Editors' Suggestion

Thermodynamic work capacity of quantum information processing

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(Received 27 October 2025; accepted 24 July 2026; published 12 August 2026)

We introduce the resource-theoretic free energy of a quantum channel as the maximal work extractable from the channel as its output equilibrates to a thermal state and its reference system remains locally intact. It is proportional to the relative entropy between the given channel and the absolutely thermal channel. It attains a clear operational meaning as twice the asymptotic rates of athermality distillation and formation under Gibbs-preserving superchannels, which map one absolutely thermal channel to another for a given bath, thereby revealing the asymptotic reversibility of the resource theory of athermality for quantum channels. Consequently, we establish that the optimal extractable work in converting one channel to another through the asymptotic athermality distillation and formation tasks equals the difference in their free energies. We call this optimal work the thermodynamic work capacity of channel conversion. Quantum information processing and computing fundamentally concern the manipulation and transformation of quantum channels, which encompass quantum states, their transformations, and measurements. A quantitative characterization of the optimal thermodynamic work gain or expenditure in quantum information processing constitutes a key step toward formulating thermodynamics of quantum processes.

DOI: 10.1103/xnzv-6975

Understanding the thermodynamic aspects of quantum systems and processes is crucial for studying natural phenomena and developing energy-efficient quantum technologies [1–4]. Thermodynamic effects impact the informational and computational capabilities of quantum processors, and the ongoing drive toward miniaturization increases the relevance of quantum thermodynamics [5–9]. Information theory provides the bridging conceptual notions between thermodynamics and quantum theory, along with tools and techniques to build the frameworks for quantum thermodynamics and analyze the energetics of quantum systems and processes [10–13].

Quantum information processing and computing primarily rely on physical transformations of quantum channels [14–17], which are completely positive, trace-preserving linear maps. Furthermore, the study of thermodynamical and informational aspects of quantum channels seems to

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readily provide a unifying framework to understand these aspects also for quantum states and measurements [4,18], as they are special examples of quantum channels. A quantum state is a preparation channel that acts on 1 and outputs the state. A quantum measurement is a quantum-to-classical channel that acts on quantum states to yield classical outputs with some probability distribution.

The free energy and work extraction are basic concepts in thermodynamics. We want to find appropriate and meaningful definitions of these concepts for quantum channels that would shed light on the thermodynamics of quantum information processing. It will help us perceive the thermodynamic utility of quantum channels and the energetics of their implementations in quantum devices. The extension of these concepts to quantum channels need not be straightforward [18–21] as the complications seem to get manifested in the notions involving channel discrimination tasks [17,22–25].

We identify the meaningful definitions of free energy and work extraction from quantum channels, and develop the resource theory of athermality of quantum channels (see also Refs. [4,9]). The resource-theoretic free energy of a quantum channel is defined as the maximum work that can be extracted when the channel output is thermalized in the presence of a bath, while the reference to the channel remains locally intact. We find that the resource-theoretic free energy of the channel is equal to the channel relative entropy with respect to the absolutely thermal channel (up to a multiplicative factor of the inverse temperature). An absolutely thermal channel always outputs a fixed thermal state with inverse temperature associated with the bath [12]. This motivates us to develop a resource theory of athermality of channels with respect to a bath at a fixed, arbitrary temperature, where the free object is an absolutely thermal channel and free operations are Gibbs-preserving superchannels (GPSCs). For a given thermal bath, a Gibbs-preserving superchannel maps one absolutely thermal channel to another at the same inverse temperature.

The relative entropy of athermality of a quantum channel is the relative entropy between the given channel and the absolutely thermal channel. It is an athermality monotone quantifying how athermal the channel is. It finds an exact operational meaning as twice the asymptotic athermality distillation and formation rates of the channel, thereby exhibiting that the resource theory of athermality of quantum channels under the allowed action of Gibbs-preserving superchannels is asymptotically reversible. As a consequence, the optimal work extractable during the asymptotic conversion of a quantum channel to another under Gibbs-preserving superchannels is equal to the difference in their free energy. We call this optimal extractable work as the *thermodynamic work capacity* of the conversion of quantum channels.

I. PRIOR WORKS

Consider a quantum system A with a Hamiltonian $\widehat{H}_A$ that is weakly interacting with the bath, such that the total energy of the system bath can be well approximated as the sum of the individual energies. Then, the equilibrium state of the system A is given by the thermal (Gibbs) state $\gamma_A^\beta := \exp(-\beta\widehat{H}_A)/Z_A^\beta$ [26], where β is the inverse temperature of the bath and $Z_A^\beta := \operatorname{tr}\exp(-\beta\widehat{H}_A)$ is the partition function. The nonequilibrium free energy of a state ρ_A is defined as $F_{\mathrm{T}}^\beta(\rho) := E(\rho) - \beta^{-1}S(\rho)$ (cf. Refs. [11,27,28]), where $S(\rho) := -\operatorname{tr}(\rho\ln\rho)$ is the von Neumann entropy and $E(\rho) = \operatorname{tr}(\rho\widehat{H}_A)$ is the internal energy of the system. We refer to $F_{\mathrm{T}}^\beta(\rho)$ as the thermodynamic free energy of the state ρ. For the thermal state, the equilibrium free energy is $F_{\mathrm{T}}^\beta(\gamma_A^\beta) = -\beta^{-1}\ln Z_A^\beta$. Incidentally, this quantity is related to the quantum relative entropy of the state with the thermal state, $F_{\mathrm{T}}^\beta(\rho) = \beta^{-1}D(\rho\|\gamma^\beta) + F_{\mathrm{T}}^\beta(\gamma^\beta) = \beta^{-1}D(\rho\|\widehat{\gamma}^\beta)$ [27,29], where $D(\rho\|\sigma) := \operatorname{tr}(\rho\ln\rho - \rho\ln\sigma)$, and $\widehat{\gamma}^\beta := \exp(-\beta\widehat{H}_A)$ is the thermal operator for given $\widehat{H}_A$ and β.

The amount of work W that can be extracted as we evolve from one equilibrium state γ_1^β to another γ_2^β is bounded by the change in the thermodynamic free energy, $W \leqslant F_{\mathrm{T}}^\beta(\gamma_2^\beta) - F_{\mathrm{T}}^\beta(\gamma_1^\beta)$, where the inequality saturates if the process is reversible. The maximum amount of work that can

be extracted from a nonequilibrium state ρ as the system equilibrates to the thermal state γ^β is given by $W^\beta_{\text{ext}}(\rho \to \gamma^\beta) = \beta^{-1} D(\rho \| \gamma^\beta)$ [30] when asymptotically many copies of ρ are available. $F^\beta(\rho) := \beta^{-1} D(\rho \| \gamma^\beta)$ is called the resource-theoretic free energy of a quantum state ρ [11,27]. The maximum extractable work through the conversion of a state ρ to a state σ under the action of Gibbs-preserving channels is given by $W^\beta_{\text{ext}}(\rho \to \sigma) = F^\beta_{\text{T}}(\rho) - F^\beta_{\text{T}}(\sigma) = F^\beta(\rho) - F^\beta(\sigma)$ when asymptotically many copies of ρ and σ are available. This is a direct consequence of the fact that the resource theory of athermality of quantum states is asymptotically reversible [31–33] under the action of Gibbs-preserving channels. The Gibbs-preserving channels map a thermal state to a thermal state with the same inverse temperature; they do not generate athermality in quantum states.

The utility of a class of athermal channels as thermal engines by the distillation of work from them has been discussed in a different resource-theoretic framework in Refs. [19,20] by considering unitary operations that commute with the thermal state as free operations. In these works, the possible use of reference to the channel input and output is ignored. On the contrary, it is desirable to consider unitary operations as athermal resources as they are purity preserving and exhibit genuine quantum behavior [18,21] unlike the absolutely thermal channels [12]. Furthermore, the task of quantum channel discrimination informs us that the reference to the channel is often crucial and can provide an advantage, which otherwise would not be feasible. From (quantum) thermodynamics, we know that even correlation carries information apart from the possible storage of information on local states. The extractable work from a quantum correlated state ρ_{AB} is more than the extractable work from the product state $\rho_A \otimes \rho_B$. Under a global entropy-preserving process, when the bath and systems are weakly interacting, the maximal extractable work from a state ρ_{AB} is given as [29,34–36]

$$W^\beta_{\text{ext}}(\rho_{AB}) = \beta^{-1} I(A;B)_\rho + F^\beta(\rho_A) + F^\beta(\rho_B) \tag{1}$$

$$= F^\beta_{\text{T}}(\rho_{AB}) - F^\beta_{\text{T}}\big(\gamma^\beta_A \otimes \gamma^\beta_B\big) \tag{2}$$

$$= \beta^{-1} D\big(\rho_{AB} \big\| \gamma^\beta_A \otimes \gamma^\beta_B\big) = F^\beta(\rho_{AB}), \tag{3}$$

where we have assumed that $\widehat{H}_{AB} = \mathbb{1}_A \otimes \widehat{H}_B + \widehat{H}_A \otimes \mathbb{1}_B$ and $I(A;B)_\rho := D(\rho_{AB} \| \rho_A \otimes \rho_B)$ are the quantum mutual information of the state ρ_{AB}, and for a state ρ_{AB}, we let $\rho_A := \text{tr}_B(\rho_{AB})$.

II. EXTRACTABLE WORK FROM A QUANTUM CHANNEL

We would like to consider the optimal work extractable from a quantum channel $\mathcal{N}_{A' \to A}$ through a thermodynamic quantity that depends on how well the channel can preserve the correlation between its input A' and the reference and while also accounting for the (resource-theoretic) free energy of the channel output A. To capture this idea, we define the extractable work from a quantum channel as the maximum possible work extractable during the partial thermalization process $\text{id}_R \otimes \mathcal{N}_{A' \to A}(\psi_{RA'}) \to \psi_R \otimes \gamma^\beta_A$ under global operations when systems weakly interact with the bath, and optimize it over all possible input states $\psi \in \text{St}(RA')$ for arbitrary dimension R,

$$W^\beta_{\text{ext}}[\mathcal{N}] := \sup_{\psi \in \text{St}(RA')} \big[F^\beta_{\text{T}}(\text{id} \otimes \mathcal{N}(\psi_{RA'})) - F^\beta_{\text{T}}\big(\psi_R \otimes \gamma^\beta_A\big)\big] \tag{4}$$

$$= \sup_{\psi \in \text{St}(RA')} [F^\beta(\text{id} \otimes \mathcal{N}(\psi_{RA'})) - F^\beta(\psi_R)] \tag{5}$$

$$= \sup_{\psi \in \text{St}(RA')} [\beta^{-1} I(R;A)_{\text{id} \otimes \mathcal{N}(\psi)} + F^\beta(\mathcal{N}(\psi_{A'}))], \tag{6}$$

where we assumed that $\widehat{H}_{RA} = \mathbb{1}_R \otimes \widehat{H}_A + \widehat{H}_R \otimes \mathbb{1}_A$. We advocate that Eq. (5) can be interpreted as extractable work from the channel $\mathcal{N}$ in a similar way as $S[\mathcal{N}] := \inf_{\psi \in \text{St}(RA')} [S(\text{id} \otimes \mathcal{N}(\psi_{RA'})) - S(\psi_R)]$ [Eq. (1.1) in Ref. [37]] finds meaningful interpretation as the entropy of the channel $\mathcal{N}$ [4,9,12,21,38].

Any transformation $\mathrm{id}_R \otimes \mathcal{N}_{A'\to A}(\psi_{RA'}) \to \psi_R \otimes \gamma_A^\beta$ for all input states $\psi_{RA'}$ is equivalent to the thermalization of the channel $\mathcal{N}$ itself, i.e., $\mathcal{N} \to \mathcal{T}^\beta$, where $\mathcal{T}^\beta_{A'\to A}(\cdot) := \mathrm{tr}(\cdot)\gamma_A^\beta$ is an absolutely thermal channel [9,12] that always outputs state in thermal equilibrium with a bath at inverse temperature β. The channel transformation $\mathcal{N} \to \mathcal{T}^\beta$ is equivalent to thermalization of the channel output while the reference system being locally intact. We can interpret $W^\beta_{\mathrm{ext}}[\mathcal{N}]$ as the extractable work when we transform the channel $\mathcal{N}$ to $\mathcal{T}^\beta$. It follows that $W^\beta_{\mathrm{ext}}[\mathcal{N}] \geqslant 0$ for an arbitrary quantum channel $\mathcal{N}$ and the inequality saturates if and only if $\mathcal{N}$ is absolutely thermal, $\mathcal{N} = \mathcal{T}^\beta$.

III. DYNAMICAL FREE ENERGY

We find that the extractable work for an arbitrary quantum channel $\mathcal{N}_{A'\to A}$ is proportional to the channel relative entropy between the channel and the absolutely thermal channel,

$$W^\beta_{\mathrm{ext}}[\mathcal{N}] = \beta^{-1} D[\mathcal{N}\|\mathcal{T}^\beta] \tag{7}$$

$$= \beta^{-1}(D[\mathcal{N}\|\widehat{\mathcal{T}}^\beta] - D[\mathcal{T}^\beta\|\widehat{\mathcal{T}}^\beta]), \tag{8}$$

where $\widehat{\mathcal{T}}^\beta_{A'\to A}(\cdot) = \mathrm{tr}(\cdot)\widehat{\gamma}_A^\beta$ and

$$D[\mathcal{N}\|\mathcal{M}] = \sup_{\psi_{RA'}} D(\mathcal{N}(\psi_{RA'})\|\mathcal{M}(\psi_{RA'})) \tag{9}$$

is the quantum relative entropy between completely positive maps $\mathcal{N}_{A'\to A}, \mathcal{M}_{A'\to A}$ and it suffices to optimize over pure states $\psi_{RA'}$ with $R \simeq A'$. We arrive at the aforementioned identities by observing that $I(A;B)_\rho + D(\rho_B\|\gamma^\beta) = D(\rho_{AB}\|\rho_A \otimes \gamma_B^\beta)$ and the fact that $D[\mathcal{T}^\beta\|\widehat{\mathcal{T}}^\beta] = D(\gamma_A^\beta\|\widehat{\gamma}_A^\beta) = -\ln Z_A^\beta$. The function $F^\beta[\mathcal{N}] := \beta^{-1}D[\mathcal{N}\|\mathcal{T}^\beta]$ (and $F^\beta_{\mathrm{T}}[\mathcal{N}] := \beta^{-1}D[\mathcal{N}\|\widehat{\mathcal{T}}^\beta]$) exhibits the following properties [9]: (1) monotonically nonincreasing under the action of Gibbs-preserving superchannels Θ^β, $\Theta^\beta(\mathcal{T}^\beta_{A'\to A}) = \mathcal{T}^\beta_{B'\to B}$, (2) reduction to the free energy of a state ω_A for a replacer (or preparation) channel $\mathcal{R}^\omega$, where $\mathcal{R}^\omega_{A'\to A}(\cdot) := \mathrm{tr}(\cdot)\omega_A$, (3) minimum if and only if the channel is absolutely thermal, (4) continuity, (5) additive under tensor product of quantum channels $\mathcal{N}_{A'\to A} \otimes \mathcal{M}_{B'\to B}$ if channel outputs are noninteracting $\widehat{H}_{AB} = \widehat{H}_A \otimes \mathbb{1}_B + \mathbb{1}_A \otimes \widehat{H}_B$, $F^\beta[\mathcal{N}\otimes\mathcal{M}] = F^\beta[\mathcal{N}] + F^\beta[\mathcal{M}]$, and (6) convexity. These are desirable properties for a free energy function of a quantum channel, analogous to quantum states (see Proposition B1 in Appendix B for proof).

