sigma||\tau)$, for all $\alpha \in \mathbb{R}$.

Proof. $2 \rightarrow 1$: We use a basic tool in single-shot thermodynamics—the embedding map [13]. Here, the embedding map Γ sends one distribution to a larger dimensional distribution. And, Γ maps the Gibbs distribution of the system to a larger uniform distribution. (To avoid technicalities, we assume the Gibbs distribution is rational.) Γ has the following properties [13].

(1) $D_\alpha(\boldsymbol{p}_\sigma \| \boldsymbol{p}_\tau) = D_\alpha(\Gamma(\boldsymbol{p}_\sigma) \| \Gamma(\boldsymbol{p}_\tau))$.

(2) $\boldsymbol{p}$ thermomajorizes $\boldsymbol{q}$ with respect to the Gibbs distribution if and only if $\Gamma(\boldsymbol{p})$ majorizes $\Gamma(\boldsymbol{q})$.

From $D_\alpha(\rho \| \tau) = D_\alpha(\sigma \| \tau)$, we have

$$D_\alpha(\Gamma(\boldsymbol{p}_\rho) \| \Gamma(\boldsymbol{p}_\tau)) = D_\alpha(\Gamma(\boldsymbol{p}_\sigma) \| \Gamma(\boldsymbol{p}_\tau)) \tag{C23}$$

for all α and $\Gamma(\boldsymbol{p}_\tau)$ is a uniform distribution. From Theorem 9,

$$\Gamma(\boldsymbol{p}_\rho) = \Gamma(\boldsymbol{p}_\sigma) \tag{C24}$$

up to a permutation. Then $\Gamma(\boldsymbol{p}_\rho)$ and $\Gamma(\boldsymbol{p}_\sigma)$ majorize each other. We have that $\boldsymbol{p}_\rho$ and $\boldsymbol{p}_\sigma$ thermomajorize each other. Hence the thermomajorization curves of ρ and σ coincide. ∎

APPENDIX D: DETAILS ON THE CONSTRUCTIONS FOR ANY STATE TRANSITIONS

Proving this requires constructing the efficient work reservoir for $(\boldsymbol{p}_S, \boldsymbol{E}_S) \rightarrow (\boldsymbol{p}'_S, \boldsymbol{E}_S)$. We denote initial and final cumulative probability distributions of the system as $\boldsymbol{P} = \{P_i\}_{i \in \{0\} \cup \mathcal{S}}$ and $\boldsymbol{P}' = \{P'_i\}_{i \in \{0\} \cup \mathcal{S}}$, where $P_0 = P'_0 = 0$. And, they satisfy $P_i - P_{i-1} = p_i$ and $P'_i - P'_{i-1} = p'_i$ for all $i \in \mathcal{S}$. Let $\boldsymbol{R} = \{R_i\}_{i \in \{0\} \cup \mathcal{W}} = \boldsymbol{P} \cup \boldsymbol{P}'$—a cumulative probability distribution where $\mathcal{W} = \{1, 2, \ldots, N\}$ and N is the dimension of corresponding probability distribution, denoted $\boldsymbol{r} = \{r_i\}_{i \in \mathcal{W}}$. Then there exist mappings $\lambda, \lambda' : \mathcal{W} \rightarrow \mathcal{S}$ from $\mathcal{W} = \{1, 2, \ldots, N\}$ to system eigenstates $\mathcal{S} = \{1, 2, \ldots n\}$ such that

$$p'_i = \sum_{j \in \lambda^{-1}(i)} r_j, \tag{D1}$$

$$p_i = \sum_{j \in \lambda'^{-1}(i)} r_j. \tag{D2}$$

Appendix E constructs the mappings λ and λ'.

The work reservoir probabilities are $\boldsymbol{p}_W$ and $\boldsymbol{p}'_W$, where $\boldsymbol{p}_W = (\boldsymbol{r}, \boldsymbol{0})$ and $\boldsymbol{p}'_W = (\boldsymbol{0}, \boldsymbol{r})$. And the energy levels are $\boldsymbol{E}_W = \{\epsilon_1, \ldots, \epsilon_N, \epsilon'_1, \ldots, \epsilon'_N\}$. To make this efficient for a n-dimensional transition $\boldsymbol{p}_S \rightarrow \boldsymbol{p}'_S$ in a system with energy levels $\boldsymbol{E}_S = \{e_1, \ldots, e_n\}$, we require that (a) there exist sets of positive numbers $\{k_i\}_{i=1}^n$ and $\{k'_i\}_{i=1}^n$ such that

$$r_j e^{\beta \epsilon_j} = k_i, \quad \text{for all } j \in \lambda^{-1}(i) \tag{D3}$$

and

$$r_j e^{\beta \epsilon'_j} = k'_i, \quad \text{for all } j \in \lambda'^{-1}(i) \tag{D4}$$

and (b)

$$p_i e^{\beta e_i} k_j = p'_j e^{\beta e_j} k'_i, \quad \text{for any pair } (i, j). \tag{D5}$$

According to Theorem 1, zero entropy is produced if and only if the thermomajorization curves of $\boldsymbol{p}_{SW} = \{p_i r_j\}_{i,j}$ over the energy levels $\boldsymbol{E}_{SW} = \{e_i + \epsilon_j\}_{i,j}$, and $\boldsymbol{p}'_{SW} = \{p'_i r_j\}_{i,j}$ over the energy levels $\boldsymbol{E}'_{SW} = \{e_i + \epsilon'_j\}_{i,j}$

are the same. (We neglect contributions from zero components in probability distribution.) From Eqs. (D1) and (D3), the thermomajorization curve $f_{\boldsymbol{p}_W, \boldsymbol{E}_W}$ has at most n distinct slopes $\{k_i\}_{i=1}^n$ with corresponding y-coordinate change $\{p'_i\}_{i=1}^n$; i.e., $\boldsymbol{f}_{\boldsymbol{p}_W, \boldsymbol{E}_W} = \{(p'_i, k_i)\}_{i=1}^n$. For the system, we have $\boldsymbol{f}_{\boldsymbol{p}_S, \boldsymbol{E}_S} = \{(p_i, p_i e^{\beta e_i})\}_{i=1}^n$. And, so, from Eq. (33) we have $\boldsymbol{f}_{\boldsymbol{p}_{SW}, \boldsymbol{E}_{SW}} = \{p_i p'_j, p_i e^{\beta e_i} k_j\}_{i,j=1}^n$. Similarly, we have $\boldsymbol{f}_{\boldsymbol{p}'_{SW}, \boldsymbol{E}_{SW}} = \{p'_i p_j, p'_i e^{\beta e_i} k'_j\}_{i,j=1}^n = \{p_i p'_j, p'_j e^{\beta e_j} k'_i\}_{i,j=1}^n$. From condition 3, $\boldsymbol{f}_{\boldsymbol{p}_{SW}, \boldsymbol{E}_{SW}} = \boldsymbol{f}_{\boldsymbol{p}'_{SW}, \boldsymbol{E}_{SW}}$. That is, the two thermomajorization curves coincide.

