PHYSICAL REVIEW A **93**, 052335 (2016)

Energy cost of creating quantum coherence

Avijit Misra,* Uttam Singh,† Samyadeb Bhattacharya,‡ and Arun Kumar Pati§
Harish-Chandra Research Institute, Chhatnag Road, Jhunsi, Allahabad 211 019, India
(Received 14 March 2016; published 26 May 2016)

We consider physical situations where the resource theories of coherence and thermodynamics play competing roles. In particular, we study the creation of quantum coherence using unitary operations with limited thermodynamic resources. We find the maximal coherence that can be created under unitary operations starting from a thermal state and find explicitly the unitary transformation that creates the maximal coherence. Since coherence is created by unitary operations starting from a thermal state, it requires some amount of energy. This motivates us to explore the trade-off between the amount of coherence that can be created and the energy cost of the unitary process. We also find the maximal achievable coherence under the constraint on the available energy. Additionally, we compare the maximal coherence and the maximal total correlation that can be created under unitary transformations with the same available energy at our disposal. We find that when maximal coherence is created with limited energy, the total correlation created in the process is upper bounded by the maximal coherence, and vice versa. For two-qubit systems we show that no unitary transformation exists that creates the maximal coherence and maximal total correlation simultaneously with a limited energy cost.

DOI: 10.1103/PhysRevA.93.052335

I. INTRODUCTION

The superposition principle in quantum physics gives rise to classically counterintuitive traits like coherence and entanglement [1]. Over the past few years, several works have been done, from quantifying quantum superposition [2] to establishing full-fledged resource theories of coherence [3–5]. The restrictions underlying a quantum resource theory (QRT) are manifestations of the physical restrictions that govern the physical processes. For example, in the QRT of entanglement, the consideration of local operations and classical communication as the allowed operations stems from the natural limitation to implementation of global operations in a multipartite quantum system with the parties separated. Considering the technological advancements towards processing of small-scale quantum systems and proposals of nanoscale heat engines, it is of utmost importance to investigate the thermodynamic perspectives of quantum features like coherence and entanglement, and this has attracted a great deal of interest (see, for example, Refs. [6–22]). Since energy conservation restricts the thermodynamic processing of coherence, a quantum state having coherence can be viewed as a resource in thermodynamics, as it allows transformations that are otherwise impossible [23,24]. These explorations have received renewed interest recently due to their possible implications in various areas such as information theory [25–29] and quantum biology [30–34]. In particular, it is also shown that quantum coherence allows for better transient cooling in absorption refrigerators and this phenomenon is dubbed coherence-assisted single-shot cooling [35].

In this work, with the aforesaid motivation, we explore the intimate connections between the resource theory of quantum coherence and thermodynamic limitations on the processing of quantum coherence. In particular, we study the creation of quantum coherence by unitary transformations with limited energy. We go even further, to present a comparative investigation of the creation of quantum coherence and mutual information within the imposed thermodynamic constraints. Considering a thermally isolated quantum system initially in a thermal state, we perform an arbitrary unitary operation on the system to create coherence. First, we find the upper bound on the coherence that can be created using arbitrary unitary operations starting from a fixed thermal state and then we show explicitly that, irrespective of the temperature of the initial thermal state, the upper bound on coherence can always be saturated. Such a physical process will cost us some amount of energy and hence it is natural to ask, if we have a limited supply of energy to invest, then what is the maximal achievable coherence in such situations? Further, we investigate whether both coherence and mutual information can be created maximally by applying a single unitary operation on a two-qubit quantum system. We find that it is not possible to achieve maximal quantum coherence and maximal mutual information simultaneously. Our results are relevant for the quantum information processing in physical systems where thermodynamic considerations cannot be ignored, as discussed in the preceding paragraph.

The organization of the paper is as follows. In Sec. II we introduce the concepts that are necessary for further exposition of our work and present the form of the unitary operation that saturates the upper bound on the amount of coherence that can be created by applying unitary transformations starting from an incoherent state. In Sec. III we provide various results on the creation of coherence when there is a limited availability of energy. In Sec. IV we compare the processes of creating maximal coherence and maximal mutual information, again with limited thermodynamic resources. Finally, we conclude with some possible implications in Sec. V.

II. MAXIMUM ACHIEVABLE COHERENCE UNDER ARBITRARY UNITARY OPERATIONS

In this section, we first discuss the QRT of coherence and then find a protocol for achieving maximal quantum coherence under unitary operations.

*avijit@hri.res.in
†uttamsingh@hri.res.in
‡samyadebbhattacharya@hri.res.in
§akpati@hri.res.in

A. Quantum coherence

Any QRT is formed by identifying the relevant physical restrictions on the set of quantum operations and preparation of quantum states. For example, in the QRT of thermodynamics the set of allowed operations is identified as the thermal operations and the only free state is the thermal state for a given fixed Hamiltonian [27,28]. The QRT of thermodynamics is well accepted and has seen enormous progress in recent years [23,24,29,36]. However, there is still ongoing debate about the possible choices of restricted operations that will define the resource theory of coherence for finite-dimensional quantum systems [3,4,37,38]. The field of QRT of coherence has advanced significantly over the past few years [37,39–65]. Measures of coherence are inherently basis dependent and the relevant reference basis is provided by the experimental situation at hand. Here we are concerned with the measures of coherence that are obtained using QRT of coherence based on incoherent operations as introduced in Ref. [3]. However, very recently a refinement over Ref. [3] of the properties that a coherence measure should satisfy was proposed in Ref. [65]. This refinement imposes an extra condition on the measures of coherence such that the set of states having the maximal coherence value with respect to the coherence measure and the set of maximally coherent states, as defined in Ref. [3], should be identical. Moreover, the unitary freedom in Kraus decomposition of a quantum channel implies that an incoherent channel with respect to a particular physical realization (Karus decomposition) may not be incoherent with respect to other realizations of the same channel. This has led to the introduction of genuinely incoherent operations [37]. Genuinely incoherent operations are those that preserve incoherent states. It is proved that the set of genuinely incoherent operations is a strict subset of the incoherent operations, therefore, every coherence monotone based on the set of incoherent operations is also a genuine coherence monotone [37].