Based on the exhibition of the aforementioned desired properties, we identify $F^\beta[\mathcal{N}] = \beta^{-1}D[\mathcal{N}\|\mathcal{T}^\beta]$ and $F^\beta_{\mathrm{T}}[\mathcal{N}] = \beta^{-1}D[\mathcal{N}\|\widehat{\mathcal{T}}^\beta]$ as the resource-theoretic and thermodynamic free energy of a quantum channel $\mathcal{N}_{A'\to A}$, respectively, so that

$$W^\beta_{\mathrm{ext}}[\mathcal{N}] = F^\beta[\mathcal{N}] = F^\beta_{\mathrm{T}}[\mathcal{N}] - F^\beta_{\mathrm{T}}[\mathcal{T}^\beta]. \tag{10}$$

This exemplifies $W^\beta_{\mathrm{ext}}[\mathcal{N}] = F^\beta[\mathcal{N}]$ as a faithful monotone of the athermality of a quantum channel $\mathcal{N}$, i.e., a valid monotone of how athermal the channel is and being zero if and only if the channel is absolutely thermal. The utility of an athermal quantum channel, a channel that is not absolutely thermal, for thermodynamic work extraction motivates us to formulate the resource theory of quantum channels.

IV. DYNAMICAL RESOURCE THEORY OF ATHERMALITY

In the real world, often the quantum systems eventually get in equilibrium with the surroundings, which acts as a thermal bath. The equilibrium state of the system A that is weakly interacting with the bath at some arbitrary inverse temperature β is given by the thermal state $\gamma_A^\beta = \exp(-\beta\widehat{H}_A)/Z_A^\beta$. This suggests that the absolutely thermal channel $\mathcal{T}^\beta$ can be considered natural or a free object [12]. For a thermal bath at inverse temperature β, the absolutely thermal channel $\mathcal{T}^\beta$ is unique, and any preparation channel $\mathcal{T}^{\beta'}$ is athermal if $\beta' \neq \beta$. Gibbs-preserving superchannels form free

operations in the resource theory of athermality, as they do not increase athermality of a quantum resource channel and preserve the thermalization property of the free object for a given thermal bath. Based on this observation, we formulate the resource theory of athermality for finite-dimensional square quantum channels under Gibbs-preserving superchannels as free operations [39].

Golden units of athermality. For a thermal bath at inverse temperature β, we denote a quantum resource channel $\mathcal{N}_{A'\to A}$, where $|A'| = |A| < +\infty$, as $(\mathcal{N}, \mathcal{T}^\beta)$. We observe that the relative entropy of athermality $D[\mathcal{N}\|\mathcal{T}^\beta]$ of a quantum channel $\mathcal{N}$ is maximum if and only if it is a unitary channel. All unitary channels $\mathcal{U}_{A'\to A}$ are equally resourceful (see Appendix C 1), and interconversions between these unitaries exist under Gibbs-preserving superchannels, which can be depicted as $(\mathcal{U}, \mathcal{T}^\beta) \sim (\mathrm{id}, \mathcal{T}^\beta)$. It can also be shown that the relative entropy of athermality $D[\mathcal{U}\|\mathcal{T}^\beta]$ of a unitary channel $\mathcal{U}_{A'\to A}$ is minimum if and only if the output Hamiltonian is fully degenerate, $\widehat{H}_A \propto \mathbb{1}_A$ (see Appendix C 1 and Proposition C1). As the output Hamiltonian of a quantum channel can be arbitrary, we advocate a golden unit of athermality of quantum channels to be a unitary channel with a fully degenerate output Hamiltonian. Without loss of generality, we choose the identity channel $(\mathrm{id}_m, \mathcal{R}^\pi)$ to be a golden unit for the resource theory of athermality of quantum channels acting on an m-dimensional system, where id_m is the identity channel on an m-dimensional system and $\mathcal{T}^\beta$ reduces to the uniformly mixing channel $\mathcal{R}^\pi(\cdot) = \mathrm{tr}(\cdot)\pi$, where π is the maximally mixed state, for $\widehat{H} \propto \mathbb{1}$.

Athermality distillation and formation. For the transformation of an arbitrary resource channel $(\mathcal{N}_{A'\to A}, \mathcal{T}^\beta_{A'\to A})$ to another arbitrary resource channel $(\mathcal{M}_{B'\to B}, \mathcal{T}^\beta_{B'\to B})$, the conversion distance under the action of GPSCs is defined as

$$d_{\mathrm{GP}}((\mathcal{N}, \mathcal{T}^\beta) \to (\mathcal{M}, \mathcal{T}^\beta)) = \inf_{\Theta} \left\{P[\mathcal{M}, \Theta(\mathcal{N})] : \Theta\left(\mathcal{T}^\beta_{A'\to A}\right) = \mathcal{T}^\beta_{B'\to B}\right\}, \tag{11}$$

where $P[\mathcal{N}, \mathcal{M}] := \sup_{\psi_{RA'}} P(\mathcal{N}(\psi), \mathcal{M}(\psi))$ is the purified distance between quantum channels $\mathcal{N}_{A'\to A}, \mathcal{M}_{A'\to A}$ and optimization can be taken over pure states $\psi_{RA'}$, and $|A'| = |A|$, $|B'| = |B|$. For an error $\varepsilon \in [0, 1]$ and a resource quantum channel $(\mathcal{N}, \mathcal{T}^\beta)$, the one-shot athermality distillation $\mathrm{Dist}^\varepsilon(\mathcal{N}, \mathcal{T}^\beta)$ and formation $\mathrm{Cost}^\varepsilon(\mathcal{N}, \mathcal{T}^\beta)$ under GPSCs are respectively defined as

$$\mathrm{Dist}^\varepsilon(\mathcal{N}, \mathcal{T}^\beta) := \sup_m \{\ln m : d_{\mathrm{GP}}((\mathcal{N}, \mathcal{T}^\beta) \to (\mathrm{id}_m, \mathcal{R}^\pi)) \leqslant \varepsilon\}, \tag{12}$$

$$\mathrm{Cost}^\varepsilon(\mathcal{N}, \mathcal{T}^\beta) := \inf_m \{\ln m : d_{\mathrm{GP}}((\mathrm{id}_m, \mathcal{R}^\pi) \to (\mathcal{N}, \mathcal{T}^\beta)) \leqslant \varepsilon\}. \tag{13}$$

That is, up to an allowed error $\varepsilon \in [0, 1]$, $\mathrm{Dist}^\varepsilon(\mathcal{N}, \mathcal{T}^\beta)$ is the maximum number of basic golden resource units $(\mathrm{id}_e, \mathcal{R}^\pi)$ distillable from $(\mathcal{N}, \mathcal{T}^\beta)$ and $\mathrm{Cost}^\varepsilon(\mathcal{N}, \mathcal{T}^\beta)$ is the minimum number of basic golden resource units $(\mathrm{id}_e, \mathcal{R}^\pi)$ required to expend to form $(\mathcal{N}, \mathcal{T}^\beta)$. For asymptotically many parallel uses of the resource channel $(\mathcal{N}, \mathcal{T}^\beta)$ and $\varepsilon \in (0, 1)$, the asymptotic distillation and formation rates are the same,

$$\limsup_{n\to\infty} \frac{1}{n}\mathrm{Dist}^\varepsilon(\mathcal{N}^{\otimes n}, \mathcal{T}^{\beta\otimes n}) = \liminf_{n\to\infty} \frac{1}{n}\mathrm{Cost}^\varepsilon(\mathcal{N}^{\otimes n}, \mathcal{T}^{\beta\otimes n}) \tag{14}$$

$$= \frac{1}{2}D[\mathcal{N}\|\mathcal{T}^\beta], \tag{15}$$

implying that the resource theory of athermality of quantum channels is reversible. Here, we consider only square quantum channels for the interconversion problem; the extension of this result to arbitrary quantum channels is discussed in Ref. [4].

The proof follows by first showing (see Appendix C 2; Theorem C1) that $\mathrm{Distill}^\varepsilon(\mathcal{N}, \mathcal{T}^\beta) = \frac{1}{2}D_H^{\varepsilon^2}[\mathcal{N}\|\mathcal{T}^\beta]$ and $\mathrm{Cost}^\varepsilon(\mathcal{N}, \mathcal{T}^\beta) = \frac{1}{2}D_\infty^\varepsilon[\mathcal{N}\|\mathcal{T}^\beta]$ [9] (also see Ref. [4]), where $D_H^\varepsilon[\mathcal{N}\|\mathcal{M}]$ and $D_\infty^\varepsilon[\mathcal{N}\|\mathcal{M}]$ are smoothed hypothesis-testing and max-relative entropies between channels $\mathcal{N}, \mathcal{M}$ [40,41], respectively. To show these relations, we used the fact that the uniformly mixing channel $\mathcal{R}^\pi_{A'\to A}$ can be expressed as the uniform mixture of Weyl unitary channels $\mathcal{W}^i_{A'\to A}$, $\mathcal{R}^\pi(\cdot) = \frac{1}{m^2}\sum_{i=0}^{m^2-1}\mathcal{W}^i(\cdot)$ for $|A'| = |A| = m$, where $\mathcal{W}^i(\cdot) := W^i(\cdot)(W^i)^\dagger$ is the set (group) $\{W^i\}_{i=0}^{m^2-1}$ of

Weyl unitaries, and $\| \mathrm{id} - \mathcal{R}^{\pi} \|_{\diamond} = 1 - \frac{1}{m^2}$ ($\|\mathcal{M}\|_{\diamond} := \sup_{\psi_{RA'}} \| \mathrm{id}_R \otimes \mathcal{M}(\psi_{RA'})\|_1$ is the diamond norm for a Hermiticity-preserving map $\mathcal{M}_{A'\to A}$). We then use the asymptotic equipartition property (see Appendix C 2 and Theorem C2) for smoothed hypothesis-testing and max-relative entropies D_{∞} between a quantum channel and a replacer channel [40,42], $\forall\, \varepsilon \in (0, 1)$

$$\lim_{n\to\infty} \frac{1}{n} D_H^{\varepsilon}[\mathcal{N}^{\otimes n} \| \mathcal{R}^{\omega\otimes n}] = \lim_{n\to\infty} \frac{1}{n} D_{\infty}^{\varepsilon}[\mathcal{N}^{\otimes n} \| \mathcal{R}^{\omega\otimes n}] = D[\mathcal{N} \| \mathcal{R}^{\omega}], \tag{16}$$

to arrive at Eq. (14).

It is known that the identity channel $\mathrm{id}_{A'\to A}$ allows for the perfect quantum communication, equivalent to the distribution of a maximally entangled state $\Phi_{RA} = \sum_{i,j=0}^{m-1} |ii\rangle\langle jj|_{RA}$ of Schmidt rank m, where $|R| = |A'| = |A| = m$. Operationally, establishing the identity channel $\mathrm{id}_{A'\to A}$ between two parties allows for the perfect distribution of $m \times m$-dimensional quantum states. A golden unit $(\mathrm{id}_m, \mathcal{R}^{\pi})$ of dynamical athermality corresponds to a golden unit $(\Phi_m, \pi_R \otimes \pi_A) \sim (|m\rangle\langle m| \otimes |m\rangle\langle m|, \pi \otimes \pi)$ of static athermality of $m \times m$-dimensional quantum system, where $|m\rangle\langle m|$ is a pure energy eigenstate. This shows that $(\mathrm{id}_m, \mathcal{R}^{\pi})$ is equivalent to the double of $(|m\rangle\langle m|, \pi_m)$, where $\pi_m = \frac{1}{m}\mathbb{1}$, in terms of athermality [9].

V. THERMODYNAMIC WORK CAPACITY OF CHANNEL CONVERSION

We define the one-shot net extractable work $W_{\beta}^{\varepsilon_1,\varepsilon_2}[\mathcal{N} \to \mathcal{M}]$ for thermodynamic channel transformation from an arbitrary square quantum channel $\mathcal{N}_{A'\to A}$ to an arbitrary square quantum channel $\mathcal{M}_{B'\to B}$ as the surplus (gain) in extractable work during the one-shot athermality distillation from $(\mathcal{N}, \mathcal{T}^{\beta})$ up to an error $\varepsilon_1 \in [0, 1]$ and the one-shot athermality formation of $(\mathcal{M}, \mathcal{T}^{\beta})$ up to an error $\varepsilon_2 \in [0, 1]$, both under GPSCs,

$$W_{\beta,\mathrm{ext}}^{\varepsilon_1,\varepsilon_2}[\mathcal{N} \to \mathcal{M}] = \frac{2}{\beta}[\mathrm{Dist}^{\varepsilon_1}(\mathcal{N}, \mathcal{T}^{\beta}) - \mathrm{Cost}^{\varepsilon_2}(\mathcal{M}, \mathcal{T}^{\beta})]. \tag{17}$$

The thermodynamic work capacity $\Delta W_{\mathrm{ext}}^{\beta}[\mathcal{N} \to \mathcal{M}]$ of the channel conversion $\mathcal{N} \to \mathcal{M}$ is defined as the difference between the asymptotic work distillation rate from $(\mathcal{N}, \mathcal{T}^{\beta})$ and the asymptotic work cost rate of $(\mathcal{M}, \mathcal{T}^{\beta})$, which is equal to the regularized net extractable work $\frac{1}{n} W_{\beta}^{\varepsilon_1,\varepsilon_2}[\mathcal{N}^{\otimes n} \to \mathcal{M}^{\otimes n}]$, for $\varepsilon_1, \varepsilon_2 \in (0, 1)$,

$$\begin{aligned} \Delta W_{\mathrm{ext}}^{\beta}[\mathcal{N} \to \mathcal{M}] &= \lim_{n\to\infty} \frac{1}{n} W_{\beta}^{\varepsilon_1,\varepsilon_2}[\mathcal{N}^{\otimes n} \to \mathcal{M}^{\otimes n}] = \beta^{-1}(D[\mathcal{N} \| \mathcal{T}^{\beta}] - D[\mathcal{M} \| \mathcal{T}^{\beta}]) \\ &= F_{\mathrm{T}}^{\beta}[\mathcal{N}] - F_{\mathrm{T}}^{\beta}[\mathcal{M}] = W_{\mathrm{ext}}^{\beta}[\mathcal{N}] - W_{\mathrm{ext}}^{\beta}[\mathcal{M}]. \end{aligned} \tag{18}$$

The reversibility of the resource theory of athermality under GPSCs ensures that $\Delta W_{\mathrm{ext}}^{\beta}[\mathcal{N}\to\mathcal{M}]$ is asymptotically the optimal net extractable work in terms of the gain in athermality golden units during the thermodynamic transformation $\mathcal{N} \to \mathcal{M}$. It follows from the reversibility that $\Delta W_{\mathrm{ext}}^{\beta}[\mathcal{N} \to \mathcal{N}] = 0$. The thermodynamic transformation is based on the distillation of $(\mathrm{id}_{m_1}, \mathcal{R}^{\pi})$ from $(\mathcal{N}^{\otimes n}, \mathcal{T}^{\beta\otimes n})$ and then expending $(\mathrm{id}_{m_2}, \mathcal{R}^{\pi})$ to form $(\mathcal{M}^{\otimes n}, \mathcal{T}^{\beta\otimes n})$, with largest possible m_1 and least possible m_2. Then, the thermodynamic work capacity is given by $\Delta W_{\mathrm{ext}}^{\beta}[\mathcal{N} \to \mathcal{M}] = \lim_{n\to\infty}(\ln m_1 - \ln m_2)/n = \lim_{n\to\infty}(1/n)\ln(m_1/m_2)$. Now, $\Delta W_{\mathrm{ext}}^{\beta}[\mathcal{N} \to \mathcal{M}] > 0$ implies $m_1 > m_2$, $\Delta W_{\mathrm{ext}}^{\beta}[\mathcal{N} \to \mathcal{M}] < 0$ implies $m_1 < m_2$, and $\Delta W_{\mathrm{ext}}^{\beta}[\mathcal{N} \to \mathcal{M}] = 0$ implies $\lim_{n\to\infty} \frac{1}{n} \ln m_1 = \lim_{n\to\infty} \frac{1}{n} \ln m_2$.