Next, we determine the energy levels $\{\epsilon_1, \ldots, \epsilon_N\}$ and $\{\epsilon'_1, \ldots, \epsilon'_N\}$ explicitly. We fix one energy level, for example ϵ_1, and express all other energy levels in terms of it. To determine k_i, from condition 3 we have

$$p_j e^{\beta e_j} k_i = p'_i e^{\beta e_i} k'_j, \tag{D6}$$

$$p_j e^{\beta e_j} k_1 = p'_1 e^{\beta e_1} k'_j. \tag{D7}$$

Dividing gives

$$k_i = k_1 \frac{p'_i e^{\beta e_i}}{p'_1 e^{\beta e_1}}, \tag{D8}$$

from which we have

$$\epsilon_x = \epsilon_1 + k_B T \log\left(\frac{r_1}{r_x} \frac{p'_i e^{\beta e_i}}{p'_1 e^{\beta e_1}}\right), \tag{D9}$$

for all $x \in \lambda^{-1}(i)$. k'_i can be determined through condition 3 by setting $j = 1$:

$$k'_i = k_1 \frac{p_i e^{\beta e_i}}{p'_1 e^{\beta e_1}}, \tag{D10}$$

from which we have

$$\epsilon'_x = \epsilon_1 + k_B T \log\left(\frac{r_1}{r_x} \frac{p_i e^{\beta e_i}}{p'_1 e^{\beta e_1}}\right), \tag{D11}$$

for all $x \in \lambda'^{-1}(i)$. The average extractable work from the state transition is

$$\langle W \rangle = \sum_{x=1}^N r_x (\epsilon'_x - \epsilon_x) \tag{D12}$$

and we have

$$\sum_{x=1}^N r_x \epsilon_x = \sum_{x=1}^N r_x \left[\epsilon_1 + k_B T \log\left(\frac{r_1}{r_x} \frac{p'_i e^{\beta e_i}}{p'_1 e^{\beta e_1}}\right) \right] \tag{D13}$$

$$= k_B T D_1(\boldsymbol{p}'_S \| \boldsymbol{\tau}_S) + C, \tag{D14}$$

$$\sum_{x=1}^N r_x \epsilon'_x = \sum_{x=1}^N r_x \left[\epsilon_1 + k_B T \log\left(\frac{r_1}{r_x} \frac{p_i e^{\beta e_i}}{p'_1 e^{\beta e_1}}\right) \right] \tag{D15}$$

$$= k_B T D_1(\boldsymbol{p}_S \| \boldsymbol{\tau}_S) + C, \tag{D16}$$

where

$$C = \epsilon_1 - e_1 + k_B T \left(\sum_x r_x \log \frac{r_1}{r_x p'_1} - Z_S \right) \tag{D17}$$

is a constant. This recovers the stochastic thermodynamics result:

$$\langle W \rangle = k_{\mathrm{B}} T [D_1(\boldsymbol{p}_S || \boldsymbol{\tau}_S) - D_1(\boldsymbol{p}'_S || \boldsymbol{\tau}_S)]. \tag{D18}$$

This gives the distribution $\{r_i\}_{i \in \mathcal{W}}$ and energy levels [Eqs. (D9) and (D11)] for the efficient work reservoir explicitly, completing the construction.

APPENDIX E: CONSTRUCTING λ AND λ'

This section constructs the mappings λ and λ' in Eqs. (D1) and (D2). We have $p'_i = P'_i - P'_{i-1}$ and P'_i, $P'_{i-1} \in \boldsymbol{R}$. We define sets $\sigma'_i \subseteq \{1, 2, \ldots N\}$ such that

$$\sum_{i \in \sigma'_i} r_i = P'_i. \tag{E1}$$

We have $\sigma'_0 = \{\}$, $\sigma'_n = \{1, 2, \ldots N\}$, and $\sigma'_0 \subset \sigma'_1 \subset \cdots \subset \sigma'_n$. $\lambda : \{1, 2, \ldots, N\} \to \{1, 2, \ldots, n\}$ is defined by $\lambda(\sigma'_i \setminus \sigma'_{i-1}) = i$ for $i = \{1, 2, \ldots, n\}$. We have

$$\sum_{j \in \lambda^{-1}(i)} r_j = \sum_{j \in \sigma'_i \setminus \sigma'_{i-1}} r_j$$

$$= \sum_{j \in \sigma'_i} r_j - \sum_{j \in \sigma'_{i-1}} r_j$$

$$= P'_i - P'_{i-1} = p_i. \tag{E2}$$

We define λ' similarly.

APPENDIX F: A DIFFERENT WAY TO CONSTRUCT EFFICIENT WORK RESERVOIRS

This section presents an alternative construction of a work reservoir for trivial Hamiltonian $\boldsymbol{E}_S = 0$. More directly, the efficient work reservoir for a transition is not unique.

Consider a $2n^2$-dimensional work reservoir of which energy levels are $\boldsymbol{E}_W = \{\epsilon_{11}, \ldots, \epsilon_{nn}, \epsilon'_{11}, \ldots \epsilon'_{nn}\}$. The initial work reservoir probability distribution is $(\boldsymbol{p} \otimes \boldsymbol{p}', \boldsymbol{0})$ and the final is $(\boldsymbol{0}, \boldsymbol{p} \otimes \boldsymbol{p}')$. The energy levels satisfy

$$p_1 p'_j e^{\beta \epsilon_{1j}} = \cdots = p_n p'_j e^{\beta \epsilon_{nj}} = k_j \quad \text{for } j = 1, \ldots, n, \tag{F1}$$

$$p_i p'_1 e^{\beta \epsilon'_{i1}} = \cdots = p_i p'_n e^{\beta \epsilon'_{in}} = k'_i \quad \text{for } i = 1, \ldots, n, \tag{F2}$$

$$k'_i p'_j = p_i k_j \quad \text{for any pair } (i, j). \tag{F3}$$

These conditions ensure that the initial total curve coincides with the final curve. We have

$$\epsilon_{ij} = k_{\mathrm{B}} T \log \frac{k_j}{p_i p'_j}, \tag{F4}$$

$$\epsilon'_{ij} = k_{\mathrm{B}} T \log \frac{k'_i}{p_i p'_j}. \tag{F5}$$

The amount of work that can be extracted is

$$\langle W \rangle = \sum_{ij} p_i p'_j (\epsilon'_{ij} - \epsilon_{ij}) \tag{F6}$$

$$= k_{\mathrm{B}} T \sum_{ij} p_i p'_j \log \frac{k'_i}{k_j} \tag{F7}$$

$$= k_{\mathrm{B}} T \sum_{ij} p_i p'_j \log \frac{p_i}{p'_j} \tag{F8}$$

$$= k_{\mathrm{B}} T (H(\boldsymbol{p}') - H(\boldsymbol{p})). \tag{F9}$$

APPENDIX G: EFFICIENT WORK RESERVOIR EXAMPLES

The following analyzes several efficient work reservoirs for nontrivial Hamiltonians and time-dependent Hamiltonians.