In this work, we consider the relative entropy of coherence as a measure of coherence, which enjoys various operational interpretations [52,66]. The relative entropy of coherence of any state ρ is defined as $C_r(\rho) = S(\rho^D) - S(\rho)$, where $S(\rho) = -\text{Tr}(\rho \log_2 \rho)$ is the von Neumann entropy and $\rho^D = \sum_i \langle i|\rho|i\rangle |i\rangle\langle i|$ is the diagonal part of ρ in the reference basis $\{|i\rangle\}$. It is to be noted that the relative entropy of coherence is also a genuine coherence monotone. Moreover, it also satisfies the additional requirement as proposed in Ref. [65].

B. Maximum achievable coherence

Let us now consider the creation of maximal coherence, which we define shortly, starting from a thermal state by unitary operations. The prime motivation for starting with a thermal initial state is that the surroundings may be considered a thermal bath, and as the system interacts with the surroundings, it eventually gets thermalized. However, our protocol for creating maximal coherence is applicable to any incoherent state. Let us now consider an arbitrary quantum system in contact with a heat bath at temperature $T = 1/\beta$ (we set the Boltzmann constant to unity and follow this convention throughout the paper). The thermal state of a system with the Hamiltonian $H = \sum_{j=1}^{d} E_j |j\rangle\langle j|$ is given by

$$\rho_T = \frac{1}{Z} e^{-\beta H}, \tag{1}$$

where d is the dimension of the Hilbert space and $Z = \text{Tr}[e^{-\beta H}]$ is the partition function. The maximum amount of coherence $C_{r,\max}(\rho_f)$ that can be created starting from ρ_T by unitary operations is given by

$$C_{r,\max}(\rho_f) = \max_{\{\rho_f | S(\rho_f) = S(\rho_T)\}} \{S(\rho_f^D) - S(\rho_T)\}. \tag{2}$$

As the maximum entropy of a quantum state in d dimensions is $\log_2 d$, the amount of coherence that can be created starting from ρ_T, by a unitary transformation, always follows the inequality

$$C_r(\rho_f) \leqslant \log_2 d - S(\rho_T). \tag{3}$$

Now the question is whether or not the bound is tight, i.e., Is there any unitary operation that can lead to the creation of $\log_2 d - S(\rho_T)$ amount of coherence starting from ρ_T? But before we answer this question, let us digress regarding its importance. Coherence in an energy eigenbasis plays a crucial role in quantum thermodynamic protocols and several quantum information processing tasks. For example in Ref. [35], it has been demonstrated that if the initial qubits of a three-qubit refrigerator possess even a small amount of coherence in an energy eigenbasis, then the cooling will be significantly better. In small-scale refrigerators, the three constituent qubits initially remain in corresponding thermal states associated with the three thermal baths. Therefore, one needs to create coherence by external means. Hence, creation of coherence from thermal states may be fruitful and far-reaching for better functioning of various nanoscale thermal machines and diverse thermodynamic protocols. These are the main motivations for studying the creation of coherence from a thermodynamic perspective. We consider closed quantum systems and hence allow only unitary operations for creating coherence. Of course, after creating coherence via the unitary transformation we have to isolate or take the system away from the heat bath so that it does not get thermalized again. Now, we show that the bound in Eq. (3) is achievable by finding the unitary operation U such that $\rho_f = U\rho_i U^\dagger$ has the maximal amount of coherence. Since the relative entropy of coherence of ρ_f is given by $S(\rho_f^D) - S(\rho_f)$, one has to maximize the entropy of the diagonal density matrix ρ_f^D. The quantum state that is the diagonal of a quantum state ρ is denoted ρ^D throughout the paper.

First, we construct a unitary transformation that results in rotating the energy eigenbasis to the maximally coherent basis as follows. The maximally coherent basis $\{|\phi_j\rangle\}_j$ is defined as $|\phi_j\rangle = \mathbb{Z}^j |\phi\rangle$, where

$$\mathbb{Z} = \sum_{m=0}^{d-1} e^{\frac{2\pi i m}{d}} |m\rangle\langle m| \tag{4}$$

and $|\phi\rangle = \frac{1}{\sqrt{d}} \sum_{i=0}^{d-1} |i\rangle$. It can be verified easily that $\langle\phi_j|\phi_k\rangle = \delta_{jk}$. Also, note that all the states in $\{|\phi_j\rangle\}_j$ and $|\phi\rangle$ are maximally coherent states [3] and have equal amounts of the relative entropy of coherence, which is equal to $\log_2 d$. Now consider the unitary operation

$$U = \sum_j |\phi_j\rangle \langle j| , \tag{5}$$

which changes energy eigenstate $|j\rangle$ to the maximally coherent state $|\phi_j\rangle$. Starting from the thermal state ρ_T, the final state ρ_f after the application of U is given by

$$\rho_f = \sum_j \frac{e^{-\beta E_j}}{Z} |\phi_j\rangle \langle \phi_j| . \tag{6}$$

Since ρ_f is a mixture of pure states that all have maximally mixed diagonals, the bound in Eq. (3) is achieved. We note that U in Eq. (5) is only one possible choice among the possible unitaries achieving the bound in Eq. (3). For example, any permutation of the indices j of $|\phi_j\rangle$ in Eq. (5) is also a valid choice to achieve the bound. It is worth mentioning that even though we consider the thermal density matrix to start with to create maximal coherence in an energy eigenbasis, following the same protocol maximal coherence can be created from any arbitrary incoherent state in any arbitrary reference basis.