VI. DISCUSSION

An arbitrary replacer channel $\mathcal{R}_{A'\to A}^{\omega}$ is an absolutely thermal channel $\mathcal{T}_{A'\to A}^{\beta}$ with respect to the channel output Hamiltonian $\widehat{H}_A = -\beta^{-1} \ln \omega_A$ and inverse temperature β. Our work provides the exact thermodynamic meaning to the generalized channel divergences like hypothesis-testing

TABLE I. Comparison between basic thermodynamic quantities of states and channels. We summarize and compare mathematical expressions for elementary thermodynamic concepts for quantum states vs channels. We consider thermal reservoir to be at inverse temperature β and $\widehat{H}$ denotes the Hamiltonian of the designated system. $\widehat{\gamma}^\beta$ is a thermal operator and γ^β is a thermal state. $\mathcal{R}^\omega_{A'\to A}(\cdot) := \mathrm{tr}[\cdot]\omega_A$, $\mathcal{T}^\beta_{A'\to A}(\cdot) := \mathrm{tr}[\cdot]\gamma^\beta_A$, $\widehat{\mathcal{T}}^\beta_{A'\to A}(\cdot) := \mathrm{tr}[\cdot]\widehat{\gamma}^\beta$. $D(\rho\|\sigma) := \lim_{\varepsilon\to 0^+} \mathrm{tr}[\rho(\ln\rho - \ln(\sigma+\varepsilon\mathbb{1}))]$ is the relative entropy between states ρ,σ and $D[\mathcal{N}\|\mathcal{M}] := \sup_{\psi\in\mathrm{St}(RA')} D(\mathrm{id}_R\otimes\mathcal{N}(\psi_{RA'})\|\,\mathrm{id}_R\otimes\mathcal{M}(\psi_{RA'}))$ is the relative entropy between channels $\mathcal{N}_{A'\to A}, \mathcal{M}_{A'\to A}$. ρ is a state of system A' and $\mathcal{N}_{A'\to A}$ is a quantum channel. The content for quantum states is known in literature [11,27–29]. The expression of the entropy of quantum channels is from Refs. [17,38]. We provide proofs in the Appendixes.

Concepts	States	Channels
Equilibration with bath	Thermal state γ^β	Absolutely thermal channel $\mathcal{T}^\beta$
Energy	$E(\rho) = \langle\widehat{H}\rangle_\rho$	$E[\mathcal{N}] = \sup_{\rho\in\mathrm{St}(A')}\langle\widehat{H}\rangle_{\mathcal{N}(\rho)}$ (for channel output noninteracting with its reference)
Entropy	$S(\rho) = -\mathrm{tr}[\rho\ln\rho] = -D(\rho\|\mathbb{1})$	$S[\mathcal{N}] = -D[\mathcal{N}\|\mathcal{R}^{\mathbb{1}}]$
Thermodynamic free energy	$F^\beta_{\mathrm{T}}(\rho) = \beta^{-1}D(\rho\|\widehat{\gamma}^\beta)$	$F^\beta_{\mathrm{T}}[\mathcal{N}] = \beta^{-1}D[\mathcal{N}\|\widehat{\mathcal{T}}^\beta]$
Resource-theoretic free energy	$F^\beta(\rho) = F^\beta_{\mathrm{T}}(\rho) - F^\beta_{\mathrm{T}}(\gamma^\beta) = \beta^{-1}D(\rho\|\gamma^\beta)$	$F^\beta[\mathcal{N}] = F^\beta_{\mathrm{T}}[\mathcal{N}] - F^\beta_{\mathrm{T}}[\mathcal{T}^\beta] = \beta^{-1}D[\mathcal{N}\|\mathcal{T}^\beta]$
Minimal free energy	Thermal state γ^β	Absolutely thermal channel $\mathcal{T}^\beta$
Maximal extractable work	$W^\beta_{\mathrm{ext}}(\rho\to\gamma^\beta) = F^\beta(\rho)$	$W^\beta_{\mathrm{ext}}[\mathcal{N}\to\mathcal{T}^\beta] = F^\beta[\mathcal{N}]$
Helmholtz equation	$F^\beta_{\mathrm{T}}(\rho) = E(\rho) - \beta^{-1}S(\rho)$	$F^\beta_{\mathrm{T}}[\mathcal{N}] \leqslant E[\mathcal{N}] - \beta^{-1}S[\mathcal{N}]$ (for channel output noninteracting with its reference; inequality saturates for replacer channels)

relative entropy, max-relative entropy, and relative entropy between an arbitrary quantum channel $\mathcal{N}_{A'\to A}$ and a replacer channel $\mathcal{R}^\omega_{A'\to A}$, where ω_A is full rank and channel output Hamiltonian $\widehat{H}_A = -\beta^{-1}\ln\omega_A$; see, for example, Eqs. (10) and (14). Also, the resource theory of purity of states and channels [31,43,44] can be seen as special cases of the resource theory of athermality of channels (see Table I for a comparison of the thermodynamic concepts between states and channels).

Work is extractable from any athermal channel $\mathcal{N}$. This allows us to assess the utility of quantum gates (processors) as quantum batteries [45–47] on the basis of their free energy. The physical transformation of a quantum channel $\mathcal{N}$ to $\mathcal{T}^\beta$ is the erasure of the channel $\mathcal{N}$ via thermalization [21], implying that the erasure cost of a channel is related to its free energy. We have detailed discussions on the quantitative relations between the free energy of a quantum channel and its private randomness distillation capacity [48] and entropy [17,38] in Appendix D. For instance, for a quantum channel $\mathcal{N}_{A'\to A}$ with $\widehat{H}_A \propto \mathbb{1}_A$, its thermodynamic free energy is proportional to its entropy, $F_{\mathrm{T}}[\mathcal{N}] = -\beta^{-1}S[\mathcal{N}]$, thus providing an exact thermodynamic interpretation of the channel entropy [17,21,38].

An interesting open question is to figure out if there exists an asymptotically reversible resource theory of athermality of quantum channels under a stricter and physically motivated class of free operations (cf. Ref. [49]). Another future direction is to study the notion of free energy of higher-order quantum processes and to define the conditional free energy of bipartite quantum channels, and study their operational meanings in thermodynamic and information processing contexts (cf. Ref. [18]).

To define the free energy of higher-order processes, one could take the approach in Secs. V and VI of Ref. [17] and define the inverse temperature times thermodynamic free energy of the nth order quantum process ($n\in\mathbb{N}$, where $n=1$ for quantum states, $n=2$ for quantum channel, $n=3$ for superchannel, and so on) as the relative entropy between the given nth-order quantum process and the absolutely thermal nth-order map. The absolutely thermal nth-order map on an input

$(n-1)$th-order physical quantum process $\mathcal{M}^{(n-1)}$ is the replacer map $\mathcal{T}^{(n),\beta}(\mathcal{M}^{(n-1)}) = \mathcal{T}^{(n-1),\beta}$, such that $\mathcal{T}^{(1),\beta} = \widehat{\gamma}^{\beta}$ and $\mathcal{T}^{(2),\beta}(\mathcal{M}^{(1)}) = \mathcal{T}^{(1),\beta}$ for all input quantum states $\mathcal{M}^{(1)}$.

ACKNOWLEDGMENTS

The authors thank Felix C. Binder, Manabendra Nath Bera, Swati Choudhary, Karol Horodecki, Yutong Luo, and Uttam Singh for discussions. H.B. acknowledges support of the Visvesvaraya Post-Doctoral Fellowship (2025–2026) in Electronics and IT from the Ministry of Electronics and Information Technology (MeitY), Government of India. D.G.S. thanks the Department of Science and Technology (DST), Government of India, for the INSPIRE fellowship. S.D. acknowledges support from the Science and Engineering Research Board (now ANRF), DST, Government of India, under Grant No. SRG/2023/000217, and MeitY, Government of India, under Grant No. 4(3)/2024-ITEA. S.D. also acknowledges support from the National Quantum Mission, an initiative of DST, Government of India.

DATA AVAILABILITY

There are no publicly available research data or software supporting this manuscript. Requests for further information or data should be sent to the authors.

APPENDIXES

In this Appendixes, we provide the elaborate proofs and discussions surrounding the main results in this article (see also Ref. [9] for related discussions from the perspective of an axiomatic resource-theoretic approach). We start by recalling the relevant definitions and notations from the literature in Appendix A. In Appendix B, we provide proofs for the expressions for the extractable work and the desirable properties exhibited by the resource-theoretic dynamical free energy $F^{\beta}[\mathcal{N}]$ claimed in this article. Along with this, we show that the unitary channels have the maximum free energy. We proceed to the detailed discussions on the resource theory of dynamical athermality in Appendix C, where we outline the motivation for defining $(\mathrm{id}, \mathcal{T}^{\beta})$ as a golden unit of the resource theory. We determine the one-shot athermality distillation and formation of a quantum channel in Theorem C1 and prove the asymptotic reversibility of the dynamical athermality under the action of Gibbs-preserving superchannels in Theorem C2. In Appendix D, we present quantitative relations between information processing capabilities of a channel and its free energy, and finally in Appendix E (Theorem E1) we provide the Helmholtz equation for quantum channels.

APPENDIX A: PRELIMINARIES

We consider quantum systems associated with separable Hilbert spaces with tensor-product structure. For a bipartite state ρ_{AB}, $\rho_A = \mathrm{tr}_B(\rho_{AB})$. The energy of a quantum state ρ_A associated with Hamiltonian $\widehat{H}_A$ is $\langle \widehat{H} \rangle_{\rho} := \mathrm{tr}[\widehat{H}_A \rho_A]$. Let $\mathrm{St}(A)$ and $\mathrm{Pos}(A)$ denote the set of all density operators (quantum states) and the set of all positive semidefinite operators on A, respectively. Let $\mathrm{Ch}(A', A)$ denote the set of all quantum channels from A' to A. Let $\mathrm{SCh}((A', A), (B', B))$ denote the set of all quantum superchannels mapping $\mathrm{Ch}(A', A)$ to $\mathrm{Ch}(B', B)$. Any quantum superchannel can be written as concatenation of preprocessing and postprocessing quantum channels [14]; i.e., for any $\Theta \in \mathrm{SCh}((A', A), (B', B))$, there exists preprocessing channel $\mathcal{P} \in \mathrm{Ch}(B', RA')$ and postprocessing channel $\mathcal{Q} \in \mathrm{Ch}(RA, B)$ such that $\Theta(\mathcal{N}) = \mathcal{Q} \circ \mathcal{N} \circ \mathcal{P}$. A unitary superchannel is composed of unitary postprocessing and preprocessing channels. Given two completely positive maps $\mathcal{N}$ and $\mathcal{M}$, we write $\mathcal{N} \geqslant \mathcal{M}$ if the linear map $\mathcal{N} - \mathcal{M}$ is also completely positive.

id_R denotes the identity channel on R and $\mathbb{1}_R$ denotes the identity operator on R. Let Γ_{RA} denote a maximally entangled operator, $\Gamma_{RA} := \sum_{i,j=0}^{d-1} |ii\rangle\langle jj|_{RA}$ for $d = \min\{|R|, |A|\}$; a maximally entangled state $\Phi_{RA} = \frac{1}{d}\Gamma_{RA}$ if $d < \infty$. For a linear supermap $\mathcal{N}_{A' \to A}$, $\Gamma^{\mathcal{N}}_{RA} = \mathrm{id}_R \otimes \mathcal{N}(\Gamma_{RA'})$ denotes

its Choi operator. If $\mathcal{N} \in \mathrm{Ch}(A', A)$ is a finite-dimensional quantum channel, then $\Phi_{RA}^{\mathcal{N}} = \frac{1}{d}\Gamma_{RA}^{\mathcal{N}}$ is its Choi state. For $|A| < \infty$, $\pi_A := \frac{1}{|A|}\mathbb{1}_A$ is the maximally mixed state. $\|X\|_p$ denotes the Schatten p norm of an operator X. For any two Hermiticity-preserving maps $\mathcal{N}, \mathcal{M}$, $\|\mathcal{N} - \mathcal{M}\|_\diamond := \sup_{\psi \in \mathrm{St}(RA')} \|\mathrm{id}_R \otimes \mathcal{N}(\psi_{RA'}) - \mathrm{id}_R \otimes \mathcal{M}(\psi_{RA'})\|_1$. The fidelity between $\rho, \sigma \in \mathrm{St}(A)$ is $F(\rho, \sigma) := \|\sqrt{\rho}\sqrt{\sigma}\|_1^2$. Let $\langle \widehat{O} \rangle_{\rho_A} := \mathrm{tr}[\widehat{O}_A \rho_A]$. For a quantum channel $\mathcal{N}_{A' \to A}$ and a bipartite state $\rho_{RA'}$, $\mathcal{N}(\rho_{RA'}) := \mathrm{id}_R \otimes \mathcal{N}(\rho_{RA'})$.

