Gibbs-preserving operations requiring infinite amount of quantum coherence

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Gibbs-preserving operations have been studied as one of the standard free processes in quantum thermodynamics. Although they admit a simple mathematical structure, their operational significance has been unclear due to the potential hidden cost to implement them using an operatioanlly motivated class of operations, such as thermal operations. Here, we show that this hidden cost can be infinite—we present a family of Gibbs-preserving operations that cannot be implemented by thermal operations aided by any finite amount of quantum coherence. Our result implies that there are uncountably many Gibbs-preserving operations that require unbounded thermodynamic resources to implement, raising a question about employing Gibbs-preserving operations as available thermodynamics processes. This finding is a consequence of the general lower bounds we provide for the coherence cost of approximately implementing a certain class of Gibbs-preserving operations with a desired accuracy. We find that our lower bound is almost tight, identifying a quantity—related to the energy change caused by the channel to implement—as a fundamental quantifier characterizing the coherence cost for the approximate implementation of Gibbs-preserving operations.

Introduction.— A central question in thermodynamics—and quantum extension thereof—is to formalize feasible state transformations under available thermodynamic operations. Recent studies have uncovered that this can effectively be studied by a resource-theoretic approach, which admits a rigorous analytical platform. There, one considers a class of operations that are "freely accessible" in thermodynamic settings and studies operational consequences, e.g., work extraction, under such operations. Therefore, the outcome of the analysis can naturally depend on the choice of the accessible operations, and it is crucial to recognize and appreciate the justification and potential drawback of those operations.

The bare minimum of the thermodynamically free operations is that they should map a thermal Gibbs state to a Gibbs state [1, 2]. One standard choice for thermodynamic operations, known as *Thermal Operations* [1, 3], is to impose an additional physical restriction, where energy-conserving unitary interacting with an ambient heat bath is only allowed. This class is operationally well supported, but at the same time it is often hard to analyze due to this additional structure. Another standard approach is to consider all operations that meet the minimum Gibbs-preserving requirement, so-called *Gibbs-preserving Operations*, as available thermodynamic processes. This rather axiomatic approach benefits from a great mathematical simplification, which allowed for several recent key findings in quantum thermodynamics [4–12].

Although these two classes have been flexibly chosen depending on the goal of the study, the precise relation between them has largely been unclear. In particular, it is not clear at all whether Gibbs-preserving Operations admit physically reasonable realization with respect to Thermal Operations—if not, the status of Gibbs-preserving Operations as thermodynamic processes would be put into question. Indeed, it has been known for a while that the set of Gibbs-preserving Operations is *strictly* larger than the set of Thermal Operations [13], making the gap between these two classes worth analyzing. In fact, Ref. [13] revealed that a key difference between these two maps resides in the capability of creating *quantum coherence*—superposition between energy eigenstates—which is known to serve as a useful thermodynamic resource [14–17]. Thermal Operations cannot create quantum coherence from incoherent states, but Gibbs-preserving Operations can. This demands that to realize Gibbs-preserving Operations with Thermal Operations, one generally needs to aid them with extra quantum coherence. Beyond this, not much is known about the implementability of Gibbs-preserving Operations, except for the limited case of trivial Hamiltonian [18]. In particular, it is crucial to clarify whether there is a universally sufficient amount of thermodynamic resources that admits implementation of any Gibbs-preserving operation of a fixed size with Thermal Operations, which would secure a certain level of physical justification of Gibbs-preserving Operations.

Here, we show that it is not the case. We present a continuous family of Gibbs-preserving Operations that cannot be implemented by any finite amount of quantum coherence. We provide an explicit way of constructing such Gibbs-preserving Operations, which can be applied to arbitrary dimensional systems and almost arbitrary Hamiltonian. Interestingly, these operations are not the ones that create coherence—like the one discussed in

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Ref. [13]—but the ones that *detect* coherence. We show that the former can actually be implemented by a finite amount of coherence, showing an intriguing asymmetry between coherence creation and detection in terms of implementation cost.

We show the phenomenon of infinite coherence cost by obtaining the general lower bounds for the coherence cost required to approximately implement a certain class of Gibbs-preserving Operations, which diverges at the limit of zero implementation error. We show that our lower bound is almost tight, where we in turn find that a quantifier introduced in Ref. [19], which is linked to the capability of changing energy, characterizes the optimal coherence cost for certain Gibbs-preserving Operations. We also find that an arbitrary (not necessarily Gibbs-preserving) quantum channel can generally be approximately implemented by Thermal Operations with a coherence cost that scales with the error in the same way as the aforementioned lower bound for Gibbs-preserving Operations, showing that some Gibbs-preserving Operations are, roughly speaking, belong to the most costly class of quantum operation.

Our results provide a partial solution to the open problem raised in Ref. [20] and particularly confirm the existence of thermodynamically infeasible Gibbs-preserving Operations. Our finding therefore implies that one needs to interpret the operational power of Gibbs-preserving Operations with extra caution in light of their physical implementability.

Preliminaries.— We begin by introducing relevant settings and frameworks. (See Appendix A for more extensive descriptions.) Throughout this work, we consider a situation where systems are surrounded by a thermal bath with an arbitrary finite inverse temperature β. We assume that the specification of a system X always comes with its Hamiltonian $H_X = \sum_{i=1}^{d_X} E_{X,i}|i\rangle\langle i|$ with dimension d_X. Then, the thermal Gibbs state in system X is written by $\tau_X = e^{-\beta H_X}/\mathrm{Tr}(e^{\beta H_X})$.

We consider a quantum channel, i.e., completely-positive trace-preserving (CPTP) map, from a system S to another system S'. A central class of quantum channels we consider is the set of Gibbs-preserving Operations. As the name suggests, these are the operations that map Gibbs states to Gibbs states. Here, we employ a generalized notion of Gibbs-preserving Operations, in which input and output systems can generally be different [1, 5, 10, 11, 21]. Namely, we call a channel $\Lambda : S \to S'$ Gibbs-preserving if $\Lambda(\tau_S) = \tau_{S'}$.

Another class, which is supported by an operational consideration, is the set of Thermal Operations. We call a channel $\Lambda : S \to S'$ Thermal Operation if there are environments E and E' such that $S \otimes E = S' \otimes E'$ and a unitary U on the whole system satisfying

$$\Lambda(\rho) = \mathrm{Tr}_{E'}\left(U\rho \otimes \tau_E U^\dagger\right), \quad [U, H_{\mathrm{tot}}] = 0 \tag{1}$$

where $H_{\mathrm{tot}} = H_S \otimes \mathbb{1}_E + \mathbb{1}_S \otimes H_E = H_{S'} \otimes \mathbb{1}_{E'} + \mathbb{1}_{S'} \otimes H_{E'}$ is the total Hamiltionian [1, 3].

It is not difficult to see that Thermal Operations are always Gibbs preserving. However, the converse is not true. Ref. [13] showed this by considering a simple example of a qubit channel $\Lambda : S \to S$ defined by

$$\Lambda(\rho) = \langle 1|\rho|1\rangle\eta + \langle 0|\rho|0\rangle\sigma \tag{2}$$

where η is some quantum state one can choose, and $\sigma = \langle 0|\tau_S|0\rangle^{-1}(\tau_S - \langle 1|\tau_S|1\rangle\eta)$. One can explicitly check that this is Gibbs preserving by definition. On the other hand, by choosing η as a state containing energetic coherence, i.e., off-diagonal term with respect to the energy eigenbasis, one can see that this channel can prepare a coherent state from the state $|1\rangle\langle 1|$, which does not have energetic coherence. Since Thermal Operations are not able to create energetic coherence from scratch, one can conclude that such a channel is Gibbs-preserving but not a Thermal Operation.

This indicates that the key notion to fill the gap between Gibbs-preserving and Thermal Operations is the energetic coherence, and we would like to formalize this quantitatively. Formally, we say that a state ρ in S has energetic coherence if $\rho \neq e^{-iH_S t}\rho e^{iH_S t}$ for some time t, which is equivalent to having a nonzero block off-diagonal element with respect to energy eigenbasis. For a quantitative analysis of energetic coherence, we employ quantum Fisher information defined for a state ρ in system S by

$$\mathcal{F}(\rho) = 2\sum_{i,j} \frac{(\lambda_i - \lambda_j)^2}{\lambda_i + \lambda_j} |\langle e_i|H_S|e_j\rangle|^2, \tag{3}$$

where $\{\lambda_i\}_i$ and $\{|e_i\rangle\}_i$ are the sets of eigenvalues and eigenstates of a state ρ such that $\rho = \sum_i \lambda_i |e_i\rangle\langle e_i|$. Quantum Fisher information is a well-known coherence quantifier that comes with a natural operational interpretation [22, 23].

Fundamental coherence cost.— We investigate how costly it is to implement Gibbs-preserving Operations by analyzing the amount of coherence needed to implement a desired Gibbs-preserving Operation by a Thermal Operation. Here, we measure the accuracy of implementation by a channel purified distance [24]

$$D_F(\Lambda_1, \Lambda_2) \coloneqq \max_\rho D_F(\mathrm{id} \otimes \Lambda_1(\rho), \mathrm{id} \otimes \Lambda_2(\rho)) \tag{4}$$

where $D_F(\rho, \sigma) = \sqrt{1 - F(\rho, \sigma)^2}$ and $F(\rho, \sigma) = \mathrm{Tr}\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}$. We particularly write $\Lambda_1 \sim_\epsilon \Lambda_2$ to denote $D_F(\Lambda_1, \Lambda_2) \leq \epsilon$.