We first study a nontrivial Hamiltonian. Consider a two-level system with the Gibbs distribution $\boldsymbol{\tau}_S = (e^{-\beta e_1}/Z_S, e^{-\beta e_2}/Z_S) = (\frac{2}{3}, \frac{1}{3})$. We begin with the distribution $\boldsymbol{p}_S = (\frac{1}{2}, \frac{1}{2})$ and end with $\boldsymbol{p}'_S = (\frac{1}{3}, \frac{2}{3})$. For the efficient work reservoir, we set $p_W = (\boldsymbol{r}, \boldsymbol{0})$ and $p'_W = (\boldsymbol{0}, \boldsymbol{r})$, where $\boldsymbol{r} = (\frac{1}{2}, \frac{1}{3}, \frac{1}{6})$. The work reservoir energy levels satisfy $\exp(-\beta \epsilon_i) = \{\frac{1}{4} a, \frac{2}{3} a, \frac{1}{12} a\}$ for $i = 1, 2, 3$ and $\exp(-\beta \epsilon'_i) = \{\frac{1}{3} a, \frac{4}{9} a, \frac{2}{9} a\}$ for $i = 1, 2, 3$ and where a is a positive number. The work reservoir's energy change is

$$\langle W \rangle = \sum_{i=1}^{3} r_i(\epsilon'_i - \epsilon_i) \tag{G1}$$

$$= \frac{1}{2} k_{\mathrm{B}} T \log \frac{3}{4} + \frac{1}{3} k_{\mathrm{B}} T \log \frac{3}{2} + \frac{1}{6} k_{\mathrm{B}} T \log \frac{3}{8} \tag{G2}$$

$$= k_{\mathrm{B}} T D_1(\boldsymbol{p}_S || \boldsymbol{\tau}_S) - k_{\mathrm{B}} T D_1(\boldsymbol{p}'_S || \boldsymbol{\tau}_S) \tag{G3}$$

$$= -0.17216 \, k_{\mathrm{B}} T. \tag{G4}$$

The amount of the work is the negative nonequilibrium free-energy difference. Table III plots the thermomajorization curves.

The second example concerns a state transition under a time-dependent Hamiltonian. The initial distribution is $\boldsymbol{p}_S = (\frac{1}{2}, \frac{1}{2})$ and the initial Gibbs distribution is $\boldsymbol{\tau}_S = (e^{-\beta e_1}/Z_S, e^{-\beta e_2}/Z_S) = (\frac{1}{3}, \frac{2}{3})$. The final distribution is $\boldsymbol{p}'_S = (\frac{2}{3}, \frac{1}{3})$ and final Gibbs distribution is $\boldsymbol{\tau}'_S = (e^{-\beta e'_1}/Z'_S, e^{-\beta e'_2}/Z'_S) = (\frac{1}{2}, \frac{1}{2})$. For the efficient work reservoir, we set $\boldsymbol{p}_W = (\boldsymbol{r}, \boldsymbol{0})$ and $\boldsymbol{p}'_W = (\boldsymbol{0}, \boldsymbol{r})$ where $\boldsymbol{r} = (\frac{1}{2}, \frac{1}{3}, \frac{1}{6})$. The work reservoir energy levels satisfy $\exp(-\beta \epsilon_i) = \{\frac{3}{8} a, \frac{1}{2} a, \frac{1}{8} a\}$ for $i = 1, 2, 3$ and $\exp(-\beta \epsilon'_i) = \{\frac{1}{3} \frac{Z_S}{Z'_S} a, \frac{4}{9} \frac{Z_S}{Z'_S} a, \frac{2}{9} \frac{Z_S}{Z'_S} a\}$ for $i = 1, 2, 3$. The work reservoir's energy change is

$$\langle W \rangle = \sum_{i=1}^{3} r_i(\epsilon'_i - \epsilon_i) \tag{G5}$$

$$= \frac{1}{2} k_{\mathrm{B}} T \log \frac{9}{8} \frac{Z'_S}{Z_S} + \frac{1}{3} k_{\mathrm{B}} T \log \frac{9}{8} \frac{Z'_S}{Z_S} \tag{G6}$$

$$+ \frac{1}{6} k_{\mathrm{B}} T \log \frac{9}{16} \frac{Z'_S}{Z_S} \tag{G7}$$

$$= k_{\mathrm{B}} T (D_1(\boldsymbol{p}_S || \boldsymbol{\tau}_S) - \log Z_S) \tag{G8}$$

$$- k_{\mathrm{B}} T (D_1(\boldsymbol{p}'_S || \boldsymbol{\tau}_S) - \log Z'_S) \tag{G9}$$

$$= \left(0.0022585 + \log \frac{Z'_S}{Z_S} \right) k_{\mathrm{B}} T. \tag{G10}$$

The amount of work is the nonequilibrium free-energy difference. Table IV plots the thermomajorization curves.

TABLE III. Thermomajorization curves with elbow point coordinates of ρ_S, ρ_W, ρ_{SW}, ρ_S', ρ_W', and ρ_{SW}' for a state transition with a nontrivial Hamiltonian. For the initial work reservoir, the red points x-axis coordinates are $\frac{1}{12}a$, $\frac{1}{3}a$, a, $\frac{11}{9}a$, $\frac{14}{9}a$, and $2a$, respectively. For initial total curves, the x-axis coordinates are $\frac{1}{36}Z_Sa$, $\frac{1}{9}Z_Sa$, $\frac{5}{36}Z_Sa$, $\frac{1}{3}Z_Sa$, $\frac{5}{9}Z_Sa$, Z_Sa, $\frac{29}{27}Z_Sa$, $\frac{32}{27}Z_Sa$, $\frac{36}{27}Z_Sa$, $\frac{40}{27}Z_Sa$, $\frac{46}{27}Z_Sa$, and $2Z_Sa$, respectively. For the final work reservoir, the red points x-axis coordinates are $\frac{1}{3}a$, $\frac{5}{9}a$, a, $\frac{13}{12}a$, $\frac{4}{3}a$, and $2a$, respectively. For the final total curve, the red points x-axis coordinates are $\frac{1}{9}Z_Sa$, $\frac{5}{27}Z_Sa$, $\frac{1}{3}Z_Sa$, $\frac{5}{9}Z_Sa$, $\frac{19}{27}Z_Sa$, Z_Sa, $\frac{37}{36}Z_Sa$, $\frac{39}{36}Z_Sa$, $\frac{42}{27}Z_Sa$, $\frac{48}{27}Z_Sa$, $\frac{56}{27}Z_Sa$, and $2Z_Sa$, respectively.