Generalized state and channel divergences. Let $\mathbf{D}(\cdot\|\cdot)$ be the generalized state divergence, i.e., for an arbitrary pair of quantum states ρ, σ and an arbitrary quantum channel $\mathcal{N}$, we have $\mathbf{D}(\rho\|\sigma) \geqslant \mathbf{D}(\mathcal{N}(\rho)\|\mathcal{N}(\sigma))$. The generalized channel divergence $\mathbf{D}[\cdot\|\cdot]$ is derived from the generalized state divergence: For any two quantum channels $\mathcal{N}, \mathcal{M} \in \mathrm{Ch}(A'A)$ and the identity channel id,

$$\mathbf{D}[\mathcal{N}\|\mathcal{M}] := \sup_{\psi \in \mathrm{St}(RA')} \mathbf{D}(\mathrm{id}_R \otimes \mathcal{N}(\psi)\|\, \mathrm{id}_R \otimes \mathcal{M}(\psi)), \tag{A1}$$

where it suffices to optimize over pure states $\psi_{RA'}$ [41]. Some examples of the generalized state divergences [50–53]: For a state ρ_A and a positive semidefinite operator σ_A, whenever $\mathrm{supp}(\rho) \subseteq \mathrm{supp}(\sigma)$ (otherwise $+\infty$) (1) the quantum relative entropy $D(\rho\|\sigma) := \mathrm{tr}[\rho(\ln\rho - \ln\sigma)]$, (2) the max-relative entropy $D_\infty(\rho\|\sigma) := \ln\|\sigma^{-1/2}\rho\,\sigma^{-1/2}\|_\infty$, (3) the sandwiched Rényi relative entropy $D_\alpha(\rho\|\sigma) := \frac{1}{\alpha-1}\ln\left(\mathrm{Tr}\left[\left(\sigma^{\frac{1-\alpha}{2\alpha}}\rho\,\sigma^{\frac{1-\alpha}{2\alpha}}\right)^\alpha\right]\right)$ for $\alpha \in [\frac{1}{2}, 1) \cup (1, \infty)$, (4) the ε-hypothesis-testing relative entropy $D_{\mathrm{H}}^\varepsilon(\rho\|\sigma) := -\ln\inf_{0\leqslant\Lambda\leqslant\mathbb{1}}\{\mathrm{tr}[\Lambda\sigma] : \mathrm{tr}[\Lambda\rho] \geqslant 1-\varepsilon\}$, and (5) the purified distance $\mathrm{P}(\rho, \sigma) := \sqrt{1 - F(\rho, \sigma)}$. ln denotes natural logarithm. We have $\lim_{\alpha\to 1} D_\alpha(\rho\|\sigma) = D(\rho\|\sigma)$ and $\lim_{\alpha\to\infty} D_\alpha(\rho\|\sigma) = D_\infty(\rho\|\sigma)$.

The generalized channel divergences are monotonically nonincreasing under the action of quantum superchannels (Theorem 1 of Ref. [18]). If the generalized state divergence is non-negative, then the corresponding channel divergence is also non-negative. If the generalized state divergence is faithful, i.e., minimum if and only if the states are equal, then the corresponding channel divergence is also faithful, i.e., attains minimum if and only if the channels are equal.

An ε-ball around a state ρ_A, for $\varepsilon \in [0, 1]$, is defined as $\mathcal{B}^\varepsilon(\rho_A) = \{\sigma_A : \sigma_A \geqslant 0, \mathrm{tr}(\sigma_A) \leqslant 1, P(\rho_A, \sigma_A) \leqslant \varepsilon\}$. For $\rho \in \mathrm{St}(A)$ and $\sigma \in \mathrm{Pos}(A)$, $D_\infty^\epsilon(\rho\|\sigma) = \inf_{\omega\in\mathcal{B}^\varepsilon(\rho)} D_\infty(\omega\|\sigma)$. An ε-ball around a channel $\mathcal{N}_{A'\to A}$ is defined as $\mathcal{B}^\varepsilon[\mathcal{N}] = \{\mathcal{M} \in \mathrm{Ch}(A', A) : P[\mathcal{N}, \mathcal{M}] \leqslant \varepsilon\}$. We use this to define smoothed channel max-relative entropy as $D_\infty^\varepsilon[\mathcal{N}\|\mathcal{M}] = \inf_{\mathcal{Q}\in\mathcal{B}^\varepsilon[\mathcal{N}]} D_\infty[\mathcal{Q}\|\mathcal{M}]$. $\mathbf{D}^\varepsilon(\cdot\|\cdot)$ is a generalized smoothed-state divergence and $\mathbf{D}^\varepsilon[\cdot\|\cdot]$ is a generalized smoothed-channel divergence.

The channel entropy $S[\mathcal{N}]$ of a quantum channel $\mathcal{N}_{A'\to A}$ is defined as $S[\mathcal{N}] := -D[\mathcal{N}\|\mathcal{R}^{\mathbb{1}}]$ [17,38], where a completely positive map $\mathcal{R}^\omega_{A'\to A}$ denotes the replacer (or preparation) map that outputs $\omega \in \mathrm{Pos}(A)$, $\mathcal{R}^\omega_{A'\to A}(\rho_{A'}) = \mathrm{tr}[\rho_{A'}]\omega_A$ for all $\rho_{A'} \in \mathrm{Pos}(A')$. The (von Neumann) entropy of a quantum state ρ_A is $S(\rho_A) := S(A)_\rho := -D(\rho\|\mathbb{1}) = -\mathrm{tr}[\rho\ln\rho]$. $\mathcal{R}^\pi$ is called a uniformly mixing or completely depolarizing channel, as it always outputs the maximally mixed state $\pi(\propto \mathbb{1})$.

APPENDIX B: EXTRACTABLE WORK AND DYNAMICAL FREE ENERGY

For a fixed inverse temperature β, the thermodynamic nonequilibrium free energy $F_{\mathrm{T}}^\beta(\rho)$ of a quantum state ρ_A is related to its entropy and energy as

$$F_{\mathrm{T}}^\beta(\rho) = E(\rho) - \beta^{-1}S(\rho) = \beta^{-1}D(\rho\|\widehat{\gamma}^\beta), \tag{B1}$$

where $\widehat{\gamma}_A^\beta = \exp(-\beta\widehat{H}_A)$ is the thermal operator (unnormalized thermal state).

Lemma B1. For a quantum state ρ_{AB} with the Hamiltonian $\widehat{H}_{AB} = \mathbb{1}_A \otimes \widehat{H}_B + \widehat{H}_A \otimes \mathbb{1}_B$ that is weakly interacting with the bath at temperature β, we have

$$F_{\mathrm{T}}^\beta(\rho_{AB}) - F_{\mathrm{T}}^\beta\left(\gamma_A^\beta \otimes \gamma_B^\beta\right) = F^\beta(\rho_{AB}) = \beta^{-1}I(A;B)_\rho + F^\beta(\rho_A) + F^\beta(\rho_B). \tag{B2}$$

Proof. Recall that $F_T^\beta(\rho) = E(\rho) + \beta^{-1}S(\rho)$, where $E(\rho) = \mathrm{tr}(\rho\widehat{H})$ is the energy of the system. For noninteracting Hamiltonian, we have $E(\rho_{AB}) = E(\rho_A) + E(\rho_B)$. Furthermore, since $S(\gamma_A^\beta \otimes$

$\gamma_B^\beta) = S(\gamma_A^\beta) + S(\gamma_B^\beta)$, we have $F_T^\beta(\gamma_A^\beta \otimes \gamma_B^\beta) = F_T^\beta(\gamma_A^\beta) + F_T^\beta(\gamma_B^\beta)$, which gives

$$F_T^\beta(\rho_{AB}) - F_T^\beta\left(\gamma_A^\beta \otimes \gamma_B^\beta\right) = E(\rho_A) + E(\rho_B) - \beta^{-1}S(\rho_{AB}) - F_T^\beta\left(\gamma_A^\beta\right) - F_T^\beta\left(\gamma_B^\beta\right) \tag{B3}$$

$$= E(\rho_A) - \beta^{-1}S(\rho_A) + E(\rho_B) - \beta^{-1}S(\rho_B) + \beta^{-1}S(\rho_A) + \beta^{-1}S(\rho_B) - \beta^{-1}S(\rho_{AB}) - F_T^\beta\left(\gamma_A^\beta\right) - F_T^\beta\left(\gamma_B^\beta\right) \tag{B4}$$

$$= F_T^\beta(\rho_A) + F_T^\beta(\rho_B) + \beta^{-1}S(\rho_A) + \beta^{-1}S(\rho_B) - \beta^{-1}S(\rho_{AB}) - F_T^\beta\left(\gamma_A^\beta\right) - F_T^\beta\left(\gamma_B^\beta\right) \tag{B5}$$

$$= F^\beta(\rho_A) + F^\beta(\rho_B) + \beta^{-1}I(A;B)_\rho. \tag{B6}$$

■

Lemma B2. The extractable work $W_{\text{ext}}^\beta[\mathcal{N}]$ from a quantum channel $\mathcal{N}_{A'\to A}$ is equal to

$$W_{\text{ext}}^\beta[\mathcal{N}] = \sup_{\psi\in\text{St}(RA')}\left[\beta^{-1}I(R;A)_{\text{id}\otimes\mathcal{N}(\psi)} + F^\beta(\mathcal{N}(\psi_{A'}))\right] = \beta^{-1}D[\mathcal{N}\|\mathcal{T}^\beta], \tag{B7}$$

where $\mathcal{T}_{A'\to A}^\beta$ is the absolutely thermal channel, $\mathcal{T}^\beta(\cdot) = \text{tr}(\cdot)\gamma_A^\beta$.

Proof. It follows from the definition of the extractable work from a channel $\mathcal{N}_{A'\to A}$ that

$$W_{\text{ext}}^\beta[\mathcal{N}] := \sup_{\psi\in\text{St}(RA')}\left[F_{\text{T}}^\beta(\text{id}\otimes\mathcal{N}(\psi)) - F_{\text{T}}^\beta\left(\psi_R\otimes\gamma_A^\beta\right)\right]$$

$$= \sup_{\psi\in\text{St}(RA')}\left[F^\beta(\text{id}\otimes\mathcal{N}(\psi)) - F^\beta\left(\psi_R\otimes\gamma_A^\beta\right)\right]$$

$$= \sup_{\psi\in\text{St}(RA')}\left[\beta^{-1}I(R;A)_{\text{id}\otimes\mathcal{N}(\psi)} + F^\beta(\mathcal{N}(\psi_{A'}))\right]. \tag{B8}$$

We know that $F^\beta(\mathcal{N}(\psi_{A'})) = \beta^{-1}D(\mathcal{N}(\psi_{A'})\|\gamma_A^\beta)$ and $I(A;B)_\rho + D(\rho_B\|\gamma^\beta) = D(\rho_{AB}\|\rho_A\otimes\gamma_B^\beta)$, which implies

$$W_{\text{ext}}^\beta[\mathcal{N}] = \sup_{\psi\in\text{St}(RA')}\left[\beta^{-1}I(R;A)_{\text{id}\otimes\mathcal{N}(\psi)} + F^\beta(\mathcal{N}(\psi_{A'}))\right] \tag{B9}$$

$$= \sup_{\psi\in\text{St}(RA')}\left[\beta^{-1}D(\text{id}\otimes\mathcal{N}(\psi)\|\,\text{id}\otimes\mathcal{T}^\beta(\psi))\right] \tag{B10}$$

$$= \beta^{-1}D[\mathcal{N}\|\mathcal{T}^\beta]. \tag{B11}$$

■

Proposition B1 (Ref. [9]). The (resource-theoretic) free energy $F^\beta[\mathcal{N}] := \beta^{-1}D[\mathcal{N}_{A'\to A}\|\mathcal{T}_{A'\to A}^\beta]$ of an arbitrary quantum channel $\mathcal{N}_{A'\to A}$ satisfies the following properties:

(P1) Monotonically nonincreasing under the action of a Gibbs-preserving superchannel Θ^β, $\Theta^\beta(\mathcal{T}_{A'\to A}^\beta) = \mathcal{T}_{B'\to B}^\beta$, $F^\beta[\Theta^\beta(\mathcal{N})] \leqslant F^\beta[\mathcal{N}]$.

(P2) Reduction to the free energy function of the output state for a replacer channel $\mathcal{R}^\omega$, $\mathcal{R}^\omega(\rho_{A'}) := \omega \in \text{St}(A)$ for all input states $\rho_{A'}$, $F^\beta[\mathcal{R}^\omega] = F^\beta(\omega)$.

(P3) Minimum is attained if and only if the channel is absolutely thermal.

(P4) Continuity: For any two channels $\mathcal{N}, \mathcal{M}$ such that $\frac{1}{2}\|\mathcal{N}-\mathcal{M}\|_\diamond \leqslant \varepsilon \in [0,1]$, we have $|F^\beta[\mathcal{N}] - F^\beta[\mathcal{M}]| \leqslant \beta^{-1}(\varepsilon K + h_2(\varepsilon))$, where K is a positive number given in Eq. (B16).

(P5) Additive under tensor-product channels $\mathcal{N}_{A_1'\to A_1}\otimes\mathcal{M}_{A_2'\to A_2}$ with $\widehat{H}_{A_1A_2} = \widehat{H}_{A_1}\otimes\mathbb{1}_{A_2} + \mathbb{1}_{A_1}\otimes\widehat{H}_{A_2}$, $F^\beta[\mathcal{N}\otimes\mathcal{M}] = F^\beta[\mathcal{N}] + F^\beta[\mathcal{M}]$.

(P6) Convexity: $F^\beta[p\mathcal{N}+(1-p)\mathcal{M}] \leqslant pF^\beta[\mathcal{N}]+(1-p)F^\beta[\mathcal{M}]$ for $p\in[0,1]$, where $\mathcal{N}_{A'\to A}$ and $\mathcal{M}_{A'\to A}$ are quantum channels.

Proof.

(P1) *Monotonicity under Gibbs-preserving superchannels*: This follows from the monotonicity of relative entropy between channels. Let Θ be a superchannel such that $\Theta(\mathcal{T}_{A'\to A}^\beta) = \mathcal{T}_{B'\to B}^\beta$, it

follows that

$$D\big[\mathcal{N}_{A'\to A}\big\|\mathcal{T}^{\beta}_{A'\to A}\big] \geqslant D\big[\Theta(\mathcal{N}_{A'\to A})\big\|\Theta\big(\mathcal{T}^{\beta}_{A'\to A}\big)\big] \tag{B12}$$

$$= D\big[\Theta(\mathcal{N}_{A'\to A})\big\|\mathcal{T}^{\beta}_{A'\to A}\big], \tag{B13}$$

which implies $F^{\beta}[\Theta(\mathcal{N}_{A'\to A})] \leqslant F^{\beta}[\mathcal{N}_{A'\to A}]$.