The primary quantity we study is the minimum coherence cost for implementing a channel Λ with error ϵ defined by

$$\mathcal{F}_c^\epsilon(\Lambda) \coloneqq \min\left\{ \mathcal{F}(\eta) \;\middle|\; \Lambda(\cdot) \sim_\epsilon \tilde{\Lambda}(\cdot \otimes \eta),\ \tilde{\Lambda} \in \mathbb{O}_{\mathrm{TO}} \right\} \tag{5}$$

where $\mathbb{O}_{\mathrm{TO}}$ is the set of Thermal Operations, and η is a state in an arbitrary ancillary system. Namely, we regard the coherence cost as the minimum amount of coherence attributed to an ancillary state that—together with a Thermal Operation—realizes the approximation implementation of the target channel Λ.

The key idea in evaluating this is to connect our setting to the recent trade-off relation between coherence cost for channel implementation and the degree of reversibility of the channel to implement [19], which was shown to unify, e.g., the Wigner-Araki-Yanase theorems on quantum processes [25–34] and the Eastin-Knill theorems on quantum error correcting codes [34–39]—see Appendix A for details. In light of this, we find that the following class of Gibbs-preserving Operations plays a central role.

Definition 1. We call a Gibbs-preserving Operation Λ *pairwise reversible* if there exists a pair $\mathbb{P} = \{\rho_1, \rho_2\}$ of orthogonal states, i.e., $\mathrm{Tr}(\rho_1\rho_2) = 0$, and a quantum channel $\mathcal{R}$ such that $\mathcal{R} \circ \Lambda(\rho_j) = \rho_j$ for $j = 1, 2$. We also call $\mathbb{P}$ a *reversible pair* of Λ.

We now introduce a central quantity for characterizing coherence cost. Let $\mathbb{P} = \{\rho_1, \rho_2\}$ be a reversible pair for a Gibbs-preserving channel $\Lambda : S \to S'$. Then, we define

$$\mathcal{C}(\Lambda, \mathbb{P}) \coloneqq \|\sqrt{\rho_1}(H_S - \Lambda^\dagger(H_{S'}))\sqrt{\rho_2}\|_2 \tag{6}$$

where $\Lambda^\dagger$ is the dual map such that $\mathrm{Tr}(\Lambda^\dagger(A)B) = \mathrm{Tr}(A\,\Lambda(B))$ for arbitrary operators A and B, and $\|X\|_2 \coloneqq \sqrt{\mathrm{Tr}(X^\dagger X)}$ is the Hilbert-Schmidt norm. This quantity particularly admits a simpler form for pure-state reversible pair $\mathbb{P} = \{\psi_1, \psi_2\}$ as

$$\mathcal{C}(\Lambda, \mathbb{P}) = |\langle\psi_1|H_S - \Lambda^\dagger(H_{S'})|\psi_2\rangle|. \tag{7}$$

The quantity $H_S - \Lambda^\dagger(H_{S'})$ is an operator that corresponds to the local energy change in the system, and the forms in (6) and (7) indicate that $\mathcal{C}(\Lambda, \mathbb{P})$ measures the off-diagonal element of this operator with respect to the reversible states. More discussions about this quantity can be found in Ref. [19].

We are now in the position to present our first main result, which establishes a universal lower bound for the coherence cost for pairwise reversible Gibbs-preserving Operations. (Proof in Appendix B.)

Theorem 2. *Let $\Lambda : S \to S'$ be a pairwise reversible Gibbs-preserving Operation with a reversible pair $\mathbb{P}$. Then,*

$$\sqrt{\mathcal{F}_c^\epsilon(\Lambda)} \geq \frac{\mathcal{C}(\Lambda, \mathbb{P})}{\epsilon} - \Delta(H_S) - 3\Delta(H_{S'}), \tag{8}$$

where $\Delta(O)$ is the difference between the minimum and maximum eigenvalues of an operator O.

This particularly establishes a demanding coherence cost in the small error regime. Notably, Theorem 2 implies that no pairwise reversible Gibbs-preserving Operation Λ with $\mathcal{C}(\Lambda, \mathbb{P}) > 0$ can be exactly implemented with a finite amount of coherence cost, as the lower bound diverges as ϵ approaches 0.

Therefore, the problem of whether cost-diverging Gibbs-preserving Operations exists reduces to whether there exists a pairwise reversible Gibbs-preserving Operation Λ and a reversible pair $\mathbb{P}$ such that $\mathcal{C}(\Lambda, \mathbb{P}) > 0$ at all. The following result not only shows the existence of such operations but provides a continuous family of those.

Theorem 3. *Let $\tau_{X,i} = \langle i|\tau_X|i\rangle_X$ be the Gibbs distribution for the Gibbs state for a system X with Hamiltonian $H_X = \sum_i E_{X,i}|i\rangle\langle i|_X$. Then, if there are integers i, j, and i' for systems S and S' such that*

$$\tau_{S,i} < \tau_{S',i'} < \tau_{S,j}, \tag{9}$$

there exists a pairwise reversible Gibbs-preserving Operation $\Lambda : S \to S'$ and a reversible pair $\mathbb{P}$ such that $\mathcal{C}(\Lambda, \mathbb{P}) > 0$.

We prove this in Appendix C, which also provides an explicit construction of the corresponding pairwise reversible Gibbs-preserving Operation. Here is an illustrative example encompassed in Theorem 3. Let S and S' be qubit systems with $H_S = |1\rangle\langle 1|$ and $H_{S'} = 0$. Since $\tau_{S,0} = 1/(1 + e^{-\beta})$, $\tau_{S,1} = e^{-\beta}/(1 + e^{-\beta})$, and $\tau_{S',0} = \tau_{S',1} = 1/2$, these systems satisfy (9) for arbitrary finite temperature. The corresponding pairwise reversible Gibbs-preserving Operation $\Lambda : S \to S'$ is

$$\Lambda(\rho) = \langle +|\rho|+\rangle|0\rangle\langle 0| + \langle -|\rho|-\rangle|1\rangle\langle 1| \tag{10}$$

where $|\pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle \pm |1\rangle)$ is the maximally coherent state on S. It is easy to see that this is Gibbs-preserving. This is also pairwise reversible with a reversible pair $\mathbb{P} = \{|+\rangle\langle +|, |-\rangle\langle -|\}$ because a recovery channel $\mathcal{R}(\cdot) = \langle 0|\cdot|0\rangle|+\rangle\langle +| + \langle 1|\cdot|1\rangle|-\rangle\langle -|$ satisfies $\mathcal{R} \circ \Lambda(|\pm\rangle\langle\pm|) = |\pm\rangle\langle\pm|$. Direct computation also shows that $\mathcal{C}(\Lambda, \mathbb{P}) = \frac{1}{2} > 0$.

It is insightful to see the structural difference between the Gibbs-preserving Operations in Eqs. (2) and (10). The one in (2) can create coherence from an incoherent state input state $|1\rangle\langle 1|$. On the other hand, the channel in (10) cannot create coherence at all—in fact, output states are always incoherent for any input states. Instead, it can perform a measurement in a coherent basis. As we show in Appendix D, the coherent cost for the channel in (2) is upper bounded by $\mathcal{F}(\eta) + \mathcal{F}(\sigma)$, which corresponds to the sum of coherence that can be created by the channel. This shows a drastic asymmetry between creation and detection of coherence when it comes to its realization.

We also remark that Theorem 3, together with Theorem 2, guarantees the existence of a Gibbs-preserving Operation with infinite coherence cost for the case when input and output systems are identical. Indeed, whenever the system's Hamiltonian comes with at least three distinct eigenenergies, the condition in Theorem 3 with S' being replaced with S is satisfied.

Theorems 2 and 3 provide an overview of the classification of Gibbs-preserving Operations (Fig. 1). We remark that not all pairwise reversible Gibbs-preserving Operations come with a diverging coherence cost (e.g., identity channel)—Theorem 2 ensures the infinite cost only when

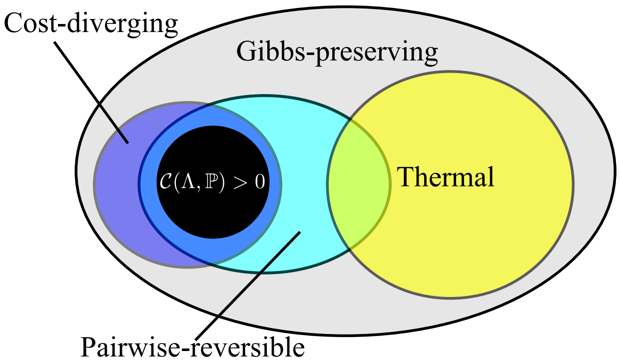

FIG. 1. Classification of Gibbs-preserving Operations. Theorem 2 ensures that pairwise reversible Gibbs-preserving Operations (Definition 1) for which there is a reversible pair $\mathbb{P}$ such that $\mathcal{C}(\Lambda,\mathbb{P})>0$ comes with diverging coherence cost, and the existence of those operations is guaranteed by Theorem 3. The existence of a cost-diverging Gibbs-preserving channel outside of $\mathcal{C}(\Lambda,\mathbb{P})>0$ circle has neither been confirmed nor ruled out.

there is a reversible pair $\mathbb{P}$ satisfying $\mathcal{C}(\Lambda,\mathbb{P})>0$. On the other hand, our results do not rule out the possibility that all cost-diverging Gibbs-preserving Operations are pairwise reversible.

Upper bounds.— A natural next question is how good the bound in Theorem 2 can be. Interestingly, we find that it is almost tight in the following sense.