	System	Work reservoir	Total = System $\otimes$ Work reservoir
Initial			
Final			
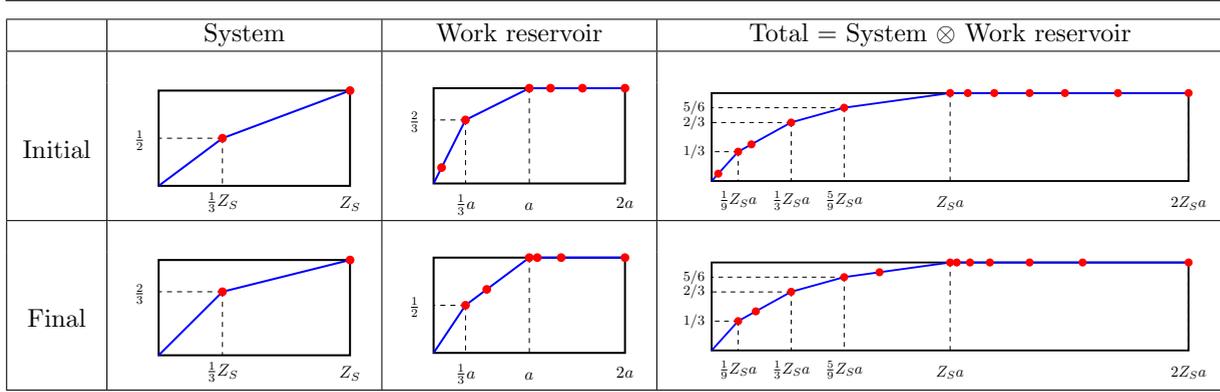
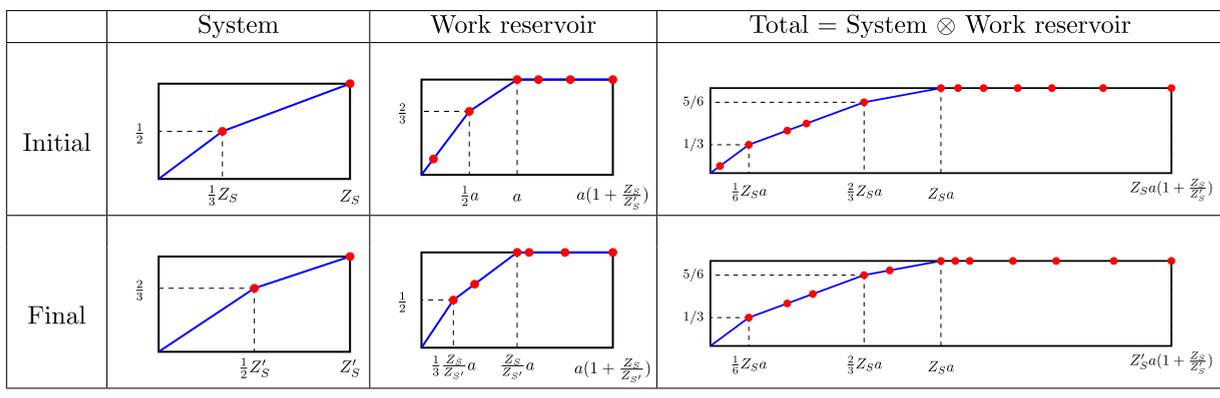

APPENDIX H: THERMOMAJORIZATION CURVES FORM A MONOID

Abstract algebra defines a *monoid M* as a set equipped with an associative binary operation and an identity element. This Appendix establishes that all possible thermomajorization curves at inverse temperature β with the regular direct product form a monoid M_β.

For a thermomajorization curve l with n distinct slopes, we use a set with n tuples to represent it:

$$l = \{(y_1, k_1), \ldots, (y_n, k_n)\}, \tag{H1}$$

where y_i and k_i are the y-coordinate change and the slope of the ith segment that satisfy $k_1 > \cdots > k_n > 0$ and $y_1 + \cdots + y_n = 1$. (We neglect subscripting with ρ and H.) Note that this definition is not one-to-one: For a thermomajorization curve l, there may be many states corresponding to curve l.

This Appendix uses the thermomajorization curve l and its representation $\boldsymbol{l}$ interchangeably.

The binary operation is defined as

$$\boldsymbol{l} \otimes \boldsymbol{m} := \left\{ \left(y_i^l y_j^m, k_i^l k_j^m \right) \right\}_{i,j} / \sim, \tag{H2}$$

where $\boldsymbol{l} = \{(y_i^l, k_i^l)\}_i$, $\boldsymbol{m} = \{(y_i^m, k_i^m)\}_i$, and $\sim$ means the segments with the same slopes are combined. The identity element is $\boldsymbol{I} = \{(1, 1)\}$.

Verifying that the set of all thermomajorization curves forms a monoid M_β is straightforward. In addition, M_β is commutative; i.e., $\boldsymbol{l} \otimes \boldsymbol{m} = \boldsymbol{m} \otimes \boldsymbol{l}$, for all $\boldsymbol{l}, \boldsymbol{m} \in M_\beta$. Not all elements in M_β have corresponding inverses. Only the elements with the form $\{(a, 1)\}$ have an inverse $\{(a^{-1}, 1)\}$. Thus, M_β is a monoid and not a group. Although the inverse may not exist, we have the following theorem.