(P2) *Reduction to states*: For a replacer channel $\mathcal{R}^{\omega}_{A'\to A}(\rho_{A'}) := \mathrm{tr}(\rho_{A'})\omega_A$, we have

$$\beta F^{\beta}[\mathcal{R}^{\omega}] = D[\mathcal{R}^{\omega}\|\mathcal{T}^{\beta}] = \sup_{\psi\in\mathrm{St}(RA')} D(\mathcal{R}^{\omega}(\psi_{RA'})\|\mathcal{T}^{\beta}(\psi_{RA'}))$$

$$= \sup_{\psi\in\mathrm{St}(RA')} D\big(\psi_R\otimes\omega_A\big\|\psi_R\otimes\gamma^{\beta}_A\big) = D\big(\omega_A\big\|\gamma^{\beta}_A\big) = \beta F^{\beta}(\omega). \tag{B14}$$

(P3) *Minimum value at absolutely thermal channel*: This follows from the fact that $D(\rho\|\sigma)\geqslant 0$ if both ρ and σ are states, and $D(\rho\|\sigma)=0$ if and only if $\rho=\sigma$. Therefore, given quantum channels $\mathcal{N}_{A'\to A}$ and $\mathcal{M}_{A'\to A}$, $D[\mathcal{N}\|\mathcal{M}] = \sup_{\psi\in\mathrm{St}(RA')} D(\mathcal{N}(\psi)\|\mathcal{M}(\psi)) = 0$ if and only if $\mathcal{N}(\varphi)=\mathcal{M}(\varphi)$ for all $\varphi\in\mathrm{St}(RA')$ or $\mathcal{N}=\mathcal{M}$. Therefore, $F^{\beta}[\mathcal{N}] = \beta^{-1}D[\mathcal{N}\|\mathcal{T}^{\beta}]\geqslant 0$ with equality if and only if $\mathcal{N}=\mathcal{T}^{\beta}$.

(P4) *Continuity:* We shall show that given two quantum channels $\mathcal{N}_{A'\to A}$ and $\mathcal{M}_{A'\to A}$ such that $\frac{1}{2}\|\mathcal{N}-\mathcal{M}\|_{\diamond}\leqslant\varepsilon$, we have

$$|F^{\beta}[\mathcal{N}] - F^{\beta}[\mathcal{M}]| \leqslant \beta^{-1}(\varepsilon K + h_2(\varepsilon)), \tag{B15}$$

where $\varepsilon\in[0,1]$ and $h_2(\varepsilon) = -\varepsilon\ln(\varepsilon) - (1-\varepsilon)\ln(1-\varepsilon)$ is the binary Shannon entropy. K is a positive real number such that

$$K \geqslant \max\left\{D_{\infty}\big(\mathcal{N}\big(\psi^0_{RA'}\big)\big\|\mathcal{T}^{\beta}\big(\psi^0_{RA'}\big)\big), D_{\infty}\big(\mathcal{M}\big(\phi^0_{RA'}\big)\big\|\mathcal{T}^{\beta}\big(\phi^0_{RA'}\big)\big)\right\}, \tag{B16}$$

where $\psi^0_{RA'}$ maximizes $D(\mathcal{N}(\psi_{RA'})\|\mathcal{T}^{\beta}(\psi_{RA'}))$ and $\phi^0_{RA'}$ maximizes $D(\mathcal{M}(\psi_{RA'})\|\mathcal{T}^{\beta}(\psi_{RA'}))$.

This can be shown by noting that the condition $\frac{1}{2}\|\mathcal{N}-\mathcal{M}\|_{\diamond}\leqslant\varepsilon$ implies that $\frac{1}{2}\|\mathcal{N}(\psi_{RA'}) - \mathcal{M}(\psi_{RA'})\|_1\leqslant\varepsilon$ for all $\psi_{RA'}$. The continuity of relative entropy in the first argument has been tightened in Refs. [54,55]. Here, we use a slightly simpler bound given in Theorem 1 of Ref. [54], from which it follows that

$$D(\mathcal{N}(\psi_{RA'})\|\mathcal{T}^{\beta}(\psi_{RA'})) - D(\mathcal{M}(\psi_{RA'})\|\mathcal{T}^{\beta}(\psi_{RA'})) \leqslant \varepsilon K + h_2(\varepsilon), \tag{B17}$$

where $K\geqslant D_{\infty}(\mathcal{N}(\psi_{RA'})\|\mathcal{T}^{\beta}(\psi_{RA'}))$ is some positive real number. Therefore, we have

$$D[\mathcal{N}\|\mathcal{T}^{\beta}] - D[\mathcal{M}\|\mathcal{T}^{\beta}] \leqslant D\big(\mathcal{N}\big(\psi^0_{RA'}\big)\big\|\mathcal{T}^{\beta}\big(\psi^0_{RA'}\big)\big) - D\big(\mathcal{M}\big(\psi^0_{RA'}\big)\big\|\mathcal{T}^{\beta}\big(\psi^0_{RA'}\big)\big) \leqslant \varepsilon K_{\mathcal{N}} + h_2(\varepsilon), \tag{B18}$$

where the state $\psi^0_{RA'}$ maximizes $D(\mathcal{N}(\psi_{RA'})\|\mathcal{T}^{\beta}(\psi_{RA'}))$ and $K_{\mathcal{N}}\geqslant D_{\infty}(\mathcal{N}(\psi^0_{RA'})\|\mathcal{T}^{\beta}(\psi^0_{RA'}))$. Following the similar steps for the channel $\mathcal{M}$,

$$D[\mathcal{M}\|\mathcal{T}^{\beta}] - D[\mathcal{N}\|\mathcal{T}^{\beta}] \leqslant \varepsilon K_{\mathcal{M}} + h_2(\varepsilon), \tag{B19}$$

where $K_{\mathcal{M}}\geqslant D_{\infty}(\mathcal{M}(\phi^0_{RA'})\|\mathcal{T}^{\beta}(\phi^0_{RA'}))$ where the state $\phi^0_{RA'}$ maximizes $D(\mathcal{M}(\psi_{RA'})\|\mathcal{T}^{\beta}(\psi_{RA'}))$. From Eqs. (B18) and (B19), we have

$$|D[\mathcal{N}\|\mathcal{T}^{\beta}] - D[\mathcal{M}\|\mathcal{T}^{\beta}]| \leqslant \varepsilon K + h_2(\varepsilon), \tag{B20}$$

where $K=\max\{K_{\mathcal{N}}, K_{\mathcal{M}}\}$. The continuity relation (B15) follows by using the definition of free energy $F^{\beta}[\mathcal{N}] = \beta^{-1}D[\mathcal{N}\|\mathcal{T}^{\beta}]$ in the above inequality.

(P5) *Additivity*: For two channels $\mathcal{N}_{A'_1\to A_1}$ and $\mathcal{M}_{A'_2\to A_2}$ such that the output interaction Hamiltonian $\widehat{H}_{A_1A_2}$ is zero, the absolutely thermal channel can be written as $\mathcal{T}^{\beta}_{A'_1A'_2\to A_1A_2} = \mathcal{T}^{\beta}_{A'_1\to A_1}\otimes\mathcal{T}^{\beta}_{A'_2\to A_2} =: \mathcal{T}^{\beta}_1\otimes\mathcal{T}^{\beta}_2$. In this case, the additivity of the generalized free energy of channel follows

from the additivity of the relative channel entropy since

$$\beta F^{\beta}[\mathcal{N}\otimes\mathcal{M}] = D\big[\mathcal{N}\otimes\mathcal{M}\big\|\mathcal{T}_1^{\beta}\otimes\mathcal{T}_2^{\beta}\big]. \tag{B21}$$

We will show that the sandwiched Rényi channel divergence is additive under tensor product with respect to the absolutely thermal channel, i.e.,

$$D\big[\mathcal{N}\otimes\mathcal{M}\big\|\mathcal{T}_1^{\beta}\otimes\mathcal{T}_2^{\beta}\big] = D\big[\mathcal{N}\big\|\mathcal{T}_1^{\beta}\big] + D\big[\mathcal{M}\big\|\mathcal{T}_2^{\beta}\big]. \tag{B22}$$

The proof of the inequality "$\geqslant$" follows from the definition of the channel relative entropy,

$$\begin{aligned} D\big[\mathcal{N}\otimes\mathcal{M}\big\|\mathcal{T}_1^{\beta}\otimes\mathcal{T}_2^{\beta}\big] &= \sup_{\psi\in\mathrm{St}(RA_1'A_2')} D\big(\mathcal{N}\otimes\mathcal{M}(\psi)\big\|\mathcal{T}_1^{\beta}\otimes\mathcal{T}_2^{\beta}(\psi)\big) \\ &\geqslant \sup_{\varphi\in\mathrm{St}(R_1A_1')\otimes\mathrm{St}(R_2A_2')} D\big(\mathcal{N}\otimes\mathcal{M}(\varphi)\big\|\mathcal{T}_1^{\beta}\otimes\mathcal{T}_2^{\beta}(\varphi)\big) \qquad \text{(B23)} \\ &= D\big[\mathcal{N}\big\|\mathcal{T}_1^{\beta}\big] + D\big[\mathcal{M}\big\|\mathcal{T}_2^{\beta}\big], \qquad \text{(B24)} \end{aligned}$$

where we have used the additivity of the relative entropy of states under the tensor product.

To prove the inequality "$\leqslant$", we use the following result from Lemma 38 of Ref. [56], for an arbitrary state $\rho_{RA'}$, a channel $\mathcal{N}_{A'\to A}$, and a replacer channel $\mathcal{R}^{\tau}_{A'\to A}$, which replaces all its input states with a state τ,

$$D(\mathcal{N}(\rho_{RA'})\|\sigma_R\otimes\tau_A) \leqslant D[\mathcal{N}\|\mathcal{R}^{\tau}] + D(\rho_{RA'}\|\sigma_{RA'}). \tag{B25}$$

Let $\psi_{RA_1'A_2'}$ be an arbitrary pure state and states $\rho_{R'A_1'}$ and $\sigma_{R'A_1'}$ be such that $R' = RA_2$, i.e., $\mathcal{M}_{A_2'\to A_2}(\psi_{RA_1'A_2'}) = \rho_{R'A_1'}$ and $\mathcal{T}^{\beta}_{A_2'\to A_2}(\psi_{RA_1'A_2'}) = \sigma_{R'A_1'}$,

$$D\big(\mathcal{N}\otimes\mathcal{M}\big(\psi_{RA_1'A_2'}\big)\big\|\mathcal{T}^{\beta}_{A_1'\to A_1}\otimes\mathcal{T}^{\beta}_{A_2'\to A_2}\big(\psi_{RA_1'A_2'}\big)\big) \leqslant D[\mathcal{N}\|\mathcal{T}^{\beta}] + D\big(\mathcal{M}\big(\psi_{RA_1'A_2'}\big)\big\|\mathcal{T}^{\beta}_{A_2'\to A_2}\big(\psi_{RA_1'A_2'}\big)\big) \tag{B26}$$

$$\leqslant D[\mathcal{N}\|\mathcal{T}^{\beta}] + D[\mathcal{M}\|\mathcal{T}^{\beta}]. \tag{B27}$$

This implies the additivity of $F^{\beta}[\mathcal{N}]$.

(P6) *Convexity*: It is known that quantum relative entropy is jointly convex, that is, for a probability distribution $\{p_x\}_x$, we have

$$\begin{aligned} D\left[\sum_x p_x\mathcal{N}^x\|\mathcal{T}^{\beta}\right] &= \sup_{\psi_{RA'}} D\left(\sum_x p_x\mathcal{N}^x(\psi)\|\mathcal{T}^{\beta}(\psi)\right) \qquad \text{(B28)} \\ &\leqslant \sup_{\psi_{RA'}}\sum_x p_x D(\mathcal{N}^x(\psi)\|\mathcal{T}^{\beta}(\psi)), \qquad \text{(B29)} \end{aligned}$$

which implies

$$F^{\beta}\left[\sum_x p_x\mathcal{N}^x\right] \leqslant \sum_x p_x F^{\beta}[\mathcal{N}^x]. \tag{B30}$$

■

1. Free energy for unitary channels

Before we show that for a given bath, unitary channels have the maximum channel resource, we prove the following lemma.

Lemma B3. Given a state $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$, the max-relative entropy is bounded as follows:

$$D_\infty(\rho\|\sigma) \geqslant \ln\left(\max_i p_i \langle\psi_i|\sigma^{-1}|\psi_i\rangle\right), \tag{B31}$$

$$D_\infty(\rho\|\sigma) \leqslant \ln\left(\sum_i p_i \langle\psi_i|\sigma^{-1}|\psi_i\rangle\right). \tag{B32}$$

Proof. The max-relative entropy $D_\infty(\rho\|\sigma)$ can be written as

$$D_\infty(\rho\|\sigma) = \ln\left\|\sum_i p_i \sigma^{-\frac{1}{2}}|\psi_i\rangle\langle\psi_i|\sigma^{-\frac{1}{2}}\right\|_\infty \tag{B33}$$

$$= \ln\|AA^\dagger\|_\infty \tag{B34}$$

$$= \ln\lambda_{\max}(AA^\dagger), \tag{B35}$$

where the matrix A is given by $A = [|v_1\rangle\ |v_2\rangle\ \cdots]$ with the vectors $|v_i\rangle := \sqrt{p_i}\sigma^{-\frac{1}{2}}|\psi_i\rangle$. The corresponding Gram matrix of matrix A is given by $G = A^\dagger A$, such that $G_{ij} = \langle v_i|v_j\rangle = \sqrt{p_i p_j}\langle\psi_i|\sigma^{-1}|\psi_j\rangle$. Note that $AA^\dagger$ and G have the same nonzero eigenvalues. Therefore, $D_\infty(\rho\|\sigma) = \ln(\lambda_{\max}(AA^\dagger)) = \ln(\lambda_{\max}(G))$. Now, for any matrix G, we have the following property:

$$\max_i(G_{ii}) \leqslant \lambda_{\max}(G) \leqslant \mathrm{tr}(G). \tag{B36}$$

Using the fact that $G_{ij} = \langle v_i|v_j\rangle = \sqrt{p_i p_j}\langle\psi_i|\sigma^{-1}|\psi_j\rangle$, we have the proof of the stated lemma. ■

Proposition B2. For $\alpha \in \{1, \infty\}$ and $|A'| = |A|$, the free energy $F_\alpha^\beta[\mathcal{N}]$ of a quantum channel $\mathcal{N}_{A'\to A}$ is maximum if and only if $\mathcal{N}$ is a unitary channel. For all unitary channels $\mathcal{U}_{A'\to A}$, $F_\alpha^\beta[\mathcal{U}] = F_\alpha^\beta[\mathrm{id}_{A'\to A}]$.

Proof. Given a state ρ_{RA} and its decomposition into pure states $\rho_{RA} = \sum_x p_x \psi_{RA}^x$, we use the joint quasiconvexity of the sandwiched Rényi entropy to observe that for $\alpha \in \{1, \infty\}$,

$$D_\alpha\left(\sum_x p_x \psi_{RA}^x \,\middle\|\, \sum_x p_x \rho_R^x \otimes \gamma_A^\beta\right) \leqslant \max_x D_\alpha\left(\psi_{RA}^x \,\|\, \rho_R^x \otimes \gamma_A^\beta\right), \tag{B37}$$

where $\rho_R^x = \mathrm{tr}_A\, \psi_{RA}^x$. Therefore, $D_\alpha(\rho_{RA}\|\rho_R \otimes \gamma_A)$ achieves the maximum value if ρ_{RA} is a pure state. This implies that $D_\alpha[\mathcal{N}\|\mathcal{T}^\beta]$ achieves the maximum value if $\mathcal{N}$ is a unitary channel.