Theorem 4. *For every real number $a>0$, there is a pairwise reversible Gibbs-preserving Operation Λ and a reversible pair $\mathbb{P}$ such that $\mathcal{C}(\Lambda,\mathbb{P})>0$ and*

$$\frac{\mathcal{C}(\Lambda,\mathbb{P})}{\epsilon}-a\leq\sqrt{\mathcal{F}_c^\epsilon(\Lambda)}\leq\frac{\sqrt{2}\mathcal{C}(\Lambda,\mathbb{P})}{\epsilon}+a. \tag{11}$$

Proof can be found in Appendix E. This particularly ensures that the quantity $\mathcal{C}(\Lambda,\mathbb{P})$ defined in (6) serves as a key quantity that characterizes the coherence cost for a certain class of Gibbs-preserving Operations, which in turn provides an operational interpretation to this quantity.

Theorem 4 ensures the existence of a Gibbs-preserving Operation that almost achieves the lower bound. However, it does not tell much about the general upper bound that could be applied to an arbitrary Gibbs-preserving Operation. In the following, we show that, by giving up obtaining the form that almost matches the lower bound, we can obtain the general sufficient coherence cost that can be universally applied to all Gibbs-preserving Operations. In fact, we find that the applicability of our bound is much beyond Gibbs-preserving Operations—it gives a sufficient coherence cost for an arbitrary quantum channel. (Proof in Appendix E.)

Theorem 5. *Let $\Lambda:S\to S'$ be an arbitrary quantum channel admitting a dilation form*

$$\Lambda(\rho)=\mathrm{Tr}_{E'}\left(V(\rho\otimes|\eta\rangle\!\langle\eta|)V^\dagger\right) \tag{12}$$

for some environments E and E' such that $S\otimes E=S'\otimes E'$, some unitary V on $S\otimes E$, and some pure incoherent state $|\eta\rangle$ on E. Then,

$$\sqrt{\mathcal{F}_c^\epsilon(\Lambda)}\leq\frac{\Delta(H_{\rm tot}-V^\dagger H_{\rm tot}V)}{2\epsilon}+\sqrt{2}\Delta(H_{\rm tot}) \tag{13}$$

where $H_{\rm tot}=H_S\otimes\mathbb{1}_E+\mathbb{1}_S\otimes H_E=H_{S'}\otimes\mathbb{1}_{E'}+\mathbb{1}_{S'}\otimes H_{E'}$, and $\Delta(O)$ is the difference between the minimum and maximum eigenvalues of an operator O.

Notably, this upper bound also scales as $\sim 1/\epsilon$ with the implementation error, which coincides with the asymptotic scaling of the lower bound in Theorem 2 for pairwise reversible Gibbs-preserving Operations. Combining these two, we can understand that the optimal coherence cost for all pairwise reversible Gibbs-preserving Operations with $\mathcal{C}(\Lambda,\mathbb{P})>0$ are roughly characterized by N/ϵ where N is an extensive quantity that grows with a particle number of the system. This, together with the fact that Theorem 5 applies to an arbitrary quantum channel, also implies that pairwise reversible Gibbs-preserving Operations are as costly as general quantum operations, putting them into the "most costly" class to implement.

Let us now remark a unique characteristic of our results in relation to the previous result for trivial Hamiltonian. When input and output states are only equipped with trivial Hamiltonian, every state becomes an incoherent state, i.e., invariant under Hamiltonian evolution, and thus coherence loses its status as a precious resource. Therefore, the meaningful question in such a setting is to ask the work cost (the minimum number of work bit required) for implementing unital channels using Noisy Operations [40], which respectively corresponds to the Gibbs-preserving and Thermal Operations for trivial Hamiltonian. Ref. [18] showed that the minimum work cost is *upper* bounded by a quantity scaling as $\sim\log(1/\epsilon)$ with implementation error ϵ, which particularly diverges at the limit of exact implementation. Nevertheless, its lower bound has still not been established, and therefore it is still unclear if this diverging cost is a fundamental phenomenon or merely an artifact of their specific construction, which is based on a decoupling technique [41]. On the other hand, our Theorem 2 provides a *lower* bound that scale with $1/\epsilon$, which is complemented by upper bounds in Theorems 4 and 5 with the same scaling. To the best of our knowledge, our results are the first ones that establish the inherently diverging thermodynamic cost for implementing Gibbs-preserving Operations.

Conclusions.— We established bounds for the minimum coherence cost for implementing Gibbs-preserving Operations with a desired target error. A major consequence of them is that there are Gibbs-preserving Operations that cannot be implemented with a Thermal Operation aided by any finite amount of quantum coherence, and the approximate implementation of these Gibbs-preserving Operations requires roughly the same amount of coherence that suffices to implement the most costly class of quantum channels. Our results therefore clarify an enormous hidden cost in Gibbs-preserving Operations, indicating their unphysical nature as thermodynamically available operations.

This particularly motivates us to revisit and scrutinize the prior results based on Gibbs-preserving Operations from a physical and operational perspective. Indeed, optimal Gibbs-preserving Operations in the standard task of state transformation, e.g., work extraction, are often found to possess a measure-and-prepare structure, which takes a similar form to the one in (10). A close investigation of the coherence cost for such channels will make an important future work. Another potential direction is to obtain a finer characterization of thermodynamic costs for Gibbs-preserving Operations. This includes the complete tight characterization of the coherence cost for all Gibbs-preserving Operations, as well as obtaining corresponding evaluation for work cost—complementary thermodynamic resource besides quantum coherence.

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Appendix A: Background and setting

1. Quantum resource theories

Quantum resource theories [42, 43] provide a useful platform on which quantitative analysis of the underlying quantum features can be performed. The core idea of resource theories is to consider relevant sets of quantum states (called *free states*) and operations (called *free operations*) that are easily accessible in the given physical setting. This results in a framework where one can quantify the amount of precious resources attributed to a given state with respect to the set of free states and investigate the feasible state transformations that can be realized by free operations.

Different physical settings of interest can be specified by appropriately choosing the sets of free states and operations, which leads to different resource theories. One standard example is to consider the set of separable states and local operations and classical communication (LOCC), resulting in an operational framework of studying quantum entanglement [3]. Here, we remark that for a given set of free states, one can consider choosing a different set of free operations while keeping the essence of the physical setting represented by the necessary requirement for free operations

$$\Lambda(\sigma) \in \mathbb{F},\ \forall \Lambda \in \mathbb{O} \tag{A1}$$

for a set $\mathbb{F}$ of free states and a set $\mathbb{O}$ of free operations. Employing the flexibility in choosing different sets of free operations is usually effective when $\mathbb{O}$ comes with a complicated structure and is difficult to analyze. For instance, in the case of entanglement, it is notoriously hard to study the full potential of LOCC, and therefore several classes of other operations, which include LOCC as their subset, were investigated. One such set is separability-preserving operations, which is the maximal set that satisfies (A1). This admits a great simplification of the analysis and results in significant insights into entanglement transformation [44–46].

The two examples of free operations in the entanglement theory mentioned above have different perspectives and focuses. In particular, LOCC is motivated by an *operational* viewpoint, which aims to reflect the reasonable operations that two distant parties can actually accomplish, while separability-preserving operations employ an *axiomatic* approach that respects the bear minimum constraint that operations should not create entanglement for free. It is clear from the definition that the latter contains the former, and the inclusion is indeed strict [46]. Although each choice is able to extract different aspects of underlying quantum resources, it is still important to clarify the relationship between them. In particular, one crucial question here is how much resources are needed for a free operation in the smaller set $\mathbb{O}_1$ to simulate the action of a free operation in the larger set $\mathbb{O}_2$, which provides the idea of how "operationally reasonable" the axiomatic free operations are. One can formalize this by asking a *channel implementation cost* for a channel $\Lambda \in \mathbb{O}_1$ defined by

$$C_{R_{\mathbb{F}}}(\Lambda) := \min\left\{ R_{\mathbb{F}}(\eta) \;\middle|\; \Lambda(\cdot) = \tilde{\Lambda}(\cdot \otimes \phi),\ \tilde{\Lambda} \in \mathbb{O}_2 \right\} \tag{A2}$$

for some resource quantifier $R_{\mathbb{F}}$ with respect to the set $\mathbb{F}$ of free states. In this work, we study this question in the setting of quantum thermodynamics.

2. Thermal and Gibbs-preserving Operations

One of the major approaches in quantum thermodynamics is to employ a resource-theoretic framework [1, 3, 14], which focuses on the ultimate operational capability of thermodynamic operations in the manipulation of quantum systems. In this approach, the thermal Gibbs state $\tau_S = e^{-\beta H_S}/\mathrm{Tr}(e^{-\beta H_S})$ for a system S with Hamiltonian H_S is considered to be a state that is freely accessible, and allowed thermodynamic operations are chosen so that they map a Gibbs state to another Gibbs state.