TABLE IV. Thermomajorization curves with elbow point coordinates of ρ_S, ρ_W, ρ_{SW}, ρ_S', ρ_W', and ρ_{SW}' for a state transition under a time-dependent Hamiltonian. For the initial work reservoir, the red points x-axis coordinates are $\frac{1}{8}a$, $\frac{1}{2}a$, a, $(1 + \frac{2}{9}\frac{Z_S}{Z_{S'}})a$, $(1 + \frac{5}{9}\frac{Z_S}{Z_{S'}})a$, and $(1 + \frac{Z_S}{Z_{S'}})a$, respectively. For initial total curves, the x-axis coordinates are $\frac{1}{24}Z_Sa$, $\frac{1}{6}Z_Sa$, $\frac{1}{3}Z_Sa$, $\frac{5}{12}Z_Sa$, $\frac{2}{3}Z_Sa$, Z_Sa, $Z_Sa(1 + \frac{2}{27}\frac{Z_S}{Z_S'})$, $Z_Sa(1 + \frac{5}{27}\frac{Z_S}{Z_S'})$, $Z_Sa(1 + \frac{9}{27}\frac{Z_S}{Z_S'})$, $Z_Sa(1 + \frac{13}{27}\frac{Z_S}{Z_S'})$, $Z_Sa(1 + \frac{19}{27}\frac{Z_S}{Z_S'})$, and $Z_Sa(1 + \frac{Z_S}{Z_S'})$, respectively. For the final work reservoir, the red points x-axis coordinates are $\frac{1}{3}\frac{Z_S}{Z_{S'}}a$, $\frac{5}{9}\frac{Z_S}{Z_{S'}}a$, $\frac{Z_S}{Z_{S'}}a$, $(\frac{1}{8} + \frac{Z_S}{Z_{S'}})a$, $(\frac{1}{2} + \frac{Z_S}{Z_{S'}})a$, and $(1 + \frac{Z_S}{Z_{S'}})a$, respectively. For the final total curve, the red points x-axis coordinates are $\frac{1}{6}Z_Sa$, $\frac{7}{18}Z_Sa$, $\frac{1}{2}Z_Sa$, $\frac{2}{3}Z_Sa$, $\frac{7}{9}Z_Sa$, Z_Sa, $Z_Sa(1 + \frac{1}{16}\frac{Z_S'}{Z_S})$, $Z_Sa(1 + \frac{2}{16}\frac{Z_S'}{Z_S})$, $Z_Sa(1 + \frac{5}{16}\frac{Z_S'}{Z_S})$, $Z_Sa(1 + \frac{8}{16}\frac{Z_S'}{Z_S})$, $Z_Sa(1 + \frac{12}{16}\frac{Z_S'}{Z_S})$, and $Z_Sa(1 + \frac{Z_S'}{Z_S})$, respectively.

	System	Work reservoir	Total = System $\otimes$ Work reservoir
Initial			
Final			

Theorem 11: Cancellative. If $\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{a} \in M_\beta$ and $\boldsymbol{a} \otimes \boldsymbol{x} = \boldsymbol{a} \otimes \boldsymbol{y}$, then $\boldsymbol{x} = \boldsymbol{y}$.

Proof. The first element in $\boldsymbol{a} \otimes \boldsymbol{x}$ is $(y_1^a y_1^x, k_1^a k_1^x)$ and the first element in $\boldsymbol{a} \otimes \boldsymbol{y}$ is $(y_1^a y_1^y, k_1^a k_1^y)$. So, we have $y_1^x = y_1^y$ and $k_1^x = k_1^y$. Since we have

$$\boldsymbol{a} \otimes \boldsymbol{x} = \boldsymbol{a} \otimes \boldsymbol{y}, \tag{H3}$$

$$\boldsymbol{a} \otimes \left(\boldsymbol{x} \setminus \left(y_1^x, k_1^x \right) \right) = \boldsymbol{a} \otimes \left(\boldsymbol{y} \setminus \left(y_1^y, k_1^y \right) \right), \tag{H4}$$

we remove the same element on both sides. If we check the first element on both sides of the new equality, we have $y_2^x = y_2^y$ and $k_2^x = k_2^y$. Continuing this procedure, $y_i^x = y_i^y$ and $k_i^x = k_i^y$ for any i. Then we have $\boldsymbol{x} = \boldsymbol{y}$. ∎

These elementary facts allow exploring all possible work reservoirs for nondissipative state formation and work extraction. For state formation $(\tau, H) \to (\rho, H)$ with zero dissipation, we know the minimum segments of the work reservoir's thermomajorization curve are equal to the segments of ρ's thermomajorization curve.

Suppose the corresponding initial work reservoir's thermomajorization curve is x_1. The final work reservoir's thermomajorization curve y_1 has only one segment. Thus, $\boldsymbol{y}_1$ has inverse $\boldsymbol{y}_1^{-1}$. Since there is no dissipation,

$$\boldsymbol{x}_1 \otimes \boldsymbol{f}_{\tau,H} = \boldsymbol{y}_1 \otimes \boldsymbol{f}_{\rho,H}. \tag{H5}$$

Suppose there is another work reservoir suited for state formation whose initial and final thermomajorization curves are $\boldsymbol{f}_{\rho_W,H_W}$ and $\boldsymbol{f}_{\rho_W',H_W}$. Then

$$\boldsymbol{f}_{\rho_W,H_W} \otimes \boldsymbol{f}_{\tau,H} = \boldsymbol{f}_{\rho_W',H_W} \otimes \boldsymbol{f}_{\rho,H}. \tag{H6}$$

Multiply $\boldsymbol{x}_1$ on both sides of Eq. (H6) and use Theorem 11 to remove $\boldsymbol{f}_{\rho,H}$. Then

$$\boldsymbol{x}_1 \otimes \boldsymbol{f}_{\rho_W',H_W} = \boldsymbol{y}_1 \otimes \boldsymbol{f}_{\rho_W,H_W}. \tag{H7}$$

Since $\boldsymbol{y}_1$ has an inverse,

$$\boldsymbol{f}_{\rho_W,H_W} = \boldsymbol{x}_1 \otimes \boldsymbol{f}_{\rho_W',H_W} \otimes \boldsymbol{y}_1^{-1} \tag{H8}$$

$$= \boldsymbol{b} \otimes \boldsymbol{x}_1, \tag{H9}$$

where $\boldsymbol{b} = \boldsymbol{f}_{\rho_W',H_W} \otimes \boldsymbol{y}_1^{-1}$ or $\boldsymbol{f}_{\rho_W',H_W} = \boldsymbol{b} \otimes \boldsymbol{y}_1$.

So, we write any general work reservoirs $\boldsymbol{f}_{\rho_W,H_W}$ and $\boldsymbol{f}_{\rho_W',H_W}$ in terms of $\boldsymbol{x}_1$ and $\boldsymbol{y}_1$:

$$\boldsymbol{f}_{\rho_W,H_W} = \boldsymbol{b} \otimes \boldsymbol{x}_1,$$
$$\boldsymbol{f}_{\rho_W',H_W} = \boldsymbol{b} \otimes \boldsymbol{y}_1. \tag{H10}$$

This means the initial thermomajorization curve must be equal to the product of $\boldsymbol{x}_1$ and an arbitrary curve $\boldsymbol{b}$ and the final thermomajorization curve must equal the product of $\boldsymbol{y}_1$ and curve $\boldsymbol{b}$. These are the most general thermomajorization curves of the work reservoir for state formation with zero dissipation.