We will show that the "only if" condition is satisfied for $\alpha \in \{1, \infty\}$ by proving that the equality in Eq. (B37) holds if and only if ρ_{RA} is a pure state. Since we know that relative entropy is jointly convex, and therefore for $\rho = \sum_i p_i \psi_i$, where $\{\psi_i\}$ are pure, we have

$$D(\rho\|\sigma) \leqslant \sum_i p_i D(\psi_i\|\sigma). \tag{B38}$$

The equality in the above holds if and only if ρ is pure [57].

For the case of $\alpha = \infty$, let the equality for the quasiconvexity condition be satisfied, i.e., $D_\infty(\rho\|\sigma) = \max_i D_\infty(\psi_i\|\sigma)$, then using Lemma B3,

$$\max_i \ln(\langle\psi_i|\sigma^{-1}|\psi_i\rangle) \leqslant \ln\left(\sum_i p_i \langle\psi_i|\sigma^{-1}|\psi_i\rangle\right) \tag{B39}$$

$$\text{or,}\quad \max_i \langle\psi_i|\sigma^{-1}|\psi_i\rangle \leqslant \sum_i p_i \langle\psi_i|\sigma^{-1}|\psi_i\rangle. \tag{B40}$$

Since the weighted average cannot be greater than the largest element of the set, the above condition is satisfied if and only if ρ is a pure state. ■

APPENDIX C: RESOURCE THEORY OF DYNAMICAL ATHERMALITY

We now introduce framework and characterization of the thermodynamic resource theory of square quantum channels. A quantum channel $\mathcal{N}_{A'\to A}$ is a square quantum channel if $|A'| = |A|$; in other words, a quantum channel with square Choi operator is called a square channel. To quantify the thermodynamic resourcefulness of a quantum channel $\mathcal{N}$, we consider its distinguishability from a thermal channel $\mathcal{T}^\beta$ whose output γ^β is in thermal equilibrium with the bath [12]. The absolutely thermal channel $\mathcal{T}^\beta$ represents thermalization process with respect to the given bath at inverse temperature β.

To characterize a resource theory of athermality of quantum channels, we identify our free object to be the absolutely thermal channel $\mathcal{T}^\beta$ and the free operations to be GPSCs. This is a relevant assumption as thermalization processes seem to be natural in practical scenarios where quantum systems inherently tend to thermalize upon interaction with the bath. The closed systems in isolation with the bath are nontrivial and idealistic. We write the athermal channel resource as $(\mathcal{N}, \mathcal{T}^\beta)$ to specify that the athermality of the channel $\mathcal{N}$ is being considered with respect to $\mathcal{T}^\beta$. We call two channel resources $(\mathcal{N}, \mathcal{T}^\beta)$ and $(\mathcal{M}, \mathcal{T}^{\beta'})$ to be equivalent, $(\mathcal{N}, \mathcal{T}^\beta) \sim (\mathcal{M}, \mathcal{T}^{\beta'})$, if they are interconvertible through some GPSCs.

For a quantum superchannel $\Theta \in \mathrm{SCh}((A', A), (B', B))$ with the following action:

$$\Theta(\mathcal{N}_{A'\to A}) = \mathcal{Q}_{A\to B} \circ \mathcal{N} \circ \mathcal{P}_{B'\to A'}, \tag{C1}$$

Θ is Gibbs preserving if and only if $\mathcal{Q}_{A\to B}$ is Gibbs-preserving channel, i.e., $\mathcal{Q}(\gamma_A^\beta) = \gamma_B^\beta$. A quantum superchannel $\widetilde{\Theta} \in \mathrm{SCh}((A', A), (B', B))$, where $\widetilde{\Theta}(\mathcal{N}) = \widetilde{\mathcal{Q}}_{PA\to B} \circ \mathcal{N} \circ \widetilde{\mathcal{P}}_{B'\to PA'}$ is also Gibbs preserving if its postprocessing channel $\widetilde{\mathcal{Q}}_{PA\to B}$ is absolutely thermal.

1. Golden unit of the dynamical athermality

For a square quantum channel $\mathcal{N}_{A'\to A}$, the free energy is maximum if and only if the channel is unitary. For an arbitrary pair $\mathcal{U}_{A'\to A}, \mathcal{V}_{A'\to A}$ of unitary channels, there always exists a GPSC $\Theta^\beta \in \mathrm{SCh}((A', A), (A', A))$ such that $\Theta^\beta(\mathcal{U}) = \mathcal{V}$, for instance, $\Theta^\beta(\mathcal{N}) = \mathcal{N} \circ (\mathcal{U}^\dagger \circ \mathcal{V})$. That is, all unitary channels $(\mathcal{U}, \mathcal{T}^\beta)$ are equally resourceful, $(\mathrm{id}_{A'\to A}, \mathcal{T}^\beta_{A'\to A}) \sim (\mathcal{U}_{A'\to A}, \mathcal{T}^\beta_{A'\to A})$. This is consistent with the free energy of all unitary channels $(\mathcal{U}, \mathcal{T}^\beta)$ being the same. We can show that the free energy of a unitary channel is minimum when the output Hamiltonian is fully degenerate. To see this, we will use the following Lemmas.

Lemma C1 (Ref. [58]). The max-free energy $F_\infty^\beta[\mathcal{U}]$ of a unitary quantum channel $\mathcal{U}_{A'\to A}$ is

$$F_\infty^\beta[\mathcal{U}] = \beta^{-1} \ln \mathrm{tr}\left[\left(\gamma_A^\beta\right)^{-1}\right]. \tag{C2}$$

If the Hamiltonian of A is fully degenerate, $\widehat{H}_A \propto \mathbb{1}_A$, then $F_\infty^\beta[\mathcal{U}] = 2\beta^{-1} \ln |A|$.

The proof follows from Corollary A.4.2 of Ref. [58], since $F_\infty^\beta[\mathcal{N}] = \beta^{-1} \ln(1 + R_T^\beta[\mathcal{N}])$. For the sake of completeness, we give a proof.

Proof. Using the property of the max-relative entropy of quantum channels

$$\beta F_\infty^\beta[\mathcal{U}] = D_\infty[\mathcal{U}\|\mathcal{T}^\beta] = D_\infty(\Phi^\mathcal{U}\|\Phi^{\mathcal{T}^\beta}), \tag{C3}$$

where $\Phi^{\mathcal{U}}$ is a pure state and $\Phi^{\mathcal{T}^\beta} = \pi_R \otimes \gamma_\beta$. Given a pure state ψ, we have $D_\infty(\psi\|\sigma) = \ln\langle\psi|\sigma^{-1}|\psi\rangle$ for a positive operator σ. Let $\mathcal{U}(\rho) = U\rho U^\dagger$, then

$$\beta F_\infty^\beta[\mathcal{U}] = D_\infty(\Phi^{\mathcal{U}}\|\Phi^{\mathcal{T}}) \tag{C4}$$

$$= \ln\left(\frac{1}{d}\sum_j(\langle j|\otimes\langle j|U^\dagger)\left(\frac{1}{d}\mathbb{1}_R\otimes\gamma_\beta\right)^{-1}\sum_i(|i\rangle\otimes U|i\rangle)\right)$$

$$= \ln\left(\sum_{i,j}\delta_{ji}\langle j|U^\dagger\gamma_\beta^{-1}U|i\rangle\right) = \ln\left(\mathrm{tr}\left[\gamma_\beta^{-1}\right]\right). \tag{C5}$$

If $\widehat{H}_A = c\mathbb{1}_A$, $\mathrm{tr}[(\gamma_A^\beta)^{-1}] = \mathrm{tr}(|A|\mathbb{1}_A) = |A|^2$ and $F_\infty^\beta[\mathcal{U}] = 2\beta^{-1}\ln|A|$. ■

Lemma C2 (Ref. [9]). Given a unitary channel $\mathcal{U}_{A'\to A}$, the minimum value of its max-free energy $F_\infty^\beta[\mathcal{U}]$ is achieved for the output with trivial Hamiltonian, $\widehat{H}_A = c\mathbb{1}_A$. In particular,

$$\min_{\widehat{H}_A} F_\infty^\beta[\mathcal{U}] = 2\beta^{-1}\ln|A|. \tag{C6}$$

Proof. From Lemma C1, we have

$$\beta F_\infty^\beta[\mathcal{U}] = \ln\mathrm{tr}\left(\gamma_\beta^{-1}\right) \tag{C7}$$

$$= \ln\mathrm{tr}\,\mathrm{e}^{\beta\widehat{H}_A} + \ln\mathrm{tr}\,\mathrm{e}^{-\beta\widehat{H}_A}. \tag{C8}$$

We analyze the vanishing conditions of the directional derivative with respect to $\widehat{H}_A$, that is $\nabla_{\widehat{H}_A}F_\infty^\beta[\mathcal{U}] = 0$, which implies that

$$\frac{\mathrm{e}^{\beta\widehat{H}_A}}{\mathrm{tr}(\mathrm{e}^{\beta\widehat{H}_A})} - \frac{\mathrm{e}^{-\beta\widehat{H}_A}}{\mathrm{tr}(\mathrm{e}^{-\beta\widehat{H}_A})} = 0. \tag{C9}$$

For all eigenvalues E_i of $\widehat{H}_A$, we have

$$\frac{\mathrm{e}^{\beta E_i}}{\mathrm{tr}(\mathrm{e}^{\beta\widehat{H}_A})} = \frac{\mathrm{e}^{-\beta E_i}}{\mathrm{tr}(\mathrm{e}^{-\beta\widehat{H}_A})} \quad\text{or}\quad \mathrm{e}^{2\beta E_i} = \frac{\mathrm{tr}(\mathrm{e}^{\beta\widehat{H}_A})}{\mathrm{tr}(\mathrm{e}^{-\beta\widehat{H}_A})}, \quad \forall i. \tag{C10}$$

Since the right-hand side is independent of i, we conclude that all the eigenvalues of $\widehat{H}_A$ must be the same, which corresponds to the Hamiltonian of the form $\widehat{H}_A = c\mathbb{1}_A$. For such Hamiltonian, we have $F_\infty^\beta[\mathcal{U}] = 2\beta^{-1}\ln|A|$. To see that this value is the global minimum for $F_\infty^\beta[\mathcal{U}]$, note that

$$\mathrm{e}^{\beta F_\infty^\beta[\mathcal{U}]} = \mathrm{tr}\,\mathrm{e}^{\beta\widehat{H}_A}\,\mathrm{tr}\,\mathrm{e}^{-\beta\widehat{H}_A} \tag{C11}$$

$$\geqslant (\mathrm{tr}\,\mathrm{e}^{\frac{1}{2}\beta\widehat{H}_A}\mathrm{e}^{-\frac{1}{2}\beta\widehat{H}_A})^2 \tag{C12}$$

$$= (\mathrm{tr}\,\mathbb{1}_A)^2 = |A|^2. \tag{C13}$$

We have used the Cauchy-Schwarz inequality for Hilbert-Schmidt inner product: $(\mathrm{tr}(A^\dagger B))^2 \leqslant \mathrm{tr}(A^\dagger A)\,\mathrm{tr}(B^\dagger B)$. We conclude that $F_\infty^\beta[\mathcal{U}] \geqslant 2\beta^{-1}\ln|A|$ and the output Hamiltonian $\widehat{H}_A = c\mathbb{1}_A$ gives the minimum free energy for unitary channels. ■

The corollary given below follows directly from Eq. (B7).

Corollary C1. The free energy $F^\beta[\mathcal{N}]$ of a quantum channel $\mathcal{N}_{A'\to A}$ is lower bounded as

$$F^\beta[\mathcal{N}] \geqslant \beta^{-1}I(R;A)_{\Phi^{\mathcal{N}}} + F^\beta(\mathcal{N}(\pi_{A'})), \tag{C14}$$

and upper bounded as

$$F^\beta[\mathcal{N}] \leqslant \beta^{-1}I[\mathcal{N}] + \sup_{\psi\in\mathrm{St}(A')} F^\beta(\mathcal{N}(\psi)). \tag{C15}$$

The free energy of a unitary channel $\mathcal{U}_{A'\to A}$ is lower bounded as

$$F^{\beta}[\mathcal{U}] \geqslant \beta^{-1}\big(\ln|A| + \ln Z_A^{\beta}\big) + \frac{1}{|A|}\operatorname{tr}[\widehat{H}_A], \tag{C16}$$

where $Z_A^{\beta} := \operatorname{tr}[\exp(-\beta\widehat{H}_A)]$.

We will now show that given a unitary channel $\mathcal{U}_{A'\to A}$, the resource $(\mathcal{U}, \mathcal{T}^{\beta})$ is minimum when the output Hamiltonian is of the form $\widehat{H}_A = c\mathbb{1}_A$.

Proposition C1 (Free energy of the golden unit). Given a unitary channel $\mathcal{U}_{A'\to A}$, the minimum free energy of the channel is achieved for the output system Hamiltonian $\widehat{H}_A = c\mathbb{1}_A$, In particular,

$$\min_{\widehat{H}_A} F_{\alpha}^{\beta}[\mathcal{U}] = 2\beta^{-1}\ln|A|, \quad \text{where } \alpha \in \{1,\infty\}. \tag{C17}$$

Proof. From Corollary C1, we have $F^{\beta}[\mathcal{U}] \geqslant f(\widehat{H}_A)$, where

$$f(\widehat{H}_A) = \beta^{-1}\left(\ln|A| + \ln Z_A^{\beta} + \frac{\beta}{|A|}\operatorname{tr}(\widehat{H}_A)\right). \tag{C18}$$

To find the global minima of the above operator function, we analyze the operator derivative $\nabla_{\widehat{H}_A} f(\widehat{H}_A)$. Using arguments similar to Lemma C2, we can show that

$$\min_{\widehat{H}_A} f(\widehat{H}_A) = f(c\mathbb{1}_A) = 2\beta^{-1}\ln|A|. \tag{C19}$$

Combining the above result with that of Lemma C2, we have the following:

$$2\beta^{-1}\ln|A| \leqslant \min_{\widehat{H}_A} F^{\beta}[\mathcal{U}] \leqslant \min_{\widehat{H}_A} F_{\infty}^{\beta}[\mathcal{U}] = 2\beta^{-1}\ln|A|. \tag{C20}$$

$$\text{This implies} \quad \min_{\widehat{H}_A} F^{\beta}[\mathcal{U}] = \min_{\widehat{H}_A} F_{\alpha}^{\beta}[\mathcal{U}] = 2\beta^{-1}\ln|A|. \tag{C21}$$

■

With freedom of choice for golden units and the fact that GPSCs are free operations in our athermality framework, we mark our golden unit as the identity resource channel $(\mathrm{id}_{A'\to A}, \mathcal{R}^{\pi})$, where $\mathcal{R}^{\pi}_{A'\to A}$ is the absolutely thermal channel for fully degenerate output Hamiltonian ($\widehat{H}_A \propto \mathbb{1}_A$). We denote $(\mathrm{id}_{A'\to A}, \mathcal{R}^{\pi}_{A'\to A})$ as $(\mathrm{id}_m, \mathcal{R}^{\pi})$ for $|A'| = |A| = m$.