To create coherence by unitary operations starting from a thermal state, some amount of energy is required. Now, let us ask how much energy is needed on average to create the maximal amount of coherence. Let $\rho_T \to V\rho_T V^\dagger$; then the energy cost of any arbitrary unitary operation V acting on the thermal state is given by

$$W = \mathrm{Tr}[H(V\rho_T V^\dagger - \rho_T)]. \tag{7}$$

Since we are dealing with an energy eigenbasis, we have $E(\rho^D) = E(\rho)$. Here $E(\rho) = \mathrm{Tr}(H\rho)$ is the average energy of the system in state ρ. The energy cost to create maximum coherence starting from the thermal state ρ_T is given by

$$W_{\max} = \mathrm{Tr}[H(U\rho_T U^\dagger - \rho_T)] = \frac{1}{d}\mathrm{Tr}[H] - \frac{1}{Z}\mathrm{Tr}[He^{-\beta H}]. \tag{8}$$

Here U is given by Eq. (5). Note that maximal coherence can always be created by unitary operations starting from a finite-dimensional thermal state at an arbitrary finite temperature, with a finite energy cost. However, it is not possible to create coherence by unitary operations starting from a thermal state at an infinite temperature, i.e., the maximally mixed state.

III. CREATING COHERENCE WITH LIMITED ENERGY

Since energy is an independent resource, it is natural to consider a scenario where creation of coherence is limited by a constraint on the available energy. In this section we consider the creation of the optimal amount of coherence at a limited energy cost ΔE starting from ρ_T. To maximize the coherence, one needs to find a final state ρ_f whose diagonal part ρ_f^D has maximum entropy with fixed average energy $E_T + \Delta E$, where E_T is the average energy of the initial thermal state ρ_T. Note that $E(\rho_f^D) = E(\rho_f)$. From the maximum entropy principle [67,68], we know that the thermal state has maximum entropy among all states with a fixed average energy. Therefore, the maximum coherence $C_{r,\max}^{\Delta E}$ that can be created with ΔE amount of available energy is upper bounded by

$$C_{r,\max}^{\Delta E} \leqslant S(\rho_{T'}) - S(\rho_T). \tag{9}$$

Here $\rho_{T'}$ is a thermal state at a higher temperature T' such that $\Delta E = \mathrm{Tr}[H(\rho_{T'} - \rho_T)]$. Thus, in order to create maximal coherence at a limited energy cost, one should look for a protocol such that the diagonal part of ρ_f is a thermal state at a higher temperature T' (depending on the energy spent ΔE), i.e., $\rho_f^D = \rho_{T'}$. Now it is obvious to inquire whether there always exists an optimal unitary U^* that serves the purpose. Theorem 1 answers this question in the affirmative.

Theorem 1. There always exists a real orthogonal transformation R that creates maximum coherence $S(\rho_{T'}) - S(\rho_T)$, starting from the thermal state ρ_T and spending only $\Delta E = \mathrm{Tr}[H(\rho_{T'} - \rho_T)]$ amount of energy.

Proof. To prove the theorem, we first show that the unitary transformations on a quantum state induce doubly stochastic [69] maps in the diagonal part of the quantum state. Note that we start from the thermal state $\rho_T = \sum_{j=0}^{d-1} \frac{e^{-\beta E_j}}{Z} |j\rangle\langle j|$. The diagonal part of ρ_T transforms under the action of a unitary U as

$$\mathrm{diag}\{U\rho_T U^\dagger\} = \sum_{i=0}^{d-1} q_i |i\rangle \langle i| , \tag{10}$$

where $q_i = \frac{1}{Z}\sum_{j=0}^{d-1} M_{ij} e^{-\beta E_j}$ and M, with entries $M_{ij} = \langle i| U |j\rangle \langle j| U^\dagger |i\rangle$, is a doubly stochastic matrix. Therefore, the diagonal part is transformed by the doubly stochastic matrix M such that

$$\vec{Q} = M\vec{P}_T, \tag{11}$$

where $\vec{P}_T = \frac{1}{Z}\{e^{-\beta E_0}, e^{-\beta E_1}, \ldots, e^{-\beta E_{d-1}}\}^T$ is the diagonal vector corresponding to the initial thermal state ρ_T and $\vec{Q}$ is the diagonal vector corresponding to the diagonal part of the final state. For two thermal states, $\rho_{T'}$ and ρ_T, corresponding to the same Hamiltonian, we have $\vec{P}_{T'} \prec \vec{P}_T$ if $T' > T$ [70]. From the results of the theory of majorization [71], it can be concluded that there always exists an orthostochastic [72] matrix B such that $\vec{P}_{T'} = B\vec{P}_T$. Hence, the real orthogonal operator R, corresponding to the orthostochastic matrix B, transforms the initial thermal state ρ_T to a final state ρ_f such that $\rho_f^D = \rho_{T'}$. Therefore, there always exists a real orthogonal transformation R that creates $S(\rho_{T'}) - S(\rho_T)$ amount of coherence, starting from the thermal state ρ_T and spending only $\Delta E = \mathrm{Tr}[H(\rho_{T'} - \rho_T)]$ amount of energy. This completes the proof.

A. Qubit system

In the following, we determine explicitly the real unitary transformation that allows the creation of maximal coherence with limited energy at our disposal for the case of a qubit system with the Hamiltonian $H = E|1\rangle\langle 1|$. The initial thermal state is given by $\rho_T = p|0\rangle\langle 0| + (1-p)|1\rangle\langle 1|$ with $p = \frac{1}{1+e^{-\beta E}}$. Now our goal is to create maximal coherence by applying an optimal unitary U^*, investing only ΔE amount of energy. The average energy of the initial thermal state ρ_T is given by $(1-p)E$. As discussed earlier, for maximal coherence creation with ΔE energy cost, the diagonal part of the final state must be a thermal state, $\rho_{T'} = q|0\rangle\langle 0| + (1-q)|1\rangle\langle 1|$, at some higher temperature T', with average energy $(1-p)E + \Delta E$. Here, q, and hence T', are determined from the energy constraint as $q = p - \frac{\Delta E}{E} = \frac{1}{1+e^{-\beta' E}}$. From Theorem 1, it is evident that there always exists a rotation operator R which creates the maximal coherence. Consider a rotation operator of the form

$$R(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \tag{12}$$

that transforms ρ_T as follows:

$$\rho_f = R(\theta)\rho_T R^T(\theta) = \begin{pmatrix} p\cos^2\theta + (1-p)\sin^2\theta & (2p-1)\sin\theta\cos\theta \\ (2p-1)\sin\theta\cos\theta & p\sin^2\theta + (1-p)\cos^2\theta \end{pmatrix}.$$