Next, we express this relation in terms of α-Rényi divergences. Recall the definition of the α free energy of state ρ:

$$F_\alpha(\rho) = F_{\text{eq}} + k_B T D_\alpha(\rho \| \tau) \tag{H11}$$

$$= F_{\text{eq}} + k_B T \frac{1}{\alpha - 1} \log \left(\sum_{i=1}^n \frac{p_i^\alpha}{q_i^{\alpha-1}} \right), \tag{H12}$$

where $\{p_i\}_{i=1}^n$ and $\{q_i\}_{i=1}^n$ are population vectors of state ρ and Gibbs distribution and $F_{\text{eq}} = -k_B T \log Z$ is the equilib-

rium free energy. The α free energy only depends on the thermomajorization curve's elbow points. Suppose ρ's thermomajorization curve is $\boldsymbol{f}_{\rho,H} = \{(y_i, k_i)\}_{i=1}^n$; then

$$D_\alpha(\rho \| \tau) = \frac{1}{\alpha - 1} \log \left(\sum_{i=1}^n \frac{p_i^\alpha}{(e^{-\beta \epsilon_i})^{\alpha-1}} Z^{\alpha-1} \right) \tag{H13}$$

$$= \frac{1}{\alpha - 1} \log \left(\sum_{i=1}^n \frac{p_i p_i^{\alpha-1}}{(e^{-\beta \epsilon_i})^{\alpha-1}} Z^{\alpha-1} \right) \tag{H14}$$

$$= \frac{1}{\alpha - 1} \log \left(\sum_{i=1}^n y_i k_i^{\alpha-1} Z^{\alpha-1} \right). \tag{H15}$$

For any state ρ and its thermomajorization curve $\boldsymbol{a}$, we use $F_\alpha(\boldsymbol{a}) = F_\alpha(\rho)$ to denote the α free energy. For the general work curves $\boldsymbol{f}_{\rho_W,H_W}$ and $\boldsymbol{f}_{\rho_W',H_W}$, from Eqs. (H5) and (H10), we have

$$F_\alpha(\boldsymbol{x}_1) + F_\alpha(\tau) = F_\alpha(\boldsymbol{y}_1) + F_\alpha(\rho), \tag{H16}$$

$$F_\alpha(\rho_W) = F_\alpha(\boldsymbol{x}_1) + F_\alpha(\boldsymbol{b}), \tag{H17}$$

$$F_\alpha(\rho_W') = F_\alpha(\boldsymbol{y}_1) + F_\alpha(\boldsymbol{b}). \tag{H18}$$

To remove $F_\alpha(\boldsymbol{b})$, we have

$$\frac{e^{F_\alpha(\rho_W')}}{e^{F_\alpha(\rho_W)}} = \frac{e^{F_\alpha(\boldsymbol{y}_1)}}{e^{F_\alpha(\boldsymbol{x}_1)}} = \frac{e^{F_\alpha(\tau)}}{e^{F_\alpha(\rho)}}, \tag{H19}$$

where

$$e^{F_\alpha(\tau)} = e^{F_{\text{eq}}}, \tag{H20}$$

$$e^{F_\alpha(\rho)} = e^{F_{\text{eq}}} Z_S \left(\sum_i p_i m_i^{\alpha-1} \right)^{\frac{1}{\alpha-1}} \tag{H21}$$

and $\boldsymbol{f}_{\rho,H} = \{(p_i, m_i)\}_i$. Then

$$\frac{e^{F_\alpha(\rho_W')}}{e^{F_\alpha(\rho_W)}} = \frac{\left(\sum_i p_i m_i^{\alpha-1} \right)^{\frac{1}{1-\alpha}}}{Z_S}. \tag{H22}$$

This relation bridges the work reservoir and the system and, thus, it is a Jarzynski-like equality in the nondissipative scenario. Thus, from information about work we learn system transitions [58]. For a general nondissipative state transition, we cannot write the general work reservoir thermomajorization curves as in Eq. (H10).

APPENDIX I: CARNOT ENGINES WITH EFFICIENT RESERVOIRS

The following introduces a qubit engine implemented with efficient work reservoirs that executes a Carnot cycle. Note that when implemented with only two-level work reservoirs, the engine's efficiency is strictly vanishing [59].

In our setup, there are two thermal baths at temperatures T_C and T_H ($T_C < T_H$), two work reservoirs W_C and W_H—that can
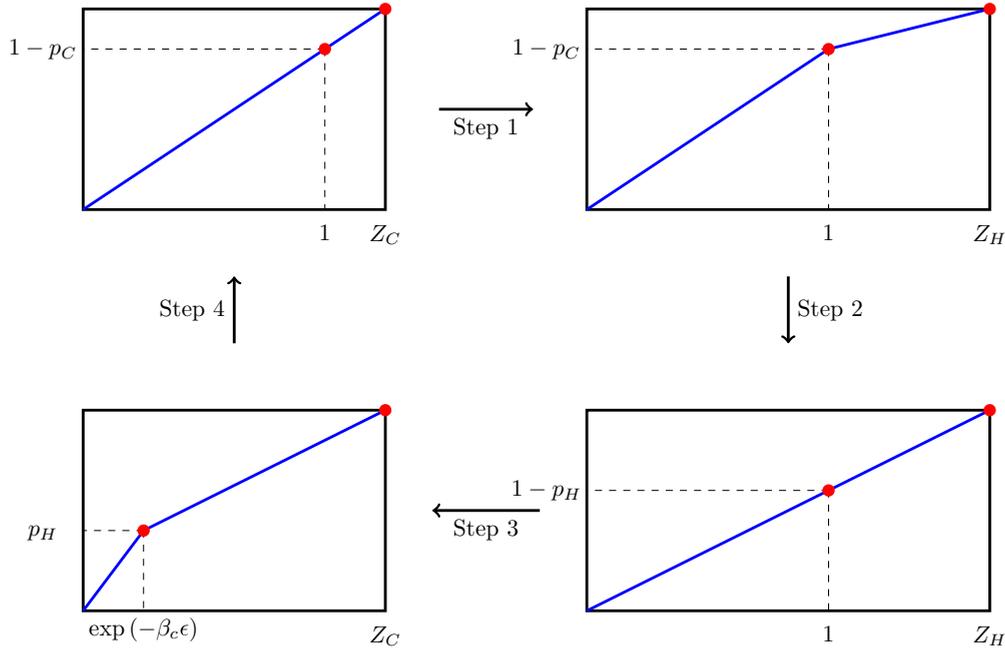
FIG. 8. Thermomajorization curves for each stage of the qubit engine, where $p_C = e^{-\beta_C \epsilon}/Z_C$ and $p_H = e^{-\beta_H \epsilon}/Z_H$. Z_C and Z_H are partition functions of the engine at temperature T_C and T_H, respectively.

be combined into one—and a system used as an engine. Since our engine and work reservoir run without dissipation, engine efficiency is $\eta = 1 - T_C/T_H$. The qubit engine's Hamiltonian is $H_S = \epsilon |1\rangle\langle 1|$.