It is evident that $(\mathrm{id}_{A'\to A}, \mathcal{R}^{\pi}_{A'\to A})$ is more resourceful than $(\mathrm{id}_{B'\to B}, \mathcal{R}^{\pi}_{B'\to B})$ if $|A| > |B|$ [12,17,38]; therefore, we will have to be considerate of the dimension of id in the golden unit. The identity channel id_m (or any equivalent unitary channel $\mathcal{U}_m$) allows for the perfect distribution of $m \times m$-dimensional quantum states between two parties [59,60], equivalent to the distribution of a maximally entangled state Φ of Schmidt rank m [60–62].

2. Distillation and conversion cost of dynamical athermality

The uniformly mixing channel $\mathcal{R}^{\pi}_{A'\to A}$, $|A'| = |A| = m$, can be obtained by the action of unitary channels $\mathcal{U}(\cdot) = U(\cdot)U^{\dagger}$ uniformly picked at random with respect to Haar measure,

$$\mathcal{R}^{\pi}(\cdot) = \int_{U\in\mathbb{U}(m)} \mathrm{d}\mu_U U(\cdot)U^{\dagger}, \tag{C22}$$

where $\mathbb{U}(m)$ is the set of all unitary operators $U_{A'\to A}$. We can also obtain $\mathcal{R}^{\pi}$ by taking a uniform mixture of Weyl unitary channels $\mathcal{W}^i(\cdot) = W^i(\cdot)W^{i\dagger}$,

$$\mathcal{R}^{\pi}(\cdot) = \frac{1}{m^2}\sum_{i=0}^{m^2-1} W^i(\cdot)W^{i\dagger}, \tag{C23}$$

where $\{W^i\}_{i=0}^{m^2-1}$ is the set (group) of Weyl unitaries; $\{W^i\}_{i=0}^{m^2-1}$ forms a complete orthonormal basis for the space of all linear operators acting on m-dimensional Hilbert space. Let $\mathcal{W}^0 = \mathrm{id}_m$ and

$\mathrm{id}_m^{\perp} := \sum_{i=1}^{m^2-1} \mathcal{W}^i$, then

$$\mathcal{R}^{\pi} = \frac{1}{m^2}\,\mathrm{id}_m + \frac{1}{m^2}\sum_{i=1}^{m^2-1}\mathcal{W}^i = \frac{1}{m^2}(\mathrm{id}_m + \mathrm{id}_m^{\perp}). \tag{C24}$$

This implies (cf. Proposition 11 of Ref. [63])

$$\frac{1}{2}\|\mathrm{id}_m - \mathcal{R}^{\pi}\|_{\diamond} = \frac{1}{2}\|\mathcal{U} - \mathcal{R}^{\pi}\|_{\diamond} = 1 - \frac{1}{m^2}. \tag{C25}$$

Channel conversion distance. For a given resource channel $(\mathcal{N}, \mathcal{T}_1^{\beta})$ being transformed to another resource channel $(\mathcal{M}, \mathcal{T}_2^{\beta})$, the conversion distance under GPSCs is defined as

$$d_{\mathrm{GP}}\big((\mathcal{N}, \mathcal{T}_1^{\beta}) \to (\mathcal{M}, \mathcal{T}_2^{\beta})\big) = \min_{\Theta}\big\{P[\mathcal{M}, \Theta(\mathcal{N})] : \Theta\big(\mathcal{T}_1^{\beta}\big) = \mathcal{T}_2^{\beta}\big\}.$$

Here, $P[\mathcal{M}, \mathcal{K}]$ is the purified channel distance between the channels $\mathcal{M}$ and $\mathcal{K}$ given by

$$P[\mathcal{M}, \mathcal{K}] := \sup_{\psi \in \mathrm{St}(RA')} P(\mathcal{M}(\psi_{RA'}), \mathcal{K}(\psi_{RA'})), \tag{C26}$$

where $P(\#, \#)$ is the purified distance, and it suffices to take $\psi_{RA'}$ to be pure.

Definition C1 (One-shot athermality distillation and formation). For an error $\varepsilon \in [0, 1]$, the single-shot athermality distillation of a resource channel $(\mathcal{N}, \mathcal{T}^{\beta})$ under GPSCs is defined as

$$\mathrm{Dist}^{\varepsilon}(\mathcal{N}, \mathcal{T}^{\beta}) := \sup_{m}\{\ln m : d_{\mathrm{GP}}((\mathcal{N}, \mathcal{T}^{\beta}) \to (\mathrm{id}_m, \mathcal{R}^{\pi})) \leqslant \varepsilon\}.$$

For an error $\varepsilon \in [0, 1]$, the single-shot athermality formation (cost) of a resource channel $(\mathcal{N}, \mathcal{T}^{\beta})$ is defined as

$$\mathrm{Cost}^{\varepsilon}(\mathcal{N}, \mathcal{T}^{\beta}) := \inf_{m}\{\ln m : d_{\mathrm{GP}}((\mathrm{id}_m, \mathcal{R}^{\pi}) \to (\mathcal{N}, \mathcal{T}^{\beta})) \leqslant \varepsilon\}.$$

The single-shot athermality distillation $\mathrm{Dist}^{\varepsilon}(\mathcal{N}, \mathcal{T}^{\beta})$ provides the largest dimensional golden unit $(\mathrm{id}_m, \mathcal{R}^{\pi})$ that can be distilled from the resource channel $(\mathcal{N}, \mathcal{T}^{\beta})$ under GPSCs, up to allowed error ε. We could possibly also interpret $(\ln 2)^{-1}\mathrm{Dist}^{\varepsilon}(\mathcal{N}, \mathcal{T}^{\beta})$ as the maximum number of elementary golden units $(\mathrm{id}_2, \mathcal{R}^{\pi})$ distillable from the resource channel $(\mathcal{N}, \mathcal{T}^{\beta})$ under GPSCs. The single-shot athermality formation $\mathrm{Cost}^{\varepsilon}(\mathcal{N}, \mathcal{T}^{\beta})$ provides the least dimensional golden unit $(\mathrm{id}_m, \mathcal{R}^{\pi})$ needed to form the resource channel $(\mathcal{N}, \mathcal{T}^{\beta})$ under GPSCs, up to allowed error ε. Therefore, we can interpret $(\ln 2)^{-1}\mathrm{Cost}^{\varepsilon}(\mathcal{N}, \mathcal{T}^{\beta})$ as the minimum number of elementary golden units $(\mathrm{id}_2, \mathcal{R}^{\pi})$ spent to form the resource channel $(\mathcal{N}, \mathcal{T}^{\beta})$ under GPSCs.

Theorem C1 (Athermality distillation and formation [9]). For any error $\varepsilon \in [0, 1]$ and a given resource channel $(\mathcal{N}, \mathcal{T}^{\beta})$, the single-shot athermality distillation and formation are proportional to the ε-hypothesis-testing free energy and the ε-max-free energy of the channel $\mathcal{N}$, respectively,

$$\mathrm{Dist}^{\varepsilon}(\mathcal{N}, \mathcal{T}^{\beta}) = \tfrac{1}{2}D_H^{\varepsilon^2}[\mathcal{N}\|\mathcal{T}^{\beta}], \tag{C27}$$

$$\mathrm{Cost}^{\varepsilon}(\mathcal{N}, \mathcal{T}^{\beta}) = \tfrac{1}{2}D_{\infty}^{\varepsilon}[\mathcal{N}\|\mathcal{T}^{\beta}], \tag{C28}$$

$F_H^{\beta,\varepsilon}[\mathcal{N}] = \frac{2}{\beta}\mathrm{Dist}^{\sqrt{\varepsilon}}(\mathcal{N}, \mathcal{T}^{\beta})$ and $F_{\infty}^{\beta,\varepsilon}[\mathcal{N}] = \frac{2}{\beta}\mathrm{Cost}^{\varepsilon}(\mathcal{N}, \mathcal{T}^{\beta})$.

Proof. Any process describing the distillation of a golden unit can be written as a measure and prepare process where an object is processed with a free operation and then a free measurement is performed; the optimal distillation rate is when the processing with free operation and measurement is optimized for maximal distillation of the golden unit. Such a process for channel distillation of the golden unit $(\mathrm{id}_m, \mathcal{R}^{\pi})$ from the resource object $(\mathcal{N}_{A'\to A}, \mathcal{T}^{\beta}_{A'\to A})$ can be described through a Gibbs-preserving superchannel Θ^{Λ}_{ψ}, defined through a pure state $\psi_{RA'}$ and an effect operator (element of a

POVM) $0 \leqslant \Lambda \leqslant \mathbb{1}_{RA}$, which can be written as the following preparation:

$$\Theta_{\psi}^{\Lambda}(\mathcal{N}) = \operatorname{tr}(\mathcal{N}(\psi)\Lambda)\,\mathrm{id} + \operatorname{tr}(\mathcal{N}(\psi)(\mathbb{1}_A - \Lambda))\frac{1}{m^2-1}\,\mathrm{id}^{\perp}. \tag{C29}$$

The Gibbs-preserving constraint on the superchannel, i.e., $\Theta_{\psi}^{\Lambda}(\mathcal{T}^{\beta}) = \mathcal{R}^{\pi}$, can be written as $\operatorname{tr}(\mathcal{T}^{\beta}(\psi)\Lambda) = \frac{1}{m^2}$, and the conversion distance $d_{\Theta_{\psi}^{\Lambda}}((\mathcal{N}, \mathcal{T}^{\beta}) \to (\mathrm{id}, \mathcal{R}^{\pi}))$ is given by $\sqrt{1 - \operatorname{tr}(\mathcal{N}(\psi)\Lambda)}$. Recalling the definition of the ε-single-shot distillation, we have the following:

$$\begin{aligned}
\mathrm{Dist}^{\varepsilon}(\mathcal{N}, \mathcal{T}^{\beta}) &= \sup_{m,\Lambda,\psi} \left\{ \ln m : \sqrt{1 - \operatorname{tr}(\mathcal{N}(\psi)\Lambda)} \leqslant \varepsilon, \operatorname{tr}(\mathcal{T}^{\beta}(\psi)\Lambda) = \frac{1}{m^2} \right\} && \text{(C30)}\\
&= \sup_{\psi,\Lambda} \left\{ -\frac{1}{2} \ln \operatorname{tr}(\mathcal{T}^{\beta}(\psi)\Lambda) : 1 - \operatorname{tr}(\mathcal{N}(\psi)\Lambda) \leqslant \varepsilon^2 \right\} && \text{(C31)}\\
&= \sup_{\psi} \left[- \inf_{\Lambda} \left\{ \frac{1}{2} \ln \operatorname{tr}(\mathcal{T}^{\beta}(\psi)\Lambda) : 1 - \operatorname{tr}(\mathcal{N}(\psi)\Lambda) \leqslant \varepsilon^2 \right\} \right] && \text{(C32)}\\
&= \sup_{\psi} \frac{1}{2} D_H^{\varepsilon^2}(\mathcal{N}(\psi) \| \mathcal{T}^{\beta}(\psi)) && \text{(C33)}\\
&= \frac{1}{2} D_H^{\varepsilon^2}[\mathcal{N} \| \mathcal{T}^{\beta}]. && \text{(C34)}
\end{aligned}$$

Now, to derive the ε-single-shot cost, we first calculate the conversion distance

$$\begin{aligned}
d_{\mathrm{GP}}((\mathrm{id}_m\, \mathcal{R}^{\pi}) \to (\mathcal{N}, \mathcal{T}^{\beta})) &= \min_{\Theta} \{ P[\mathcal{N}, \Theta(\mathrm{id}_m)] : \Theta(\mathcal{R}^{\pi}) = \mathcal{T}^{\beta} \} && \text{(C35)}\\
&= \min_{\Theta} \left\{ P[\mathcal{N}, \Theta(\mathrm{id}_m)] : \mathcal{T}^{\beta} = \frac{1}{m^2}\Theta(\mathrm{id}_m) + \frac{1}{m^2}\Theta(\mathrm{id}_m^{\perp}) \right\} && \text{(C36)}\\
&= \min_{\mathcal{E}} \{ P[\mathcal{N}, \mathcal{E}] : m^2 \mathcal{T}^{\beta} \geqslant \mathcal{E} \} && \text{(C37)}\\
&= \min_{\mathcal{E}} \{ P[\mathcal{N}, \mathcal{E}] : 2 \ln m \geqslant D_{\infty}[\mathcal{E} \| \mathcal{T}^{\beta}] \}, && \text{(C38)}
\end{aligned}$$

where we have replaced $\mathcal{E} = \Theta(\mathrm{id}_m)$. Note that $\mathcal{E}$ can be any channel such that $m^2\mathcal{T}^{\beta} \geqslant \mathcal{E}$ and is not constrained by the Gibbs-preserving property of Θ. This is because the quantity that we are optimizing is a function of the variable $\Theta(\mathrm{id}_m)$, and the range of this variable is fully captured by the constraint $m^2\mathcal{T}^{\beta} \geqslant \Theta(\mathrm{id}_m)$. The ε-single-shot cost can be written as

$$\begin{aligned}
\mathrm{Cost}^{\varepsilon}(\mathcal{N}, \mathcal{T}^{\beta}) &= \inf_{m} \{ \ln m : d_{\mathrm{GP}}((\mathrm{id}_m\, \mathcal{R}^{\pi}) \to (\mathcal{N}, \mathcal{T}^{\beta})) \leqslant \varepsilon \} && \text{(C39)}\\
&= \inf_{m} \{ \ln m : P[\mathcal{N}, \mathcal{E}] \leqslant \varepsilon, 2 \ln m \geqslant D_{\infty}[\mathcal{E} \| \mathcal{T}^{\beta}] \} && \text{(C40)}\\
&= \inf_{\mathcal{E}} \left\{ \tfrac{1}{2} D_{\infty}[\mathcal{E} \| \mathcal{T}^{\beta}] : P[\mathcal{N}, \mathcal{E}] \leqslant \varepsilon \right\} && \text{(C41)}\\
&= \tfrac{1}{2} D_{\infty}^{\varepsilon}[\mathcal{N} \| \mathcal{T}^{\beta}]. && \text{(C42)}
\end{aligned}$$

■

The one-shot athermality distillation and formation of a resource channel $(\mathcal{N}, \mathcal{T}^{\beta})$ are associated with how well the channel $\mathcal{N}$ can be discriminated from $\mathcal{T}^{\beta}$ in an asymmetric channel discrimination task [24,40,56,64], where $\mathcal{N}$ is null hypothesis and $\mathcal{T}^{\beta}$ is alternate hypothesis.

Based on the assistance of parallel strategies for the channel discrimination tasks (see Refs. [25,40,64] for formal discussion), for an error $\varepsilon \in (0, 1)$, we define the adaptive (ad) and nonadaptive asymptotic athermality distillation and formation rates of a resource channel $(\mathcal{N}, \mathcal{T}^\beta)$ as

$$\mathscr{C}^{\varepsilon}_{\text{distill}}[\mathcal{N}] := \lim_{n\to\infty} \frac{1}{n} \text{Distill}^{\varepsilon}(\mathcal{N}^{\otimes n}, (\mathcal{T}^\beta)^{\otimes n}), \tag{C43}$$

$$\mathscr{C}^{\varepsilon}_{\text{cost}}[\mathcal{N}] := \lim_{n\to\infty} \frac{1}{n} \text{Cost}^{\varepsilon}(\mathcal{N}^{\otimes n}, (\mathcal{T}^\beta)^{\otimes n}). \tag{C44}$$

It directly follows from the definitions that $\mathscr{C}^{\varepsilon}_{\text{distill}}[\mathcal{N}] \leqslant \mathscr{C}^{\varepsilon}_{\text{cost}}[\mathcal{N}]$. We prove that the asymptotic distillation and formation rates are equal under nonadaptive strategies.