One of the standard choices for such thermodynamic operations is based on an operational motivation and is known as *Thermal Operations* [2, 3, 47]. A channel $\Lambda : S \to S'$ is called a Thermal Operation if there exists an environment E and E' with $S \otimes E = S' \otimes E'$ and an energy-conserving unitary U on $S \otimes E$ such that

$$\Lambda(\rho) = \mathrm{Tr}_{E'}\left(U\rho \otimes \tau_S U^\dagger\right), \quad [U, H_{\mathrm{tot}}] = 0 \tag{A3}$$

where $H_{\rm tot} = H_S \otimes \mathbb{1}_E + \mathbb{1}_S \otimes H_E = H_{S'} \otimes \mathbb{1}_{E'} + \mathbb{1}_{S'} \otimes H_{E'}$ is the total Hamiltonian. On the other hand, one can also consider a broader class based on the axiomatic formulation, which is only restricted by the minimum requirement that they should map Gibbs states to Gibbs states. This is known as *Gibbs-preserving Operations*—a channel $\Lambda : S \to S'$ is called a Gibbs-preserving operation if

$$\Lambda(\tau_S) = \tau_{S'}. \tag{A4}$$

We remark that we here allow the final system S' to differ from the initial system S. This setting is motivated by the observation that discarding an arbitrary subsystem should operationally be allowed, which may result in a different system from the initial one [1, 3, 21, 47]. One could also formulate the change in the initial and final systems by inducing different Hamiltonians by introducing ancillary systems working as a switch [3, 11, 48], which generally comes with a different work cost to realize state transformation. Although these distinctions should carefully be taken into account when one investigates the work cost, here we do not delve into this discussion further, as our main focus here is the coherence cost, which is not affected by these subtleties. We also note that the main consequences of our results, i.e., diverging coherence cost and its bounds for approximate implementation, still hold for the restricted settings with identical initial and final systems, particularly because of the broad applicability of Theorem 3. See the main text for relevant discussions.

It is elementary to see that any thermal operation is Gibbs-preserving, and therefore the set $\mathbb{O}_{\rm TO}$ of thermal operations and the set $\mathbb{O}_{\rm GP}$ of Gibbs-preserving operations satisfy the inclusion relation $\mathbb{O}_{\rm TO} \subseteq \mathbb{O}_{\rm GP}$. Furthermore, this inclusion is shown to be strict, i.e., $\mathbb{O}_{\rm TO} \subsetneq \mathbb{O}_{\rm GP}$ [13]. A key observation to see this strict inclusion relation is to study energetic coherence, which we review in the following.

3. Quantum coherence in energy eigenbasis

Recent studies found that, in the realm of quantum thermodynamics, quantum coherence also plays a major role that allows one to extract work and thus serves as another type of quantum resource besides out-of-equilibrium energy distribution [14–17]. To formalize quantum coherence, let $H = \sum_n E_n |n\rangle\langle n|$ be a Hamiltonian where $\{E_n\}_n$ is the set of (possibly degenerate) energy eigenvalues and $\{|n\rangle\}_n$ is the orthonormal set of energy eigenstates. We say that a state ρ has *quantum coherence* or *energetic coherence* if ρ has an off-diagonal term, i.e., superposition, for different energy levels. Formally, let Π_E be a projector onto the subspace with energy E given by

$$\Pi_E = \sum_{n:E_n=E} |n\rangle\langle n|. \tag{A5}$$

Then, a state ρ has energetic coherence if $\sum_E \Pi_E \rho \Pi_E \neq \rho$. Equivalently, a state ρ has nonzero coherence if $e^{-Ht} \rho e^{iHt} \neq \rho$ for some $t \in \mathbb{R}$.

The letter expression particularly allows us to formalize energetic coherence in relation to a group action represented by a unitary representation of U(1) (or $\mathbb{R}$ if the Hamiltonian contains relatively irrational eigenvalues). Namely, *incoherent states*—states that do not have coherence—are equivalent to the states invariant under a unitary representation $\{e^{-iHt}\}_t$. This observation provides a way of quantifying the amount of energetic coherence employing the resource theory of asymmetry [42, 49], which considers states invariant under action of a unitary representation of a group G as free states, i.e., $\mathbb{F} = \{\sigma \,|\, U_g \sigma U_g^\dagger = \sigma,\ \forall g \in G\}$, and the operations covariant with such group actions as free operations, i.e., $\mathbb{O} = \{\Lambda : S \to S' \,|\, U_{S',g} \Lambda(\rho) U_{S',g}^\dagger = \Lambda(U_{S,g} \rho U_{S,g}^\dagger),\ \forall g \in G\}$ where $U_{X,g}$ is a unitary representation acting on a system X. One can then realize that incoherent states coincide with the set of free states in the framework of resource theory of asymmetry with U(1) group with the representation $U_t = e^{-iHt}$, equipped with

$$\mathbb{F}_{\rm inc} = \{\sigma \,|\, e^{-iHt} \sigma e^{iHt} = \sigma,\ \forall t\} \tag{A6}$$

and free operation called *Covariant Operations*

$$\mathbb{O}_{\rm cov} = \{\Lambda : S \to S' \,|\, e^{-iH_{S'}t} \Lambda(\rho) e^{iH_{S'}t} = \Lambda(e^{-iH_S t} \rho e^{iH_S t})\ \forall t\}. \tag{A7}$$

It is easy to check that covariant operations are indeed free operations for energetic coherence in the sense that it does not create a state with nonzero energetic coherence from an incoherent state.

Another insightful characterization of covariant operations is that an arbitrary covariant operation $\Lambda : S \to S'$ admits the following dilation form [49, 50]

$$\Lambda(\rho) = \mathrm{Tr}_{E'}\left(U\rho \otimes \sigma U^\dagger\right), \quad [U, H_S \otimes \mathbb{1}_E + \mathbb{1}_S \otimes H_E] = 0,\ \sigma \in \mathbb{F}_{\mathrm{inc}} \tag{A8}$$

for some systems E and E'. The similarity between (A3) and (A8) represents an intriguing interplay between resource theories for quantum thermodynamics and energetic coherence. Indeed, since Gibbs states do not have energetic coherence by definition, we immediately notice that

$$\mathbb{O}_{\mathrm{TO}} \subseteq \mathbb{O}_{\mathrm{cov}}. \tag{A9}$$

On the other hand, Ref. [13] presented a Gibbs-preserving operation $\Lambda \in \mathbb{O}_{\mathrm{GP}}$ that can create a coherent state from an incoherent state, showing $\Lambda \notin \mathbb{O}_{\mathrm{cov}}$. This shows the strict inclusion $\mathbb{O}_{\mathrm{TO}} \subsetneq \mathbb{O}_{\mathrm{GP}}$. In other words, in an operationally driven approach with thermal operations, energetic coherence serves as a precious resource that cannot be created for free, while in an axiomatic approach with Gibbs-preserving operations, energetic coherence loses the status of the precious resource.

4. Coherence cost for Gibbs-preserving operations

The aforementioned gap between thermal and Gibbs-preserving operations naturally raises a question [20]: what is the coherence cost for thermal operations to implement Gibbs-preserving operations? Indeed, Gibbs-preserving operations have been widely studied because of their simple mathematical structure [4–12]. However, if it requires unreasonable additional resource costs to implement, it would lose the physical ground as a reasonable set of free operations from an operational perspective.

This motivates us to study the channel implementation cost introduced in Sec. A 1 in our setting, which corresponds to $\mathbb{F} = \mathbb{F}_{\mathrm{inc}}$, $\mathbb{O}_1 = \mathbb{O}_{\mathrm{GP}}$, and $\mathbb{O}_2 = \mathbb{O}_{\mathrm{TO}}$. For a coherence quantifier $R_{\mathbb{F}_{\mathrm{inc}}}$, we employ quantum Fisher information, the standard measure of coherence (and asymmetry in general), defined for an arbitrary state ρ by

$$\mathcal{F}(\rho) = 2\sum_{i,j} \frac{(p_i - p_j)^2}{p_i + p_j} |\langle i|H|j\rangle|^2 \tag{A10}$$

where H is the Hamiltonian of the system that ρ acts on, and $\{p_j\}_j$ and $\{|j\rangle\}_j$ are the eigenvalues and eigenstates of $\rho = \sum_j p_j |j\rangle\langle j|$. The coherence cost of a channel Λ is then

$$\mathcal{F}_c(\Lambda) \coloneqq \min\left\{ \mathcal{F}(\eta) \;\middle|\; \Lambda = \tilde{\Lambda}(\cdot \otimes \eta),\ \tilde{\Lambda} \in \mathbb{O}_{\mathrm{TO}} \right\}. \tag{A11}$$

To encompass general and practical scenarios, we extend this quantity to the cost for approximate implementation, admitting some error ϵ. Here, we measure the error by a channel purified distance [24]

$$D_F(\Lambda_1, \Lambda_2) \coloneqq \max_\rho D_F(\mathrm{id} \otimes \Lambda_1(\rho), \mathrm{id} \otimes \Lambda_2(\rho)) \tag{A12}$$

where

$$D_F(\rho, \sigma) = \sqrt{1 - F(\rho,\sigma)^2}, \quad F(\rho, \sigma) = \mathrm{Tr}\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}. \tag{A13}$$

We particularly write $\Lambda_1 \sim_\epsilon \Lambda_2$ to denote $D_F(\Lambda_1, \Lambda_2) \le \epsilon$. We then define the approximate implementation cost for a channel Λ by

$$\mathcal{F}_c^\epsilon(\Lambda) \coloneqq \min\left\{ \mathcal{F}(\eta) \;\middle|\; \Lambda \sim_\epsilon \tilde{\Lambda}(\cdot \otimes \eta),\ \tilde{\Lambda} \in \mathbb{O}_{\mathrm{TO}} \right\}. \tag{A14}$$

5. Trade-off relation between symmetry, irreversibility, and quantum coherence

The main goal of this work is to evaluate the coherence cost in (A14) for Gibbs-preserving Operations. In particular, we are interested in the fundamental limitations on the implementation of Gibbs-preserving Operations, which could be analyzed by obtaining lower bounds for $\mathcal{F}_c^\epsilon$. Lower bounds can never obtained by studying specific implementation protocols, and we thus need an approach that can put general restrictions on all feasible implementation strategies.