Initially, the engine is in thermal state τ_C at temperature T_C, being in contact with the cold bath. Next, τ_C is brought to the hot bath (step 1) to extract work with work reservoir W_H and ends in thermal state τ_H at temperature T_H (step 2). The work extracted from the hot thermal bath is $W_H = k_B T_H D(\tau_C || \tau_H)$. Then, the system returns to the cold bath (step 3) and extracts work with reservoir W_C and ends in thermal state τ_C at temperature T_C (step 4). The work that can be extracted from the cold thermal bath is $W_C = k_B T_C D(\tau_H || \tau_C)$. The cycle completes when the engine returns to the thermal state at T_C.

Now, let us construct the corresponding work reservoir for this Carnot cycle. The work reservoir's state only changes during steps 2 and 4. Step 2 is a work extraction process. We use the minimal work reservoir W_1 to extract work without dissipation. In step 4, we also use the minimal work reservoir W_2 to extract work without dissipation. Figure 8 shows the system's thermomajorization curves for each step. And Table V shows the work reservoirs W_C and W_H used in the Carnot cycle. We can combine W_C and W_H into a single work reservoir. (See Table VI for details.) Since there is no dissipation in steps 2 and step 4, the heat transferred to the hot bath Q_H during step 2 and to the cold bath Q_C during step 4 satisfy

$$\beta_H Q_H + S(\tau_H) - S(\tau_C) = 0, \tag{I1}$$

$$\beta_C Q_C + S(\tau_C) - S(\tau_H) = 0. \tag{I2}$$

Then we have $\beta_C Q_C + \beta_H Q_H = 0$.

From energy conservation, the work done in one cycle is given by $W = -Q_H - Q_C$. And, the efficiency of this cycle is

given by

$$\eta = \frac{W}{-Q_H} \tag{I3}$$

$$= \frac{-Q_H - Q_C}{-Q_H} \tag{I4}$$

$$= 1 - \frac{T_C}{T_H}. \tag{I5}$$

For any engine operating with efficient work reservoirs, we always have

$$\beta_C Q_C + \beta_H Q_H = 0. \tag{I6}$$

As a result, the efficiency of an engine with efficient work reservoirs is always the Carnot efficiency $1 - T_C/T_H$. Similar results are considered in Ref. [60].

TABLE V. Qubit engine thermomajorization curves of initial and final W_H and W_C. c_1 and c_2 are arbitrary positive numbers. Here, we ignore flat portions in thermomajorization curves.

TABLE VI. Qubit engine efficient work reservoir energy levels: Here, we combine W_C and W_H into a single work reservoir. The work reservoir begins with ρ_{W1}. In step 2, the work reservoir changes from ρ_{W1} to ρ_{W2}. And, in step 4, the work reservoir changes from ρ_{W2} to ρ_{W3}. The nonzero components of probability distributions are $p_C p_H$, $p_C(1 - p_H)$, $(1 - p_C)p_H$, and $(1 - p_C)(1 - p_H)$. We list the corresponding energy levels in each work reservoir state, where c_1 and c_2 are two arbitrary positive constants.

	ρ_{W1}	ρ_{W2}	ρ_{W3}
$p_C p_H$	$-\frac{1}{\beta_H}\log(c_1 p_C) - \frac{1}{\beta_C}\log(c_2 p_H)$	$-\frac{1}{\beta_H}\log(c_1 p_H) - \frac{1}{\beta_C}\log(c_2 p_H)$	$-\frac{1}{\beta_H}\log(c_1 p_H) - \frac{1}{\beta_C}\log(c_2 p_C)$
$p_C(1 - p_H)$	$-\frac{1}{\beta_H}\log(c_1 p_C) - \frac{1}{\beta_C}\log(c_2(1 - p_H))$	$-\frac{1}{\beta_H}\log(c_1 p_H) - \frac{1}{\beta_C}\log(c_2(1 - p_H))$	$-\frac{1}{\beta_H}\log(c_1 p_H) - \frac{1}{\beta_C}\log(c_2(1 - p_C))$
$(1 - p_C)p_H$	$-\frac{1}{\beta_H}\log(c_1(1 - p_C)) - \frac{1}{\beta_C}\log(c_2 p_H)$	$-\frac{1}{\beta_H}\log(c_1(1 - p_H)) - \frac{1}{\beta_C}\log(c_2 p_H)$	$-\frac{1}{\beta_H}\log(c_1(1 - p_H)) - \frac{1}{\beta_C}\log(c_2 p_C)$
$(1 - p_C)(1 - p_H)$	$-\frac{1}{\beta_H}\log(c_1(1 - p_C)) - \frac{1}{\beta_C}\log(c_2(1 - p_H))$	$-\frac{1}{\beta_H}\log(c_1(1 - p_H)) - \frac{1}{\beta_C}\log(c_2(1 - p_H))$	$-\frac{1}{\beta_H}\log(c_1(1 - p_H)) - \frac{1}{\beta_C}\log(c_2(1 - p_C))$

APPENDIX J: REALIZATION OF EFFICIENT STATE TRANSITIONS

In studying the possibility of realizing the state transitions by using multilevel work reservoirs, we may ask whether it is possible to construct an explicit joint unitary operator U on the system, work reservoir, and thermal bath to implement the transition. In this Appendix, we give one example.

We consider the well-known Landauer erasure beginning with the probability distribution $(\frac{1}{2}, \frac{1}{2})$ storing in a trivial two-level system spanned by $\{|0\rangle, |1\rangle\}$ with Hamiltonian $H_S = 0$. The work reservoir's is a two-level system spanned by $\{|g\rangle, |e\rangle\}$ with Hamiltonian $H_W = \epsilon|e\rangle\langle e|$. Let us consider a special thermal bath with energy levels $\{0, 1\epsilon, \ldots, N\epsilon\}$ of which corresponding degeneracies are $\{2^0, 2^1, \ldots, 2^N\}$, respectively. The Hamiltonian of the bath is

$$H_B = \sum_{n=0}^{N} \sum_{i=1}^{2^n} n\epsilon|n, i\rangle\langle n, i| \tag{J1}$$

where $|n, i\rangle$ is the ith degenerated eigenstate with the eigenvalue $n\epsilon$. The partition function of the bath is

$$Z_B = \frac{1 - e^{-(N+1)\delta}}{1 - e^{-\delta}} \tag{J2}$$

where $\delta = \beta\epsilon - \log 2$. We construct the joint energy preserving unitary U such that