We need the diagonal part of the final state to be the thermal state $\rho_{T'}$ at a higher temperature T'. Therefore,

$$q = p\cos^2\theta + (1-p)\sin^2\theta. \tag{13}$$

As the right-hand side of Eq. (13) is a convex combination of p and $(1-p)$ and $p \geqslant q \geqslant 1/2 \geqslant (1-p)$, by suitably choosing θ one can reach the desired final state ρ_f such that $\rho_f^D = \rho_{T'}$. The angle of rotation θ is given by

$$\theta = \cos^{-1}\left(\sqrt{\frac{p+q-1}{2p-1}}\right). \tag{14}$$

Thus, the maximal coherence at constrained energy cost ΔE can be created from a qubit thermal state by a two-dimensional rotation operator as given by Eq. (12).

B. Qutrit system

For qubit systems, a two-dimensional rotation with the suitably chosen θ is required to create maximum coherence starting from a thermal state at a finite temperature with limited available energy. For higher dimensional systems, it follows from Theorem 1 that there always exists a rotation which serves the purpose of maximal coherence creation. However, finding the exact rotation operator for a given initial thermal density matrix and energy constraint is not an easy task. Even for a qutrit system, finding the optimal rotation is nontrivial. In what follows, we demonstrate the protocol for creating maximal coherence with energy constraint starting from a thermal state for qutrit systems. Note that by applying a unitary operation on a thermal qubit, one has to invest some energy, and thus the excited-state population corresponding to the diagonal part of the final qubit is always increased. Therefore, for the case of qubit systems, one only has to give a rotation by an angle θ, depending on the available energy, to create the maximal coherence starting from a given thermal state. For a thermal state in higher dimensions, we know that with an increment in the temperature (energy), the occupation probability of the ground state will always decrease and the occupation probability will increase for the highest excited state. But what will happen for the intermediate energy levels? Let us first answer this particular question considering an initial thermal state of the form

$$\rho_T = \sum_{j=1}^{d} p_j |j\rangle\langle j|, \tag{15}$$

where $p_j = \frac{e^{-E_j/T}}{\sum_j e^{-E_j/T}}$ is the occupation probability of the jth energy level. Differentiating p_j with respect to the temperature, we get

$$\frac{\partial p_j}{\partial T} = -\frac{(\langle E\rangle_T - E_j)}{T^2} p_j. \tag{16}$$

Therefore, for energy levels lying below the average energy of the thermal state, the occupation probabilities will decrease with an increase in temperature and the occupation probabilities will increase for energy levels lying above the average energy. Making use of this change in occupation probabilities, we now provide a protocol for maximum coherence creation in thermal qutrit systems with a constraint on the available energy. We consider a qutrit system with the system Hamiltonian $H = E|1\rangle\langle 1| + 2E|2\rangle\langle 2|$. The initial thermal qutrit state is given by $\rho_T = p|0\rangle\langle 0| + (1-p-q)|1\rangle\langle 1| + q|2\rangle\langle 2|$ with average energy $\langle E\rangle_T = (1-p-q)E + 2qE$. Here $p = 1/Z$ and $q = e^{-2\beta E}/Z$, where $Z = 1 + e^{-\beta E} + e^{-2\beta E}$ is the partition function. The diagonal density matrix of the final state is a thermal qutrit state at temperature T' with average energy $\langle E\rangle'_T = (1-p-q)E + 2qE + \Delta E$, when we create coherence with ΔE energy constraint.

We show that just two successive rotations in two dimensions suffice the purpose of creating the maximum amount of coherence. For equal energy spacing of $\{0, E, 2E\}$, the average energy at infinite temperature is given by $\langle E\rangle_\infty = E$. So, for an arbitrary finite temperature, the condition $E > \langle E\rangle_T$ holds true. Thus for the aforementioned qutrit thermal system, with an increase in temperature, the occupation probabilities of the first and second excited states will always increase at the expense of a decrease in the occupation probability for the ground state. The diagonal elements of the final state should be the occupation probabilities of the thermal state at a higher temperature T', given by p', $1-p'-q'$, and q' for the ground, first excited, and second excited states, respectively. From the conservation of probabilities, it follows that

$$\begin{aligned} -\Delta p = p - p' &= (q'-q) + (1-p'-q') - (1-p-q) \\ &= \Delta q + \Delta(1-p-q). \end{aligned} \tag{17}$$

Note that we always have $-\Delta p > \Delta q > 0$.

Now, let us first apply a rotation about $|1\rangle$. Physically, this rotation creates coherence between basis states $|0\rangle$ and $|2\rangle$. The rotation can be expressed by the unitary $R_1(\alpha) = e^{-i\alpha J_1}$, where

$$J_1 = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix} \tag{18}$$

is the generator of the rotation. Then another rotation is applied about $|2\rangle$, which is given by $R_2(\delta) = e^{-i\delta J_2}$, where

$$J_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{19}$$

After the action of two successive rotations, given by $R_2(\delta)R_1(\alpha)$, we have

$$q' = q\cos^2\alpha + p\sin^2\alpha \tag{20}$$

and

$$p' = (q\sin^2\alpha + p\cos^2\alpha)\cos^2\delta + (1-p-q)\sin^2\delta$$
$$= (p-\Delta q)\cos^2\delta + (1-p-q)\sin^2\delta. \quad (21)$$

From Eq. (20), it is clear that q' is a convex combination of p and q, and since $q < q' < p$, there always exists an angle of rotation α, depending on the available energy, so that the protocol can be realized. The angle of rotation is given by $\alpha = \cos^{-1}\sqrt{\frac{p-q'}{p-q}}$, where $\alpha \in [0,\pi/2]$. Similarly, Eq. (21) suggests that p' is a convex combination of $(p-\Delta q)$ and $(1-p-q)$, and since $1-p-q < p' < p-\Delta q$ [Eq. (17)], one can always achieve any desired value of p' by suitably choosing $\delta \in [0,\pi/2]$, with $\delta = \cos^{-1}\sqrt{\frac{p'-(1-p-q)}{(p-\Delta q)-(1-p-q)}}$. Thus, maximal coherence at a finite energy cost can be created by two successive two-dimensional rotations starting from a thermal state of a qutrit system. Note that we have considered equal energy spacing $\{0,E,2E\}$, however, the above protocol will hold for any energy spacing for which the condition $E_1 > \langle E\rangle_T$ holds, where E_1 is the energy of the energy eigenstate $|1\rangle$.