The key technique we employ to this end is the universal trade-off relation between symmetry, irreversibility, and quantum coherence recently found in Ref. [19]. Let us define a measure of the irreversibility of a channel $\Lambda : S \to S'$ for an orthogonal state pair $\mathbb{P} := \{\rho_1, \rho_2\}$ on S satisfying $F(\rho_1, \rho_2) = 0$ as follows:

$$\delta(\Lambda, \mathbb{P}) := \min_{\mathcal{R}:S'\to S} \sqrt{\sum_{j=1}^{2} \frac{1}{2} D_F(\rho_j, \mathcal{R} \circ \Lambda(\rho_j))^2}. \tag{A15}$$

Here $\mathcal{R}$ runs over all CPTP maps from S' to S. This irreversibility measure gives lower bounds for other relevant quantities, e.g., the entropy production and recovery errors of error-correcting codes [19], and various errors and disturbances of quantum measurements and the out-of-time-ordered correlators (OTOC) [30].

For an arbitrary orthogonal state pair $\mathbb{P} = \{\rho_1, \rho_2\}$, we define

$$\mathcal{C}(\Lambda, \mathbb{P}) := \|\sqrt{\rho_1}(H_S - \Lambda^\dagger(H_{S'}))\sqrt{\rho_2}\|_2, \tag{A16}$$

where $\|O\|_2 = \sqrt{\mathrm{Tr}(O^\dagger O)}$ is the Hilbert-Schmidt norm. We also define coherence cost for channel implementation by covariant operations

$$\mathcal{F}_{c,\mathrm{cov}}(\Lambda) := \min\left\{ \mathcal{F}(\eta) \;\middle|\; \Lambda = \tilde{\Lambda}(\cdot \otimes \eta),\ \tilde{\Lambda} \in \mathbb{O}_{\mathrm{cov}} \right\}. \tag{A17}$$

Then, it turns out that there is a fundamental trade-off relation between these quantities and the coherence cost for exact channel implementation.

Theorem S.1 (in Ref. [19])**.** *For an arbitrary quantum channel $\Lambda : S \to S'$ and an arbitrary orthogonal state pair $\mathbb{P}$, the following inequality holds:*

$$\frac{\mathcal{C}(\Lambda, \mathbb{P})}{\sqrt{\mathcal{F}_{c,\mathrm{cov}}(\Lambda)} + \Delta(H_S) + \Delta(H_{S'})} \leq \delta(\Lambda, \mathbb{P}), \tag{A18}$$

where $\Delta(O)$ is the difference between the minimum and maximum eigenvalues of an operator O.

We remark that the above relation can be extended to a general state ensemble $\{p_j, \rho_j\}_j$ that may not be orthogonal to each other [19]. The relation (A18) is given as a unification between the Wigner-Araki-Yanase (WAY) theorems on quantum measurements [25–29] and unitary gates [31–34] and the Eastin-Knill theorems on quantum error correcting codes [34–39]. It also allows restrictions on the classical information recovery in the Hayden-Preskill thought experiments [51] imposed by the energy conservation [19] and extends the WAY theorem to various errors and disturbances of quantum measurements and the out-of-time-ordered correlators [30]. Here, we utilize this relation to obtain a lower bound for coherence cost for approximately implementing Gibbs-preserving Operations by Thermal Operations.

Appendix B: Lower bound for pairwise reversible Gibbs-preserving Operations (Proof of Theorem 2)

Recall that we call a channel Λ pairwise reversible with a reversible pair $\mathbb{P}$ if each state in $\mathbb{P}$ is perfectly reversible, i.e., $\delta(\Lambda, \mathbb{P}) = 0$. (See Definition 1 in the main text.) We then obtain the following lower bound for coherence cost.

Theorem S.2 (Theorem 2 in the main text)**.** *Let $\Lambda : S \to S'$ be a pairwise reversible Gibbs-preserving Operation with a reversible pair $\mathbb{P}$. Then,*

$$\sqrt{\mathcal{F}_c^\epsilon(\Lambda)} \geq \frac{\mathcal{C}(\Lambda, \mathbb{P})}{\epsilon} - \Delta(H_S) - 3\Delta(H_{S'}), \tag{B1}$$

where $\Delta(O)$ is the difference between the minimum and maximum eigenvalues of an operator O.

Proof. Let Λ_ϵ be a channel that approximates Λ with error ϵ, i.e., $D_F(\Lambda_\epsilon,\Lambda)\leq\epsilon$ (recall (A12)). We aim to apply Theorem S.1 to Λ_ϵ while expressing each term by the quantities in (B1) relevant to the desired channel Λ and the accuracy of implementation.

We first bound $\delta(\Lambda_\epsilon,\mathbb{P})$ by the implementation error ϵ. Let $\mathcal{R}$ be a recovery channel such that $\mathcal{R}\circ\Lambda(\rho)=\rho$ for each state $\rho\in\mathbb{P}$, whose existence is ensured by assumption. Then, for each state ρ in $\mathbb{P}$, we have

$$\begin{aligned}D_F(\mathcal{R}\circ\Lambda_\epsilon(\rho),\rho)&\leq D_F(\mathcal{R}\circ\Lambda_\epsilon(\rho),\mathcal{R}\circ\Lambda(\rho))+D_F(\mathcal{R}\circ\Lambda(\rho),\rho)\\&=D_F(\mathcal{R}\circ\Lambda_\epsilon(\rho),\mathcal{R}\circ\Lambda(\rho))\\&\leq D_F(\Lambda_\epsilon(\rho),\Lambda(\rho))\\&\leq\max_\rho D_F(\mathrm{id}\otimes\Lambda_\epsilon(\rho),\mathrm{id}\otimes\Lambda(\rho))\\&\leq\epsilon\end{aligned}\tag{B2}$$

where in the first line we used the triangle inequality of the purified distance [24], the second line is because of the perfect reversibility of ρ with $\mathcal{R}$, the third line follows from the data-processing inequality of the purified distance, and the fifth line is because of the assumption that $\Lambda_\epsilon\sim_\epsilon\Lambda$. This particularly means that

$$\delta(\Lambda_\epsilon,\mathbb{P})\leq\sqrt{\frac{1}{2}D_F(\mathcal{R}\circ\Lambda_\epsilon(\rho_1),\rho_1)^2+\frac{1}{2}D_F(\mathcal{R}\circ\Lambda_\epsilon(\rho_2),\rho_2)^2}\leq\epsilon.\tag{B3}$$

We next obtain an expression of $\mathcal{C}(\Lambda_\epsilon,\mathbb{P})$ in terms of $\mathcal{C}(\Lambda,\mathbb{P})$. We first get

$$\begin{aligned}\mathcal{C}(\Lambda_\epsilon,\mathbb{P})&=\|\sqrt{\rho_1}(H_S-\Lambda_\epsilon^\dagger(H_{S'}))\sqrt{\rho_2}\|_2\\&\geq\|\sqrt{\rho_1}(H_S-\Lambda^\dagger(H_{S'}))\sqrt{\rho_2}\|_2-\|\sqrt{\rho_1}(\Lambda^\dagger(H_{S'})-\Lambda_\epsilon^\dagger(H_{S'}))\sqrt{\rho_2}\|_2\\&=\mathcal{C}(\Lambda,\mathbb{P})-\|\sqrt{\rho_1}(\Lambda^\dagger(H_{S'})-\Lambda_\epsilon^\dagger(H_{S'}))\sqrt{\rho_2}\|_2\end{aligned}\tag{B4}$$

where in the second line we used the triangle inequality of the Hilbert-Schmidt norm. We therefore focus on upper bounding the second term $\|\sqrt{\rho_1}(\Lambda^\dagger(H_{S'})-\Lambda_\epsilon^\dagger(H_{S'}))\sqrt{\rho_2}\|_2$. For states $\rho_1,\rho_2\in\mathbb{P}$, let $\rho_1=\sum_k q_k\psi_k$ and $\rho_2=\sum_k q'_k\phi_k$ be their spectral decompositions, i.e., $\langle\psi_{k_1}|\psi_{k_2}\rangle=\delta_{k_1k_2}$ and $\langle\phi_{k'_1}|\phi_{k'_2}\rangle=\delta_{k'_1k'_2}$. Then, direct computation gives

$$\begin{aligned}\|\sqrt{\rho_1}(\Lambda^\dagger(H_{S'})-\Lambda_\epsilon^\dagger(H_{S'}))\sqrt{\rho_2}\|_2&=\left\|\sum_{k,k'}\sqrt{q_k}\sqrt{q'_k}\psi_k(\Lambda^\dagger(H_{S'})-\Lambda_\epsilon^\dagger(H_{S'}))\phi_{k'}\right\|_2\\&=\sqrt{\sum_{k,k'}q_kq_{k'}\left|\langle\psi_k|(\Lambda^\dagger(H_S)-\Lambda_\epsilon^\dagger(H_{S'}))|\phi_{k'}\rangle\right|^2}.\end{aligned}\tag{B5}$$