Theorem C2 (Asymptotic reversibility [9]). The resource theory of athermality of quantum channels with GPSCs as free operations is asymptotically reversible under parallel uses of channels, i.e., for any $\varepsilon \in (0, 1)$ and an arbitrary (square) quantum resource channel $(\mathcal{N}, \mathcal{T}^\beta)$,

$$\mathscr{C}^{\sqrt{\varepsilon}}_{\text{distill}}[\mathcal{N}] = \mathscr{C}^{\varepsilon}_{\text{cost}}[\mathcal{N}] = \frac{1}{2} D[\mathcal{N}\|\mathcal{T}^\beta] = \frac{\beta}{2} F^\beta[\mathcal{N}]. \tag{C45}$$

Proof. For any $\varepsilon \in (0, 1)$, we have from Theorem 1 of Ref. [40],

$$\mathscr{C}^{\sqrt{\varepsilon}}_{\text{distill}}[\mathcal{N}] = \tfrac{1}{2} D[\mathcal{N}\|\mathcal{T}^\beta], \tag{C46}$$

and from Theorem 4.1 of Ref. [42],

$$\mathscr{C}^{\varepsilon}_{\text{cost}}[\mathcal{N}] = \tfrac{1}{2} D[\mathcal{N}\|\mathcal{T}^\beta]. \tag{C47}$$

We conclude the proof by recalling that $F^\beta[\mathcal{N}] = \beta^{-1} D[\mathcal{N}\|\mathcal{T}^\beta]$. ■

It follows from Theorem 2 of Ref. [40] that for any athermality distillation scheme, which seeks to distill at a rate strictly higher than $\frac{1}{2} D[\mathcal{N}\|\mathcal{T}^\beta]$, the probability of successful distillation decays to zero exponentially fast with the number of channel uses of $\mathcal{N}$. That is, $\frac{1}{2} D[\mathcal{N}\|\mathcal{T}^\beta]$ also serves as the strong converse bound on the asymptotic athermality distillation rate of the channel $\mathcal{N}$, irrespective of whether the strategy used is adaptive or nonadaptive.

APPENDIX D: INFORMATIONAL ASPECTS OF FREE ENERGY

We discuss connection of the dynamical free energy with the channel capacity and the free energy of the channel output. We observe connections of the resource theory of athermality with the information processing tasks of private randomness and purity distillation.

Private randomness distillation. The private randomness capacity of a channel $\mathcal{N}_{A'\to A}$ is the maximum rate, in an asymptotic setting of i.i.d. uses of the channel, at which the receiver accessing output A can extract private randomness, against an eavesdropper accessing extension E of an isometric channel extension $\mathcal{V}^{\mathcal{N}}_{A'\to AE}$ of the channel $\mathcal{N}$, when the sender sends states through the channel [48]. The private randomness capacity is given by $P[\mathcal{N}] = D[\mathcal{N}\|\mathcal{R}^\pi] = \lim_{\beta\to 0^+} D[\mathcal{N}\|\mathcal{T}^\beta]$. Therefore, the private randomness capacity of a square quantum channel is twice its asymptotic thermodynamic distillation or formation rate under the action of GPSCs in the limit inverse temperature tends to vanish.

Dynamical resource theory of purity. By considering $\beta \to 0^+$ or the Hamiltonian of the channel output to be proportional to $\mathbb{1}$ in our dynamical resource theory of athermality, we obtain the dynamical resource theory of purity [44,48,65,66] where unitary channels are golden units and the uniformly mixing channels are free objects. When $\widehat{H}_A \propto \mathbb{1}_A$, then $\mathcal{T}^\beta_{A'\to A} = \mathcal{R}^\pi_{A'\to A}$ as $\gamma^\beta_A = \pi_A$ due to $\widehat{H}_A$ being fully degenerate Hamiltonian, i.e., all energy eigenstates have the same eigenvalue. The asymptotic purity distillation and formation rate of a square quantum channel $\mathcal{N}_{A'\to A}$ is equal to $\frac{1}{2} D[\mathcal{N}\|\mathcal{R}^\pi] = \frac{1}{2} \lim_{\beta\to 0^+} D[\mathcal{N}\|\mathcal{T}^\beta]$ [38,44,48].

Entropy and thermal entropy. The entropy $S[\mathcal{N}]$ of a quantum channel $\mathcal{N}_{A'\to A}$ and its private randomness capacity $P[\mathcal{N}]$ satisfy the following duality or trade-off relation [12,18]:

$$S[\mathcal{N}] + P[\mathcal{N}] = \ln |A|. \tag{D1}$$

We have a similar dual relationship between the thermal entropy $S^\beta[\mathcal{N}] := \ln Z_A^\beta - D[\mathcal{N}\|\mathcal{T}^\beta]$ [17] and the resource-theoretic free energy $F^\beta[\mathcal{N}]$ of a quantum channel $\mathcal{N}_{A'\to A}$:

$$S^\beta[\mathcal{N}] + \beta F^\beta[\mathcal{N}] = \ln Z_A^\beta, \tag{D2}$$

where $Z_A^\beta = \mathrm{tr}[\exp(-\beta \widehat{H}_A)]$. A similar relation exists between the min-channel entropy and the min-free energy of a channel. In particular, if the output Hamiltonian is trivial $\widehat{H}_A = 0$ and $\widehat{H}_{RA} = \widehat{H}_R \otimes \mathbb{1}_A$, we have

$$S_\infty[\mathcal{N}] + \beta F_\infty^\beta[\mathcal{N}] = \ln |A|. \tag{D3}$$

The min-entropy $S_\infty[\mathcal{N}]$ of a quantum channel $\mathcal{N}_{A'\to A}$ is associated with the decoupling ability of the channel (Theorem 1 and Proposition 1 of Ref. [21]) and the environment-assisted erasure cost $W[A|E]_\mathcal{N}$ of the output A of the channel when access to the environment E is provided to the erasure (Theorem 3 and Proposition 2 of Ref. [21]). These operational interpretations of the min-entropy of a quantum channel $\mathcal{N}_{A'\to A}$ directly provide operational interpretations for the max-free energy $F_\infty^\beta[\mathcal{N}]$ of the channel when $\widehat{H}_A = 0$.

APPENDIX E: THERMODYNAMIC FREE ENERGY AND WORK EXTRACTION

For a quantum state ρ_A, the entropy $S(\rho)$ is $S(\rho) := S(A)_\rho := -D(\rho_A\|\mathbb{1}_A)$ and the energy $E(\rho)$ is $E(\rho) = \langle \widehat{H}_A\rangle_\rho = \mathrm{tr}[\widehat{H}_A\rho_A]$. The entropy $S[\mathcal{N}]$ of a quantum channel $\mathcal{N}_{A'\to A}$ is defined as [17,37,38,67]

$$S[\mathcal{N}] := -D[\mathcal{N}\|\mathcal{R}^\mathbb{1}] = \inf_{\psi\in \mathrm{St}(RA')} [S(RA)_{\mathcal{N}(\psi)} - S(R)_\psi], \tag{E1}$$

where it suffices to optimize only over pure states $\psi_{RA'}$.

Definition E1 (Thermodynamic free energy). The thermodynamic (nonequilibrium) free energy $F_\mathrm{T}^\beta[\mathcal{N}]$ of an arbitrary quantum channel $\mathcal{N}_{A'\to A}$ is defined as

$$F_\mathrm{T}^\beta[\mathcal{N}] := \beta^{-1} D[\mathcal{N}\|\widehat{\mathcal{T}}^\beta], \tag{E2}$$

where $\widehat{\mathcal{T}}^\beta = \mathcal{R}^{\widehat{\gamma}^\beta}$, i.e., $\widehat{\mathcal{T}}^\beta(\rho_{A'}) = \mathrm{tr}[\rho_{A'}]\widehat{\gamma}_A^\beta$ is a replacer map that is completely positive but not trace preserving.

The function $D[\mathcal{N}\|\widehat{\mathcal{T}}^\beta] = -S^\beta[\mathcal{N}]$, where $S^\beta[\mathcal{N}]$ is the thermal entropy of the channel $\mathcal{N}$ [17]. We see that $F_\mathrm{T}^\beta[\mathcal{N}] = \beta^{-1} S^\beta[\mathcal{N}]$.

Based on the "channelized" entropy and free energy definitions, we define an energy function called the thermodynamic energy $E[\mathcal{N}]$ of a quantum channel $\mathcal{N}$ [9,12].

Definition E2. The thermodynamic energy $E[\mathcal{N}]$ of a quantum channel $\mathcal{N}$ is defined as

$$E[\mathcal{N}] := \sup_{\psi\in \mathrm{St}(RA')} [E(\mathcal{N}(\psi_{RA'})) - E(\psi_R)], \tag{E3}$$

where it suffices to optimize only over pure states $\psi_{RA'}$ and $|R| = |A'|$.

Proposition E1 (Ref. [9]). The thermodynamic energy $E[\mathcal{N}]$ of a quantum channel $\mathcal{N}_{A'\to A}$, with the reference-output Hamiltonian as $\widehat{H}_{RA} = \mathbb{1}_R \otimes \widehat{H}_A + \widehat{H}_R \otimes \mathbb{1}_A + \widehat{H}_{RA}^\mathrm{int}$, is

$$E[\mathcal{N}] = \sup_{\psi\in \mathrm{St}(RA')} \left[\langle \widehat{H}_A\rangle_{\mathcal{N}(\psi_{A'})} + \left\langle \widehat{H}_{RA}^\mathrm{int}\right\rangle_{\mathcal{N}(\psi_{RA'})}\right], \tag{E4}$$

where it suffices to optimize over pure states $\psi_{RA'}$.

Proof. The proof follows from the definition of $E[\mathcal{N}]$ and the fact that, for state $\mathcal{N}_{A'\to A}(\psi_{RA'})$ and Hamiltonian $\widehat{H}_{RA}$, we have

$$\begin{aligned} E(\mathcal{N}(\psi_{RA'})) - E(\psi_R) &= \mathrm{tr}[\widehat{H}_{RA}\mathcal{N}(\psi_{RA'})] - \mathrm{tr}[\widehat{H}_R\psi_R] \\ &= \mathrm{tr}[(\widehat{H}_R\otimes\mathbb{1}_A)\mathcal{N}(\psi_{RA'})] + \mathrm{tr}[(\mathbb{1}_R\otimes\widehat{H}_A)\mathcal{N}(\psi_{RA'})] \\ &\quad + \mathrm{tr}\left[\widehat{H}^{\mathrm{int}}_{RA}\mathcal{N}(\psi_{RA'})\right] - \mathrm{tr}[\widehat{H}_R\psi_R] \\ &= \mathrm{tr}[\widehat{H}_R\psi_R] + \mathrm{tr}[\widehat{H}_A\mathcal{N}(\psi_{A'})] + \mathrm{tr}\left[\widehat{H}^{\mathrm{int}}_{RA}\mathcal{N}(\psi_{RA'})\right] - \mathrm{tr}[\widehat{H}_R\psi_R] \\ &= \mathrm{tr}[\widehat{H}_A\mathcal{N}(\psi_{A'})] + \mathrm{tr}\left[\widehat{H}^{\mathrm{int}}_{RA}\mathcal{N}(\psi_{RA'})\right]. \end{aligned} \tag{E5}$$

■

The following corollary directly follows from the above proposition.

Corollary E1. For an arbitrary quantum channel $\mathcal{N}_{A'\to A}$, when the reference output has noninteracting Hamiltonian $\widehat{H}_{RA} = \mathbb{1}_R\otimes\widehat{H}_A + \widehat{H}_R\otimes\mathbb{1}_A$ ($\widehat{H}^{\mathrm{int}}_{RA} = 0$), then

$$E[\mathcal{N}] = \sup_{\psi\in\mathrm{St}(A')} \langle\widehat{H}\rangle_{\mathcal{N}(\psi)}, \tag{E6}$$

where it suffices to consider optimization over all pure states $\psi_{A'}$.

Theorem E1. The thermal free energy $F^\beta_{\mathrm{T}}[\mathcal{N}]$ of a quantum channel $\mathcal{N}_{A'\to A}$ is upper bounded as, when the reference R is noninteracting with A ($\widehat{H}_{RA} = \widehat{H}_R\otimes\mathbb{1}_A + \mathbb{1}_R\otimes\widehat{H}_A$),

$$F^\beta_{\mathrm{T}}[\mathcal{N}] \leqslant E[\mathcal{N}] - \beta^{-1}S[\mathcal{N}]. \tag{E7}$$

The bound is saturated for the replacer channels $\mathcal{R}^\omega_{A'\to A}$, for $\omega\in\mathrm{St}(A)$ and $\widehat{H}^{\mathrm{int}}_{RA} = 0$, $F^\beta_{\mathrm{T}}[\mathcal{R}^\omega] = E[\mathcal{R}^\omega] - \beta^{-1}S[\mathcal{R}^\omega]$.

Proof. It follows from the definition of the free energy $F^\beta[\mathcal{N}]$ that

$$F^\beta[\mathcal{N}] = \sup_{\psi\in\mathrm{St}(RA')}\left[E(\mathcal{N}(\psi_{RA'})) - E(\psi_R) - \beta^{-1}(S(\mathcal{N}(\psi_{RA'})) - S(\psi_R)) + \beta^{-1}\left(\ln Z^\beta_{RA} - \ln Z^\beta_R\right)\right]$$

and $F^\beta[\mathcal{N}] = F^\beta_{\mathrm{T}}[\mathcal{N}] + \beta^{-1}\ln Z^\beta_A$.

If $\widehat{H}_{RA} = \widehat{H}_R\otimes\mathbb{1}_A + \mathbb{1}_R\otimes\widehat{H}_A$, then $\ln Z^\beta_{RA} = \ln Z^\beta_R + \ln Z^\beta_A$, and

$$F^\beta_{\mathrm{T}}[\mathcal{N}] = \sup_{\psi\in\mathrm{St}(RA')}\left[E(\mathcal{N}(\psi_{RA'})) - E(\psi_R) - \beta^{-1}(S(\mathcal{N}(\psi_{RA'})) - S(\psi_R))\right] \leqslant E[\mathcal{N}] - \beta^{-1}S[\mathcal{N}]. \tag{E8}$$

We conclude the proof by observing that for a replacer channel $\mathcal{R}^\omega$, $F^\beta_{\mathrm{T}}[\mathcal{R}^\omega] = F^\beta_{\mathrm{T}}(\omega) = E(\omega) - \beta^{-1}S(\omega) = E[\mathcal{R}^\omega] - \beta^{-1}S[\mathcal{R}^\omega]$, using the fact that R and A are noninteracting. ■

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