IV. COHERENCE VERSUS CORRELATION

In this section we carry out a comparative study between maximal coherence creation and maximal total correlation creation (also see Ref. [16]) with limited available energy. We consider an arbitrary N-party system acting on a Hilbert space $\mathcal{H}^{d_1}\otimes\mathcal{H}^{d_2}\otimes\cdots\otimes\mathcal{H}^{d_N}$. The Hamiltonian of the composite system is noninteracting and given by $H_{\rm tot} = H_1 + H_2 + \cdots + H_N$. For the sake of simplicity, we consider $H_1 = H_2 = \cdots = H_N = H$. However, our results hold in general. Suppose there exists an optimal unitary operator U^* which creates the maximal total correlation from initial thermal state ρ_T with ΔE energy cost. It is shown in Ref. [16] that the maximal correlation (multipartite mutual information) that can be created by a unitary transformation with energy cost ΔE is given by

$$I_{\rm max}^{\Delta E} = \sum_i \left[S\left(\rho_{T'}^i\right) - S\left(\rho_T^i\right)\right]. \quad (22)$$

In the protocol to achieve the maximal correlation, the subsystems of the composite system ρ_T^N transform to the thermal states $\rho_{T'}^i$ of the corresponding individual systems at some higher temperature T' [16]. It is interesting to inquire how much coherence is created during this process, as in several quantum information processing tasks it may be necessary to create both the coherence and the correlation simultaneously. The amount of coherence created, $C_r|_{I_{\rm max}^{\Delta E}}$, when the unitary transformation creates the maximal correlation is given by

$$C_r|_{I_{\rm max}^{\Delta E}} = S\left(\rho_f^D\right) - \sum_i S\left(\rho_T^i\right). \quad (23)$$

As the Hamiltonian is noninteracting, ρ_f^D and the product of the marginals $(\prod^{\otimes i}\rho_{T'}^i)$ have the same average energy. Since the product of the marginals is the thermal state of the composite system at temperature T', the maximum entropy principle implies that $\sum_i S(\rho_{T'}^i) \geqslant S(\rho_f^D)$. Hence, $C_r|_{I_{\rm max}^{\Delta E}} \leqslant I_{\rm max}^{\Delta E}$. Therefore, when one aims for maximal correlation creation the coherence created is always bounded by the amount of correlation created. Now, we ask the converse, i.e., How much correlation can be created when one creates maximal coherence by a unitary operation with the same energy constraint ΔE? The maximal coherence that can be created in this scenario by unitary transformation with energy constraint is given by

$$C_{r,\rm max}^{\Delta E} = \sum_i \left[S\left(\rho_{T'}^i\right) - S\left(\rho_T^i\right)\right]. \quad (24)$$

Note that the maximal achievable coherence is equal to the maximal achievable correlation [cf. Eq. (22)], but the protocols to achieve them are completely different. When the maximal coherence is created, the diagonal of the final density matrix is a thermal state at some higher temperature, while the maximal correlation is created when the product of the marginals of the final state is a thermal state at some higher temperature. Therefore, when the maximum amount of coherence $C_{r,\rm max}^{\Delta E}$ is created, the correlation $I|_{C_{r,\rm max}^{\Delta E}}$ that is created simultaneously always satisfies

$$I|_{C_{r,\rm max}^{\Delta E}} \leqslant C_{r,\rm max}^{\Delta E}. \quad (25)$$

The above equation again follows from the maximum entropy principle and the fact that the diagonal part and the product of the marginals have the same average energy. Therefore, when one aims for maximal coherence creation, the amount of correlation that can be created at the same time is always bounded by the maximal coherence created, and vice versa.

It is also interesting to inquire whether one can create the maximal coherence and the maximal correlation simultaneously. In the following, we partially answer this question. For two-qubit systems we show no unitary transformation exists which maximizes both the coherence and the correlation simultaneously. Let the Hamiltonian of the two-qubit system be given by $H_{AB} = H_A + H_B$, with $H_A \neq H_B$, in general. Later, we also consider $H_A = H_B$. The initial state is the thermal state at temperature T and is given by

$$\rho_{AB,T} = \text{diag}\{pq, p(1-q), (1-p)q, (1-p)(1-q)\}, \quad (26)$$

where $p = 1/(1+e^{-\beta E_A})$, $q = 1/(1+e^{-\beta E_B})$, $H_A = E_A|1\rangle\langle 1|$, and $H_B = E_B|1\rangle\langle 1|$. Consider the protocol in Ref. [16] for creating the maximum correlation. In that scenario, the marginals are the thermal states at a higher temperature T'. Let the final state of the two-qubit system after the unitary transformation be given by

$$\rho_{AB}^f = \sum_{ijkl} a_{ijkl}|i\rangle\langle j|\otimes|k\rangle\langle l|. \quad (27)$$

As the marginals are thermal, $a_{iikl} = 0$ if $k \neq l$ and $a_{ijkk} = 0$ if $i \neq j$. Thus, the maximally correlated state that is created by investing a limited amount of energy is an X state [73], while for maximal coherence creation, the diagonal part of the final state is a thermal state at a higher temperature T'. Therefore, the diagonal part of the final state must be of the form

$$\rho_{AB,T'}^{fD} = \text{diag}\{p'q', p'(1-q'), (1-p')q', (1-p')(1-q')\},$$

where $p' = 1/(1+e^{-\beta' E_A})$, $q' = 1/(1+e^{-\beta' E_B})$, and $p' < p$ and $q' < q$ as $\beta' < \beta$. We show in the Appendix, separately for $E_A = E_B$ (Sec. 1) and $E_A \neq E_B$ (Sec. 2), that there is no such unitary transformation which serves the purpose. It will be interesting to explore what happens for higher dimensional systems.