We further remark that $\langle\psi_k|\phi_{k'}\rangle=0$ for all k and k' because $\mathrm{Tr}(\rho_1\rho_2)=0$ by the definition of reversible pairs. For arbitrary orthogonal pure states ψ and ϕ, the following relation holds:

$$
\begin{aligned}
|\langle\psi|\Lambda_\epsilon^\dagger(H_{S'})-\Lambda^\dagger(H_{S'})|\phi\rangle| &\leq \frac{1}{2}|\langle\psi|\Lambda_\epsilon^\dagger(H_{S'})-\Lambda^\dagger(H_{S'})|\phi\rangle+\langle\phi|\Lambda_\epsilon^\dagger(H_{S'})-\Lambda^\dagger(H_{S'})|\psi\rangle| \\
&\quad+\frac{1}{2}|\langle\psi|\Lambda_\epsilon^\dagger(H_{S'})-\Lambda^\dagger(H_{S'})|\phi\rangle-\langle\phi|\Lambda_\epsilon^\dagger(H_{S'})-\Lambda^\dagger(H_{S'})|\psi\rangle| \\
&= \frac{1}{2}\left|\mathrm{Tr}(H_{S'}(\Lambda_\epsilon-\Lambda)(|\psi\rangle\langle\phi|+|\phi\rangle\langle\psi|))\right|+\frac{1}{2}\left|\mathrm{Tr}(H_{S'}(\Lambda_\epsilon-\Lambda)(|\psi\rangle\langle\phi|-|\phi\rangle\langle\psi|))\right| \\
&= \frac{1}{2}\left|\mathrm{Tr}((H_{S'}-a\mathbb{1}_{S'})(\Lambda_\epsilon-\Lambda)(|\psi\rangle\langle\phi|+|\phi\rangle\langle\psi|))\right| \\
&\quad+\frac{1}{2}\left|\mathrm{Tr}((H_{S'}-a\mathbb{1}_{S'})(\Lambda_\epsilon-\Lambda)(|\psi\rangle\langle\phi|-|\phi\rangle\langle\psi|))\right| \\
&\leq \frac{1}{2}\|H_{S'}-a\mathbb{1}_{S'}\|_\infty\|(\Lambda_\epsilon-\Lambda)(|\psi\rangle\langle\phi|+|\phi\rangle\langle\psi|)\|_1 \\
&\quad+\frac{1}{2}\|H_{S'}-a\mathbb{1}_{S'}\|_\infty\|(\Lambda_\epsilon-\Lambda)(|\psi\rangle\langle\phi|-|\phi\rangle\langle\psi|)\|_1 \\
&= \frac{1}{2}\|H_{S'}-a\mathbb{1}_{S'}\|_\infty\|(\Lambda_\epsilon-\Lambda)(|\eta_+\rangle\langle\eta_+|-|\eta_-\rangle\langle\eta_-|)\|_1 \\
&\quad+\frac{1}{2}\|H_{S'}-a\mathbb{1}_{S'}\|_\infty\|(\Lambda_\epsilon-\Lambda)(|\eta'_+\rangle\langle\eta'_+|-|\eta'_-\rangle\langle\eta'_-|)\|_1 \\
&\leq 4\|H_{S'}-a\mathbb{1}_{S'}\|_\infty\epsilon \\
&\leq 2\Delta(H_{S'})\epsilon
\end{aligned}
\tag{B6}
$$

where a is an arbitrary real number, and $|\eta_\pm\rangle \coloneqq \frac{1}{\sqrt{2}}(|\psi\rangle \pm |\phi\rangle)$ and $|\eta'_\pm\rangle \coloneqq \frac{1}{\sqrt{2}}(|\psi\rangle \pm i|\phi\rangle)$. In the second last line, we used the triangle inequality for the trace norm and $\frac{1}{2}\|\rho-\sigma\|_1 \leq D_F(\rho,\sigma)$. In the last line, we fixed a to satisfy $\|H_{S'}\|_\infty = \Delta(H_{S'})/2$.

Together with (B5), this particularly implies

$$
\begin{aligned}
\|\sqrt{\rho_1}(\Lambda^\dagger(H_{S'})-\Lambda_\epsilon^\dagger(H_{S'}))\sqrt{\rho_2}\|_2 &\leq \sqrt{\sum_{k,k'}q_kq_{k'}}2\Delta(H_{S'})\epsilon \\
&= 2\Delta(H_{S'})\epsilon.
\end{aligned}
\tag{B7}
$$

Combining this with (B4), we get

$$
\mathcal{C}(\Lambda_\epsilon,\mathbb{P}) \geq \mathcal{C}(\Lambda,\mathbb{P})-2\Delta(H_{S'})\epsilon. \tag{B8}
$$

We finally note that since $\mathbb{O}_{\rm TO} \subseteq \mathbb{O}_{\rm cov}$ as in (A9), $\mathcal{F}_c^\epsilon(\Lambda) \geq \mathcal{F}_{c,\rm cov}^\epsilon(\Lambda)$ always holds. We conclude the proof by combining all these observations. Let us particularly take Λ_ϵ to be the optimal channel achieving the coherence cost with error ϵ, i.e., $\Lambda_\epsilon \sim_\epsilon \Lambda$ and $\mathcal{F}_{c,\rm cov}(\Lambda_\epsilon) = \mathcal{F}_{c,\rm cov}^\epsilon(\Lambda)$. Then,

$$
\begin{aligned}
\sqrt{\mathcal{F}_c^\epsilon(\Lambda)} &\geq \sqrt{\mathcal{F}_{c,\rm cov}^\epsilon(\Lambda)} \\
&= \sqrt{\mathcal{F}_{c,\rm cov}(\Lambda_\epsilon)} \\
&\geq \frac{\mathcal{C}(\Lambda_\epsilon,\mathbb{P})}{\delta(\Lambda_\epsilon,\mathbb{P})}-\Delta(H_S)-\Delta(H_{S'}) \\
&\geq \frac{\mathcal{C}(\Lambda,\mathbb{P})}{\epsilon}-\Delta(H_S)-3\Delta(H_{S'})
\end{aligned}
\tag{B9}
$$

where we used Theorem S.1 in the third line and (B3) and (B8) in the fourth line.

□

Appendix C: Construction of pairwise reversible Gibbs-preserving Operations (Proof of Theorem 3)

We first show a general sufficient condition for the existence of pairwise reversible Gibbs-preserving Operations. To this end, let ψ be a pure state in S. We define the min-relative entropy with respect to the Gibbs state by [6, 8, 52, 53]

$$
D_{\min}(\psi\|\tau_S) = -\log\mathrm{Tr}(\psi\tau_S). \tag{C1}
$$

Also, for an arbitrary state ρ in S, max-relative entropy with respect to the Gibbs state is defined by [6, 8, 52, 53]

$$D_{\max}(\rho\|\tau_S) = \log\min\left\{ s \;\middle|\; \rho \le s\tau_S \right\}. \tag{C2}$$

We then obtain the following result.

Theorem S.3. *Let S be a system with Hamiltonian $H_S = \sum_n E_{n,S}|n\rangle\langle n|$ and S' be a system with some arbitrary Hamiltonian. If there exists a pair of pure states $\psi \in S$ and $\phi \in S'$ such that*

$$\langle i|\psi|i\rangle \neq 0, \quad \langle j|\psi|j\rangle \neq 0, \quad E_{i,S} \neq E_{j,S} \tag{C3}$$

and

$$D_{\min}(\psi\|\tau_S) = D_{\min}(\phi\|\tau_{S'}) = D_{\max}(\phi\|\tau_{S'}), \tag{C4}$$

there exists a pairwise reversible Gibbs-preserving Operation from S to S'.

Proof. Let ψ and ϕ be the pure states in (C3) and (C4). Define

$$\Lambda(\rho) = \mathrm{Tr}(\psi\rho)\phi + \mathrm{Tr}\left[(\mathbb{1}-\psi)\rho\right]\eta \tag{C5}$$

where

$$\eta = \frac{\tau_{S'} - \mathrm{Tr}(\psi\tau_S)\phi}{\mathrm{Tr}\left[(\mathbb{1}-\psi)\tau_S\right]}. \tag{C6}$$

The operator η is a valid state because it clearly has the unit trace and

$$\phi \le 2^{D_{\max}(\phi\|\tau_{S'})}\tau_{S'} = 2^{D_{\min}(\psi\|\tau_S)}\tau_{S'} = \mathrm{Tr}(\psi\tau_S)^{-1}\tau_{S'} \tag{C7}$$

where the first inequality is by definition of $D_{\max}$, the first equality is due to (C4), and the last equality is by definition of $D_{\min}$. This ensures that $\eta \ge 0$ and that Λ is a valid Gibbs-preserving channel.

Moreover,

$$\mathrm{Tr}(\phi\eta) \propto \mathrm{Tr}(\phi\tau_{S'}) - \mathrm{Tr}(\psi\tau_S) = 2^{-D_{\min}(\phi\|\tau_{S'})} - 2^{-D_{\min}(\psi\|\tau_S)} = 0 \tag{C8}$$

where the final equality is due to (C4). This implies that ϕ and η are perfectly distinguishable and thus ensures that $\delta(\Lambda,\mathbb{P}) = 0$ for a choice of state pair $\mathbb{P} = \{\psi,\sigma\}$ where σ is an arbitrary state in S such that $\mathrm{Tr}(\psi\sigma) = 0$.

As a choice of σ, we can particularly choose an orthogonal pure state $\psi^\perp$ defined as follows. Let $a_i \coloneqq \langle i|\psi\rangle$ and $a_j \coloneqq \langle j|\psi\rangle$ be the coefficients for i th and j th energy of ψ, where i and j are the labels in (C3). We assume $a_{i,j} \in \mathbb{R}$ without loss of generality, as incoherent unitary—which can arbitrarily adjust the relative phase—is energy conserving. We then choose

$$|\psi^\perp\rangle = \frac{1}{\sqrt{|a_j|^2 + |a_i|^2}}\left(a_j|i\rangle - a_i|j\rangle\right), \tag{C9}$$

for which one can directly check that the condition $\mathrm{Tr}(\psi\psi^\perp) = 0$ is satisfied. Since

$$\Lambda^\dagger(H_{S'}) = \mathrm{Tr}(\phi H_{S'})\psi + \mathrm{Tr}(\eta H_{S'})(\mathbb{1}-\psi), \tag{C10}$$

we get

$$\langle\psi|\Lambda^\dagger(H_{S'})|\psi^\perp\rangle = 0. \tag{C11}$$

Therefore,

$$\left|\langle\psi|H - \Lambda^\dagger(H_{S'})|\psi^\perp\rangle\right| = \left|\langle\psi|H|\psi^\perp\rangle\right| = \frac{|a_i a_j|}{\sqrt{a_i^2 + a_j^2}}|E_{i,S} - E_{j,s}| > 0 \tag{C12}$$

where the last inequality is because of the assumption that $E_{i,S} \neq E_{j,S}$. This ensures

$$\mathcal{C}(\Lambda,\mathbb{P}) = \left|\langle\psi|H - \Lambda^\dagger(H_{S'})|\psi^\perp\rangle\right| > 0 \tag{C13}$$

with a reversible pair $\mathbb{P} = \{\psi,\psi^\perp\}$, concluding the proof. □

Theorem S.3 admits the following simple sufficient condition.