$$U|0e\rangle \otimes |n, i\rangle = |0g\rangle \otimes |n + 1, i\rangle, \tag{J3}$$

$$U|1e\rangle \otimes |n, i\rangle = |0g\rangle \otimes |n + 1, 2^n + i\rangle \tag{J4}$$

for $n = 0, 1, \ldots, N - 1$ and for $n = N$

$$U|0e\rangle \otimes |N, i\rangle = |0e\rangle \otimes |N, i\rangle, \tag{J5}$$

$$U|1e\rangle \otimes |N, i\rangle = |1e\rangle \otimes |N, i\rangle. \tag{J6}$$

There are undetermined degrees of freedom in this unitary operator U. But the conditions above are sufficient to determine our final state if the initial state is $\rho_{SWB} = (\frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1|) \otimes |e\rangle\langle e| \otimes \tau_B$. The final state of the system and work reservoir is given by tracing out the thermal bath degrees of freedom:

$$\rho'_{SW} = \text{Tr}_B(U\rho_{SWB}U^\dagger). \tag{J7}$$

This leads to the final state of the system plus work reservoir:

$$\rho'_{SW} = p|0g\rangle\langle 0g| + \frac{1}{2}(1 - p)|0e\rangle\langle 0e| + \frac{1}{2}(1 - p)|1e\rangle\langle 1e| \tag{J8}$$

where

$$p = \frac{1 - e^{-N(\beta\epsilon - \log 2)}}{1 - e^{-(N+1)(\beta\epsilon - \log 2)}} = \frac{1 - e^{-N\delta}}{1 - e^{-(N+1)\delta}}. \tag{J9}$$

The norm-1 distance between ρ'_{SW} and desired final state $|0g\rangle\langle 0g|$ is

$$\|\rho'_{SW} - |0g\rangle\langle 0g|\|_1 = 2(1 - p). \tag{J10}$$

The energy change in the work reservoir is

$$W = -k_B T(\delta + \log 2)\frac{1 - e^{-N\delta}}{1 - e^{-(N+1)\delta}}. \tag{J11}$$

As long as $\delta = \beta\epsilon - \log 2 > 0$, the partition function of the bath is finite for any N. And the norm-1 distance can be arbitrarily small as $N \to \infty$. The corresponding energy change in the work reservoir can be arbitrarily close to $k_B T \log 2$.

APPENDIX K: CORRELATED CATALYSTS FOR A TRIVIAL HAMILTONIAN

In this section, we show an interesting result on correlated catalysts. The catalysts can be used to decrease the entropy productions in state transitions in a trivial Hamiltonian.

Theorem 12. Consider a m-dimensional system with Hamiltonian $H = 0$. Given a state ρ_S, a thermal operation $\mathcal{E}$, and $\mathcal{E}(\rho_S) = \sigma_S$, then there exists a catalyst ω_C such that we have the following.

(1) $\mathcal{T}(\rho_S \otimes \omega_C) = \sigma_{SC}$.

(2) $\text{Tr}_C \sigma_{SC} = \sigma_S$ and $\text{Tr}_S \sigma_{SC} = \omega_C$.

(3) The entropy production of $\rho_S \otimes \omega_C \to \mathcal{T}(\rho_S \otimes \omega_C)$ is zero.

We use probability distribution to replace the density matrix and prove a theorem first.

Theorem 13. Let p_X and q_X be distributions on a finite set X and σ_Y be probability distribution on a finite set Y and T be a doubly stochastic matrix such that $T p_X = q_X$. Then there exists a distribution q_{XY} on $X \times Y$ such that

$$p_X \otimes \sigma_Y = q_{XY} \tag{K1}$$

and q_{XY}'s marginal distribution of X is q_X and the marginal distribution of Y is σ_Y. Here, two probability distributions being equal to each other means that they are the same up to a reorder.

Proof. We prove this by directly constructing q_{XY}. From the Birkhoff–von Neumann theorem, any doubly stochastic matrix T can be written as a convex combination of

permutation matrices:

$$T = \sum_{i=1}^{\alpha} \theta_i P_{\pi_i} \qquad (\text{K2})$$

where $\sum_i \theta_i = 1$ and P_{π_i} is the permutation matrix corresponding to permutation π_i. Without loss of generality, we can assume θ_i are rational, i.e., $\theta_i = m_i/N$ where $m_i, N \in \mathbb{Z}$. Here, we take

$$\sigma_Y = \frac{1}{N} \underbrace{(1, \ldots, 1)}_{\text{No. of 1s} = N}. \qquad (\text{K3})$$

And we introduce a $m \times N$ matrix C to express $p_X \otimes \sigma_Y$:

$$p_X \otimes \sigma_Y = C = \begin{pmatrix} \frac{p_{X1}}{N} & \cdots & \frac{p_{X1}}{N} \\ \vdots & \vdots & \vdots \\ \frac{p_{Xm}}{N} & \cdots & \frac{p_{Xm}}{N} \end{pmatrix}. \qquad (\text{K4})$$

In this matrix, if we add all components in each column together, we have probability distribution σ_Y and if we add all components in each row together, we have probability distribution p_X. We know

$$q_X = T p_X = \sum_i \theta_i P_{\pi_i} p_X = \sum_i \frac{m_i}{N} P_{\pi_i} p_X$$

$$= \sum_i \frac{m_i}{N} \pi_i(p_X) \qquad (\text{K5})$$

where $\pi_i(p_X)$ is the probability distribution after the permutation π_i taking effect on p_X. Now we permute components in each column of C to get C':

$$C' = (\pi_1(p_X)/N \quad \cdots \quad \pi_\alpha(p_X)/N) \qquad (\text{K6})$$

where for each $\pi_i(p_X)$ there are m_i copies in C'. We let q_{XY} be C'. Since we only permute components in each column, so we have the same σ_Y after we trace out X and we have q_X after we trace out Y. We only reorder the components in the matrix so we have

$$p_X \otimes \sigma_Y = q_{XY}. \qquad (\text{K7})$$

∎

From the theorem proved above, we see that for any state ρ and σ and letting $\mathcal{E}$ be a thermal operation, such that $\mathcal{E}(\rho) = \sigma$, we can find a catalyst ω such that the entropy production of the transition $\rho \otimes \omega \to \sigma'$ through a thermal operation is zero and $\omega = \text{tr}_1[\sigma']$, $\sigma = \text{tr}_2[\sigma']$ if the Hamiltonian of the system is trivial. From Theorem 13, we can achieve this by only reordering the eigenvalues of $\rho \otimes \omega$. So we can even only use a unitary operator U to achieve this, i.e., $U \rho \otimes \omega U^\dagger = \sigma'$. For the nontrivial Hamiltonian in general, this is not correct. We cannot do arbitrary permutations since it violates energy conservation.

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