V. CONCLUSION

In this article, we have studied the creation of quantum coherence by unitary transformations starting from a thermal state. This is important from a practical viewpoint, as most systems interact with the environment and get thermalized eventually. We find the maximal amount of coherence that can be created from a thermal state at a given temperature and find a protocol to achieve this. Moreover, we find the amount of coherence that can be created with limited available energy. Thus, our study establishes a link between coherence and thermodynamic resource theories and reveals the limitations imposed by thermodynamics on the processing of the coherence. Additionally, we have performed a comparative study between coherence creation and total correlation creation with the same amount of energy at our disposal. We show that when one creates the maximum coherence with limited energy, the total correlation created in the process is always upper bounded by the amount of coherence created, and vice versa. As correlation and coherence both are useful resources, processing them simultaneously is fruitful. However, our result shows that, at least in two-qubit systems, there is no way to create the maximal coherence and the maximal correlation simultaneously via unitary transformations. Recently, the importance of coherence for improving the performance of thermal machines has been explicitly established and the implications of coherence for the thermodynamic behavior of quantum systems have been studied. Therefore, it is justified to believe that the study of the thermodynamic cost and limitations of thermodynamic laws in the processing of quantum coherence can be far reaching. The results in this paper are a step in this direction.

ACKNOWLEDGMENTS

A.M., U.S., and S.B. acknowledge the research fellowship from the Department of Atomic Energy, Government of India.

APPENDIX: COHERENCE VS CORRELATION IN TWO-QUBIT SYSTEMS

Here, for two-qubit states with the Hamiltonian $H = H_A + H_B$, we show that maximum correlation and maximum coherence cannot be created simultaneously via a unitary transformation, starting from a thermal state with limited available energy. We consider the two cases where $E_A = E_B$ and $E_A \neq E_B$.

1. $E_A = E_B$

This is the case where the initial state is $\rho_T^{\otimes 2}$ with $\rho_T = \rho_T^A = \rho_T^B = \text{diag}\{p, 1-p\}$ and the final state is in the X-state form, given by

$$\rho_f = \begin{pmatrix} q^2 & 0 & 0 & Y \\ 0 & q(1-q) & X & 0 \\ 0 & X^* & q(1-q) & 0 \\ Y^* & 0 & 0 & (1-q)^2 \end{pmatrix}. \quad \text{(A1)}$$

Note that $p \geqslant q \geqslant 1/2 \geqslant (1-q) \geqslant (1-p)$. Here, $|Y| \leqslant q(1-q)$ and $|X| \leqslant q(1-q)$, so that ρ_f is positive semidefinite. Let $p = \frac{1}{2} + \epsilon$ and $q = \frac{1}{2} + \epsilon'$, where $\frac{1}{2} > \epsilon > \epsilon' > 0$. The eigenvalues of this final density matrix are given by

$$\lambda_{1,4} = \tfrac{1}{2}(q^2 + (1-q)^2 \pm \sqrt{(q^2 - (1-q)^2)^2 + 4|Y|^2}), \quad \text{(A2)}$$

$$\lambda_{2,3} = q(1-q) \pm |X|. \quad \text{(A3)}$$

As the unitary transformation preserves the eigenvalues, two of the eigenvalues of the final density matrix must be equal to $p(1-p)$ and the other two must be equal to p^2 and $(1-p)^2$, respectively.

a. Case 1

Let us first assume that $\lambda_2 = \lambda_3 = p(1-p)$. Then we find that $|X| = 0$ and $q = p$ or $q = 1 - p$. Since we know that $p \geqslant 1/2$, then $q \leqslant 1/2$ for $q = 1 - p$. Hence, $q \neq 1 - p$. $q = p$ can only happen under identity operation. Therefore, $\lambda_2 \neq \lambda_3$.

b. Case 2

Assume that $\lambda_1 = \lambda_4 = p(1-p)$; then we have

$$p(1-p) = \frac{q^2 + (1-q)^2}{2} + \frac{q^2 - (1-q)^2}{2} M = \frac{q^2 + (1-q)^2}{2} - \frac{q^2 - (1-q)^2}{2} M, \quad \text{(A4)}$$

where $M = \sqrt{1 + \frac{4|Y|^2}{(2q-1)^2}}$. From Eq. (A4), we have $M = 0$, which is a contradiction since $M \geqslant 1$. Therefore, Eq. (A4) cannot be satisfied.

c. Case 3

As $p^2 \geqslant p(1-p) \geqslant (1-p)^2$, two other possibilities are $\lambda_1 = \lambda_3 = p(1-p)$ and $\lambda_4 = \lambda_2 = p(1-p)$. Note that we always have $\lambda_1 > \lambda_3$. Therefore, the only possibility we have to check is $\lambda_4 = \lambda_2 = p(1-p)$. For this we have

$$\lambda_2 = p(1-p) \Rightarrow |X| = p(1-p) - q(1-q) \Rightarrow |X| = -(\epsilon^2 - \epsilon'^2), \quad \text{(A5)}$$

which is a contradiction, as the right-hand side is negative since $\epsilon > \epsilon'$. Therefore, it is also not possible.

2. $E_A \neq E_B$

Let us relabel the diagonal entries of the initial density matrix as

$$\rho_T^{AB} = a_1|00\rangle\langle 00| + a_2|01\rangle\langle 01| + a_3|10\rangle\langle 10| + a_4|11\rangle\langle 11|.$$

Here, $\{a_i\}$ is an arbitrary probability distribution that depends on the energy levels E_A and E_B and the initial temperature T.