Corollary S.4 (Theorem 3 in the main text). *Let $\tau_{X,i} = \langle i|\tau_X|i\rangle_X$ be the Gibbs distribution for the Gibbs state for a system X with Hamiltonian $H_X = \sum_i E_{X,i}|i\rangle\langle i|_X$. Then, if there are integers i, j, and i' for systems S and S' such that*

$$\tau_{S,i} < \tau_{S',i'} < \tau_{S,j}, \tag{C14}$$

there exists a pairwise reversible Gibbs-preserving Operation $\Lambda : S \to S'$ and a reversible pair $\mathbb{P}$ such that $\mathcal{C}(\Lambda, \mathbb{P}) > 0$.

Proof. Let $r \in (0, 1)$ be a real positive number satisfying

$$\tau_{S',i'} = r\tau_{S,i} + (1-r)\tau_{S,j}, \tag{C15}$$

whose existence is guaranteed because of (C14). Let ψ and ϕ be the pure states defined by

$$|\psi\rangle := \sqrt{r}|i\rangle_S + \sqrt{1-r}|j\rangle_S, \tag{C16}$$

$$|\phi\rangle := |i'\rangle_{S'}. \tag{C17}$$

It suffices to show that ψ and ϕ satisfy (C3) and (C4). It is straightforward to check (C3) noting $0 < r < 1$. Eq. (C4) can be checked as follows:

$$\begin{aligned}
D_{\min}(\psi\|\tau_S) &= -\log \operatorname{Tr}(\psi\tau_S) \\
&= -\log(r\tau_{S,i} + (1-r)\tau_{S,j}) \\
&= -\log \tau_{S',i'} \\
&= -\log \operatorname{Tr}[\phi\tau_{S'}] = D_{\min}(\phi\|\tau_{S'}) \\
&= \log \min\left\{ s \,\middle|\, |i'\rangle\langle i'|_{S'} \le s\tau_{S'} \right\} = D_{\max}(\phi\|\tau_{S'}).
\end{aligned} \tag{C18}$$

□

We also provide an alternative construction.

Proposition S.5. *For a countably infinite series $\{E_n\}_n$ of real numbers, let $S_d(\{E_n\}_n)$ be an arbitrary d-dimensional system equipped with Hamiltonian $H_d = \sum_{n=0}^{d-1} E_n|n\rangle\langle n|$. Then, for arbitrary $d \ge 3$ and $d' \le d$, and an arbitrary energy spectrum $\{E_n\}_n$ with $E_i \ge E_j$, $\forall i, j$ such that it is not fully degenerate above the ground energy, i.e., there exists $1 \le i \le d-1$ such that $E_{i+1} > E_i$, there exists a pairwise reversible Gibbs-preserving map $\Lambda : S_d(\{E_n\}_n) \to S_{d'}(\{E_n\}_n)$ with a reversible pair $\mathbb{P}$ such that $\mathcal{C}(\Lambda, \mathbb{P}) > 0$.*

Proof. Let $\tau_S = \sum_n \tau_{S,n}$ be the Gibbs state for $S_d(\{E_n\}_n)$ and $\tau_{S'} = \sum_n \tau_{S',n}$ be the Gibbs state for $S_{d'}(\{E_n\}_n)$. Let i be an integer such that $1 \le i \le d-1$ and $E_{i+1} > E_i$ ensured by the assumption. Define

$$\Lambda(\rho) = \operatorname{Tr}(|+\rangle\langle +|_{i,i+1}\rho)|0\rangle\langle 0| + \operatorname{Tr}(|-\rangle\langle -|_{i,i+1}\rho)|1\rangle\langle 1| + \operatorname{Tr}(P^\perp_{i,i+1}\rho)\eta \tag{C19}$$

where $P^\perp_{i,i+1} = \mathbb{1}_d - (|i\rangle\langle i| + |i+1\rangle\langle i+1|)$ is the projector onto the input space complement to $\mathrm{span}\{|i\rangle, |i+1\rangle\}$, and

$$\eta := \frac{\tau_{S'} - \operatorname{Tr}(|+\rangle\langle +|_{i,i+1}\tau_S)|0\rangle\langle 0| - \operatorname{Tr}(|-\rangle\langle -|_{i,i+1}\tau_S)|1\rangle\langle 1|}{\operatorname{Tr}(P^\perp_{i,i+1}\tau_S)}. \tag{C20}$$

The operator η is a valid state because it clearly has a unit trace and

$$\eta \propto \left(\tau_{S',0} - \frac{\tau_{S,i} + \tau_{S,i+1}}{2}\right)|0\rangle\langle 0| + \left(\tau_{S',1} - \frac{\tau_{S,i} + \tau_{S,i+1}}{2}\right)|1\rangle\langle 1| + \sum_{j\ge 2} \tau_{S',j}|j\rangle\langle j| \ge 0 \tag{C21}$$

where we used the fact that for any k,

$$\tau_{S',k} - \tau_{S,k} = \frac{(Z - Z')e^{-\beta E_k}}{ZZ'} \ge 0, \quad Z := \sum_{n=0}^{d-1} e^{-\beta E_n}, Z' := \sum_{n=0}^{d'-1} e^{-\beta E_n} \tag{C22}$$

because $d \geq d'$ by assumption, which implies $Z \geq Z'$. We then get

$$\begin{aligned}\tau_{S',0} - \frac{\tau_{S,i}+\tau_{S,i+1}}{2} &\geq \tau_{S,0} - \frac{\tau_{S,i}+\tau_{S,i+1}}{2} \geq 0 \\ \tau_{S',1} - \frac{\tau_{S,i}+\tau_{S,i+1}}{2} &\geq \tau_{S,1} - \frac{\tau_{S,i}+\tau_{S,i+1}}{2} \geq 0\end{aligned} \tag{C23}$$

where the last inequalities hold because $E_{i+1} \geq E_i \geq E_1 \geq E_0$ and thus $\tau_{S,i+1} \leq \tau_{S,i} \leq \tau_{S,1} \leq \tau_{S,0}$. This ensures that Λ is a measure-and-prepare channel, and due to the definition of η, Λ is Gibbs-preserving.

In addition, a state pair $\{|+\rangle\langle+|_{i,i+1}, |-\rangle\langle-|_{i,i+1}\}$ is reversible because $\Lambda(|+\rangle\langle+|_{i,i+1}) = |0\rangle\langle 0|$ and $\Lambda(|-\rangle\langle-|_{i,i+1}) = |1\rangle\langle 1|$ are perfectly distinguishable. This ensures $\delta(\Lambda, \mathbb{P}) = 0$ for $\mathbb{P} = \{|+\rangle\langle+|_{i,i+1}, |-\rangle\langle-|_{i,i+1}\}$.

One can also check $\mathcal{C}(\Lambda, \mathbb{P}) > 0$ as follows. We have

$$\Lambda^\dagger(H_{d'}) = \mathrm{Tr}(H_{d'}|0\rangle\langle 0|)|+\rangle\langle+|_{i,i+1} + \mathrm{Tr}(H_{d'}|1\rangle\langle 1|)|-\rangle\langle-|_{i,i+1} + \mathrm{Tr}(H_{d'}\eta)P^{\perp}_{i,i+1} \tag{C24}$$

resulting in

$${}_{i,i+1}\langle+|\Lambda^\dagger(H_{d'})|-\rangle_{i,i+1} = 0. \tag{C25}$$

On the other hand,

$$|{}_{i,i+1}\langle+|H_d|-\rangle_{i,i+1}| = \frac{E_{i+1}-E_i}{2} > 0 \tag{C26}$$

because $E_{i+1} > E_i$ by assumption. This ensures $\mathcal{C}(\Lambda, \mathbb{P}) > 0$.

□

Appendix D: Upper bound for the coherence cost of Eq. (2)

We show that the coherence cost $\mathcal{F}_c(\Lambda)$ for the channel $\Lambda : S \to S'$ defined by

$$\Lambda(\rho) = \langle 1|\rho|1\rangle\eta + \langle 0|\rho|0\rangle\sigma \tag{D1}$$

satisfies the upper bound

$$\mathcal{F}_c(\Lambda) \leq \mathcal{F}(\eta) + \mathcal{F}(\sigma). \tag{D2}$$

Proof. Let E be an ancillary system with $H_E = 0$. Let $\Lambda_1 : S \to E$ and $\Lambda_2 : E \to S'$ be the channels defined by

$$\Lambda_1(\kappa_S) := \langle 1|\kappa_S|1\rangle|1\rangle\langle 1|_E + \langle 0|\kappa_S|0\rangle|0\rangle\langle 0|_E \tag{D3}$$

and

$$\Lambda_2(\kappa_E) := \langle 1|\kappa_E|1\rangle\eta + \langle 0|\kappa_E|0\rangle\sigma \tag{D4}$$

for arbitrary states κ_S in S and κ_E in E.

Let $\tilde{S}$ be a system identical to S (equipped with Hamiltonian H_S). The channels Λ_1 and Λ_2 can be implemented by unitaries U on SE and V on $ES\tilde{S}$ by

$$\Lambda_1(\kappa_S) = \mathrm{Tr}_S[U\kappa_S \otimes |0\rangle\langle 0|_E U^\dagger] \tag{D5}$$

$$\Lambda_2(\kappa_E) = \mathrm{Tr}_{E\tilde{S}}[V\kappa_E \otimes \eta \otimes \sigma V^\dagger] \tag{D6}$$

where

$$U := |00\rangle\langle 00|_{SE} + |11\rangle\langle 10|_{SE} + |01\rangle\langle 01|_{SE} + |10\rangle\langle 11|_{SE}, \tag{D7}$$

$$V := |0\rangle\langle 0|_E \otimes \mathbb{1}_{S\tilde{S}} + |1\rangle\langle 1|_E \otimes U_{\mathrm{SWAP}} \tag{D8}$$

where U_{SWAP} is the swap operator between S and $\tilde{S}$. Because of $H_E = 0$ and $H_S = H_{\tilde{S}}$, the relations $[U, H_S + H_E] = 0$ and $[V, H_E + H_S + H_{\tilde{S}}] = 0$ are satisfied. Therefore, we obtain

$$\mathcal{F}_c(\Lambda_1) \leq \mathcal{F}(|0\rangle\langle 0|) = 0 \tag{D9}$$

$$\mathcal{F}_c(\Lambda_2) \leq \mathcal{F}(\eta \otimes \sigma) = \mathcal{F}(\eta) + \mathcal{F}(\sigma). \tag{D10}$$

Since $\mathcal{F}_c(\Lambda) \leq \mathcal{F}_c(\Lambda_1) + \mathcal{F}_c(\Lambda_2)$, we obtain (D2). □

Appendix E: Upper bounds (Proofs of Theorems 4 and 5)

We first show Theorem 5, which we later utilize to prove Theorem 4.

Theorem S.6 (Theorem 5 in the main text)**.** *Let $\Lambda : S \to S'$ be an arbitrary quantum channel admitting a dilation form*

$$\Lambda(\rho) = \mathrm{Tr}_{E'}\left(V(\rho \otimes |\eta\rangle\langle\eta|)V^\dagger\right) \tag{E1}$$

for some environments E and E' such that $S \otimes E = S' \otimes E'$, some unitary V on $S \otimes E$, and some pure incoherent state $|\eta\rangle$ on E. Then,

$$\sqrt{\mathcal{F}_c^\epsilon(\Lambda)} \leq \frac{\Delta(H_{\rm tot} - V^\dagger H_{\rm tot} V)}{2\epsilon} + \sqrt{2}\Delta(H_{\rm tot}) \tag{E2}$$

where $H_{\rm tot} = H_S \otimes \mathbb{1}_E + \mathbb{1}_S \otimes H_E = H_{S'} \otimes \mathbb{1}_{E'} + \mathbb{1}_{S'} \otimes H_{E'}$, and $\Delta(O)$ is the difference between the minimum and maximum eigenvalues of an operator O.

Proof. Ref. [33, Theorem 2] shows that an arbitrary unitary channel $\mathcal{V}(\cdot) = V \cdot V$ on a system with Hamiltonian H can be implemented with error ϵ with coherence cost $\frac{\Delta(H - V^\dagger HV)}{2\epsilon} + \sqrt{2}\Delta(H)$. Let $\mathcal{V}_\epsilon$ be such a channel approximating $\mathcal{V}$ satisfying $D_F(\mathcal{V}_\epsilon, \mathcal{V}) \leq \epsilon$, and define $\Lambda_\epsilon := \mathrm{Tr}_{E'} \circ \mathcal{V}_\epsilon \circ \mathcal{P}_{|\eta\rangle}$ where $\mathcal{P}_{|\eta\rangle}(\rho) = \rho \otimes |\eta\rangle\langle\eta|$ is a state preparation channel. Noting that $\mathcal{P}_{|\eta\rangle}$ and $\mathrm{Tr}_{E'}$ can be implemented with no coherence cost, we get

$$\sqrt{\mathcal{F}_c(\Lambda_\epsilon)} \leq \sqrt{\mathcal{F}_c(\mathcal{V}_\epsilon)} \leq \frac{\Delta(H_{\rm tot} - V^\dagger H_{\rm tot} V)}{2\epsilon} + \sqrt{2}\Delta(H_{\rm tot}). \tag{E3}$$

Therefore, it suffices to show that $D_F(\Lambda_\epsilon, \Lambda) \leq \epsilon$, which would ensure that $\sqrt{\mathcal{F}_c^\epsilon(\Lambda)} \leq \sqrt{\mathcal{F}_c(\Lambda_\epsilon)}$ and result in the advertised upper bound. This can indeed be checked by

$$\begin{aligned} D_F(\Lambda_\epsilon, \Lambda) &= D_F(\mathrm{Tr}_{E'} \circ \mathcal{V}_\epsilon \circ \mathcal{P}_{|\eta\rangle}, \mathrm{Tr}_{E'} \circ \mathcal{V} \circ \mathcal{P}_{|\eta\rangle}) \\ &\leq D_F(\mathrm{Tr}_{E'} \circ \mathcal{V}_\epsilon, \mathrm{Tr}_{E'} \circ \mathcal{V}) \\ &\leq D_F(\mathcal{V}_\epsilon, \mathcal{V}) \\ &\leq \epsilon \end{aligned} \tag{E4}$$

where the second line comes from the definition of the channel purified distance (A12), the third line is because of the data-processing inequality of the purified distance, and the fourth line follows from the assumption of $\mathcal{V}_\epsilon$. □

We next show Theorem 4, which shows that the lower bound in Theorem 2 is almost tight, where $\mathcal{C}(\Lambda, \mathbb{P})$ serves as a fundamental quantity that characterizes the coherence cost for a Gibbs-preserving operation.

Theorem S.7 (Theorem 4 in the main text)**.** *For every real number $a > 0$, there is a pairwise reversible Gibbs-preserving Operation Λ and a reversible pair $\mathbb{P}$ such that $\mathcal{C}(\Lambda, \mathbb{P}) > 0$ and*

$$\frac{\mathcal{C}(\Lambda, \mathbb{P})}{\epsilon} - a \leq \sqrt{\mathcal{F}_c^\epsilon(\Lambda)} \leq \frac{\sqrt{2}\mathcal{C}(\Lambda, \mathbb{P})}{\epsilon} + a. \tag{E5}$$

Proof. For a given $a > 0$, consider a qubit system S with Hamiltonian $H_S = \tilde{a}|1\rangle\langle 1|$ with $\tilde{a} = a/\sqrt{2}$ and another qubit system S' with trivial Hamiltonian $H_{S'} = 0$. Consider a channel $\Lambda : S \to S'$ defined by

$$\Lambda(\rho) = \langle +|\rho|+\rangle |0\rangle\langle 0| + \langle -|\rho|-\rangle |1\rangle\langle 1|. \tag{E6}$$

This is evidently a Gibbs-preserving operation, noting that $H_{S'} = 0$. Take the state pair $\mathbb{P} = \{|+\rangle\langle +|, |-\rangle\langle -|\}$. Since both states are reversible under Λ, we have $\delta(\Lambda, \mathbb{P}) = 0$, and $\mathcal{C}(\Lambda, \mathbb{P}) > 0$ can be checked by direct computation. This ensures that Theorem S.2 can be applied, and the lower bound in (E5) then immediately follows noting that $\Delta(H_S) = \tilde{a} \leq a$ and $H_{S'} = 0$.

To get the upper bound, notice that the channel Λ can be implemented by

$$\Lambda(\rho) = \mathrm{Tr}_S(V\rho \otimes |0\rangle\langle 0|_{S'} V^\dagger) \tag{E7}$$

where $V = \mathrm{CNOT}_{SS'}\, U_H \otimes \mathbb{1}_{S'}$ is a unitary on SS' where U_H is the Hadamard gate and $\mathrm{CNOT}_{SS'}$ is the CNOT gate controlled on S. Noting that $H_{S'} = 0$ and thus $H_{\mathrm{tot}} = H_S \otimes \mathbb{1}_{S'}$, we get

$$H_{\mathrm{tot}} - V^\dagger H_{\mathrm{tot}} V = H_S \otimes \mathbb{1} - V^\dagger (H_S \otimes \mathbb{1}) V = (H_S - U_H H_S U_H) \otimes \mathbb{1}. \tag{E8}$$

This gives

$$\Delta(H_{\mathrm{tot}} - V^\dagger H_{\mathrm{tot}} V) = \Delta(H_S - U_H H_S U_H) = \sqrt{2}\tilde{a}. \tag{E9}$$

On the other hand,

$$\mathcal{C}(\Lambda, \mathbb{P}) = |\langle + | H_S - U_H H_S U_H | - \rangle| = \frac{\tilde{a}}{2}. \tag{E10}$$

Combining (E9) and (E10) gives

$$\Delta(H_{\mathrm{tot}} - V^\dagger H_{\mathrm{tot}} V) = 2\sqrt{2}\, \mathcal{C}(\Lambda, \mathbb{P}), \tag{E11}$$

from which the upper bound in (E5) follows by using Theorem S.6 and noting $\Delta(H_S) = \tilde{a} = a/\sqrt{2}$ and $\Delta(H_{S'}) = 0$. $\square$