We argue that the unitary transformations that map the initial state into an X state, starting from a two-qubit thermal state at arbitrary finite temperature T, are only allowed to create correlation among the subspaces spanned by $\{|00\rangle,|11\rangle\}$ and $\{|01\rangle,|10\rangle\}$, separately; i.e., no correlation can be created between these two subspaces. Thus, the unitary transformation that maximizes the total correlation acts on the blocks spanned by $\{|00\rangle,|11\rangle\}$ and $\{|01\rangle,|10\rangle\}$, separately. Given this, again from comparing eigenvalues, it can be argued that the total correlation and the coherence cannot be maximized simultaneously by unitary transformations in two-qubit systems when the Hamiltonians of the systems are not the same.

[1] R. Horodecki, P. Horodecki, M. Horodecki, and K. Horodecki, Rev. Mod. Phys. **81**, 865 (2009).
[2] J. Åberg, arXiv:quant-ph/0612146.
[3] T. Baumgratz, M. Cramer, and M. B. Plenio, Phys. Rev. Lett. **113**, 140401 (2014).
[4] I. Marvian and R. W. Spekkens, Phys. Rev. A **90**, 062110 (2014).
[5] G. Gour and R. W. Spekkens, New J. Phys. **10**, 033023 (2008).
[6] R. Alicki and M. Fannes, Phys. Rev. E **87**, 042123 (2013).
[7] K. V. Hovhannisyan, M. Perarnau-Llobet, M. Huber, and A. Acín, Phys. Rev. Lett. **111**, 240401 (2013).
[8] N. Brunner, M. Huber, N. Linden, S. Popescu, R. Silva, and P. Skrzypczyk, Phys. Rev. E **89**, 032115 (2014).
[9] J. Roßnagel, O. Abah, F. Schmidt-Kaler, K. Singer, and E. Lutz, Phys. Rev. Lett. **112**, 030602 (2014).
[10] L. A. Correa, J. P. Palao, D. Alonso, and G. Adesso, Sci. Rep. **4**, 3949 (2014).
[11] R. Gallego, A. Riera, and J. Eisert, New J. Phys. **16**, 125009 (2014).
[12] F. Galve and E. Lutz, Phys. Rev. A **79**, 032327 (2009).
[13] A. Carlisle, L. Mazzola, M. Campisi, J. Goold, F. L. Semião, A. Ferraro, F. Plastina, V. Vedral, G. De Chiara, and M. Paternostro, arXiv:1403.0629.
[14] V. Scarani, M. Ziman, P. Štelmachovič, N. Gisin, and V. Bužek, Phys. Rev. Lett. **88**, 097905 (2002).
[15] J. Eisert, M. B. Plenio, S. Bose, and J. Hartley, Phys. Rev. Lett. **93**, 190402 (2004).
[16] M. Huber, M. Perarnau-Llobet, K. V. Hovhannisyan, P. Skrzypczyk, C. Klöckl, N. Brunner, and A. Acín, New J. Phys. **17**, 065008 (2015).
[17] D. E. Bruschi, M. Perarnau-Llobet, N. Friis, K. V. Hovhannisyan, and M. Huber, Phys. Rev. E **91**, 032118 (2015).
[18] S. Vinjanampathy and J. Anders, arXiv:1508.06099.
[19] J. Goold, M. Huber, A. Riera, L. del Rio, and P. Skrzypczyk, J. Phys. A: Math. Theor. **49**, 143001 (2016).
[20] P. Kammerlander and J. Anders, Sci. Rep. **6**, 22174 (2016).
[21] M. Perarnau-Llobet, K. V. Hovhannisyan, M. Huber, P. Skrzypczyk, N. Brunner, and A. Acín, Phys. Rev. X **5**, 041011 (2015).
[22] K. Korzekwa, M. Lostaglio, J. Oppenheim, and D. Jennings, New J. Phys. **18**, 023045 (2016).
[23] M. Lostaglio, K. Korzekwa, D. Jennings, and T. Rudolph, Phys. Rev. X **5**, 021001 (2015).
[24] M. Lostaglio, D. Jennings, and T. Rudolph, Nat. Commun. **6**, 6383 (2015).
[25] K. Maruyama, F. Nori, and V. Vedral, Rev. Mod. Phys. **81**, 1 (2009).
[26] L. del Rio, J. Aberg, R. Renner, O. Dahlsten, and V. Vedral, Nature **474**, 61 (2011).
[27] F. G. S. L. Brandão, M. Horodecki, J. Oppenheim, J. M. Renes, and R. W. Spekkens, Phys. Rev. Lett. **111**, 250404 (2013).
[28] M. Horodecki and J. Oppenheim, Int. J. Mod. Phys. B **27**, 1345019 (2013).
[29] F. Brandão, M. Horodecki, N. Ng, J. Oppenheim, and S. Wehner, Proc. Natl. Acad. Sci. USA **112**, 3275 (2015).
[30] G. S. Engel, T. R. Calhoun, E. L. Read, T.-K. Ahn, T. Mancal, Y.-C. Cheng, R. E. Blankenship, and G. R. Fleming, Nature **446**, 782 (2007).
[31] S. Lloyd, J. Phys.: Conf. Ser. **302**, 012037 (2011).
[32] E. Collini, C. Y. Wong, K. E. Wilk, P. M. G. Curmi, P. Brumer, and G. D. Scholes, Nature **463**, 644 (2010).
[33] N. Lambert, Y.-N. Chen, Y.-C. Cheng, C.-M. Li, G.-Y. Chen, and F. Nori, Nat. Phys. **9**, 10 (2013).
[34] A. W. Chin, S. F. Huelga, and M. B. Plenio, Philos. Trans. Roy. Soc. London A: Math. Phys. Eng. Sci. **370**, 3638 (2012).
[35] M. T. Mitchison, M. P. Woods, J. Prior, and M. Huber, New J. Phys. **17**, 115013 (2015).
[36] V. Narasimhachar and G. Gour, Nat. Commun. **6**, 7689 (2015).
[37] A. Streltsov, arXiv:1511.08346.
[38] B. Yadin, J. Ma, D. Girolami, M. Gu, and V. Vedral, arXiv:1512.02085.
[39] A. Streltsov, U. Singh, H. S. Dhar, M. N. Bera, and G. Adesso, Phys. Rev. Lett. **115**, 020403 (2015).
[40] M. N. Bera, T. Qureshi, M. A. Siddiqui, and A. K. Pati, Phys. Rev. A **92**, 012118 (2015).
[41] R. Angelo and A. Ribeiro, Found. Phys. **45**, 1407 (2015).
[42] U. Singh, M. N. Bera, H. S. Dhar, and A. K. Pati, Phys. Rev. A **91**, 052115 (2015).
[43] L.-H. Shao, Z. Xi, H. Fan, and Y. Li, Phys. Rev. A **91**, 042120 (2015).
[44] D. P. Pires, L. C. Céleri, and D. O. Soares-Pinto, Phys. Rev. A **91**, 042330 (2015).
[45] S. Du, Z. Bai, and Y. Guo, Phys. Rev. A **91**, 052120 (2015).
[46] Y. Yao, X. Xiao, L. Ge, and C. P. Sun, Phys. Rev. A **92**, 022112 (2015).
[47] Z. Xi, Y. Li, and H. Fan, Sci. Rep. **5**, 10922 (2015).
[48] D. Girolami, Phys. Rev. Lett. **113**, 170401 (2014).
[49] T. R. Bromley, M. Cianciaruso, and G. Adesso, Phys. Rev. Lett. **114**, 210401 (2015).
[50] N. Killoran, F. E. S. Steinhoff, and M. B. Plenio, Phys. Rev. Lett. **116**, 080402 (2016).
[51] L. Zhang, A. K. Pati, and J. Wu, Phys. Rev. A **92**, 022316 (2015).
[52] U. Singh, M. N. Bera, A. Misra, and A. K. Pati, arXiv:1506.08186.
[53] S. Cheng and M. J. W. Hall, Phys. Rev. A **92**, 042101 (2015).
[54] D. Mondal, T. Pramanik, and A. K. Pati, arXiv:1508.03770.
[55] D. Mondal, C. Datta, and S. K. Sazim, Phys. Lett. A **380**, 689 (2016).
[56] A. Kumar, arXiv:1508.00262.
[57] A. Mani and V. Karimipour, Phys. Rev. A **92**, 032331 (2015).

[58] K. Bu, L. Zhang, and J. Wu, arXiv:1509.09109.
[59] E. Chitambar, A. Streltsov, S. Rana, M. N. Bera, G. Adesso, and M. Lewenstein, Phys. Rev. Lett. **116**, 070402 (2016).
[60] E. Chitambar and M.-H. Hsieh, arXiv:1509.07458.
[61] K. Bu, U. Singh, and J. Wu, Phys. Rev. A **93**, 042326 (2016).
[62] A. Streltsov, S. Rana, M. Nath Bera, and M. Lewenstein, arXiv:1509.07456.
[63] E. Chitambar and G. Gour, arXiv:1602.06969.
[64] I. Marvian and R. W. Spekkens, arXiv:1602.08049.
[65] Y. Peng, Y. Jiang, and H. Fan, Phys. Rev. A **93**, 032326 (2016).
[66] A. Winter and D. Yang, Phys. Rev. Lett. **116**, 120404 (2016).
[67] E. T. Jaynes, Phys. Rev. **106**, 620 (1957).
[68] E. T. Jaynes, Phys. Rev. **108**, 171 (1957).
[69] A $d \times d$ matrix $M = (M_{ab})(a \in \{1,\ldots,d\}, b \in \{1,\ldots,d\}$, and $M_{ab} \geqslant 0)$ is called a doubly stochastic matrix if $\sum_a M_{ab} = 1$ for all b and $\sum_b M_{ab} = 1$ for all a [71] .
[70] N. Canosa, R. Rossignoli, and M. Portesi, Physica A: Stat. Mech. Appl. **368**, 435 (2006).
[71] R. Bhatia, *Matrix Analysis* (Springer-Verlag, New York, 1997).
[72] Consider a $d \times d$ real orthogonal matrix $O = (O_{ab})$ $(a \in \{1,\ldots,d\}$, $b \in \{1,\ldots,d\}$, and $O_{ab} \geqslant 0)$ such that $O^T O = \mathbb{I}$. Here the superscript T denotes the transpose and $\mathbb{I}$ is a $d \times d$ identity matrix. The matrix (O_{ab}^2) forms a doubly stochastic matrix and such a matrix is called an orthostochastic matrix [71].
[73] X states are a special class of states that have been analyzed in great detail in the context of analytical calculations of quantum discord [74,75] among others. The term X states was coined in Ref. [76], for their visual appearance. For bipartite qubit quantum systems, states ρ_X of the form

$$\rho_X := \begin{pmatrix} \rho_{00} & 0 & 0 & \rho_{03} \\ 0 & \rho_{11} & \rho_{12} & 0 \\ 0 & \rho_{21} & \rho_{22} & 0 \\ \rho_{30} & 0 & 0 & \rho_{33} \end{pmatrix}$$

are called X states. In general, any density matrix that has nonzero elements only at the diagonals and antidiagonals is called an X state. For a detailed exposition of X states see Ref. [77].
[74] L. Henderson and V. Vedral, J. Phys. A: Math. Gen. **34**, 6899 (2001).
[75] H. Ollivier and W. H. Zurek, Phys. Rev. Lett. **88**, 017901 (2001).
[76] T. Yu and J. H. Eberly, Quantum Info. Comput. **7**, 459 (2007).
[77] A. R. P. Rau, J. Phys. A: Math. Theor. **42**, 412002 (2009).