# Role of quantum coherence in the thermodynamics of energy transfer

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Recent research on the thermodynamic arrow of time, at the microscopic scale, has questioned the universality of its direction. Theoretical studies showed that quantum correlations can be used to revert the natural heat flow (from the hot body to the cold one), posing an apparent challenge to the second law of thermodynamics. Such an "anomalous" heat current was observed in a recent experiment (K. Micadei *et al.*, arXiv:1711.03323), by employing two spin systems initially quantum correlated. Nevertheless, the precise relationship between this intriguing phenomenon and the initial conditions that allow it is not fully evident. Here, we address energy transfer in a wider perspective, identifying a nonclassical contribution that applies to the reversion of the heat flow as well as to more general forms of energy exchange. We derive three theorems that describe the energy transfer between two microscopic systems, for arbitrary initial bipartite states. Using these theorems, we obtain an analytical bound showing that certain type of quantum coherence can optimize such a process, outperforming incoherent states. This genuine quantum advantage is corroborated through a characterization of the energy transfer between two qubits. For this system, it is shown that a large enough amount of coherence is necessary and sufficient to revert the thermodynamic arrow of time. As a second crucial consequence of the presented theorems, we introduce a class of nonequilibrium states that only allow unidirectional energy flow. In this way, we broaden the set where the standard Clausius statement of the second law applies.

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## I. INTRODUCTION

Since Carnot discovered the fundamental limit that governs the efficiency of heat engines, the second law of thermodynamics has been discussed and explored in different ways. One of them refers to the celebrated Clausius statement that heat must flow from a hot system to a cold one, when the whole system is isolated. This preferred direction of the heat flux may be interpreted as a "thermodynamic arrow" that characterizes the time ordering of physical events [1–3]. More recently, developments on quantum thermodynamics have allowed the thermodynamic description of microscopic quantum systems. Fluctuation relations [4,5] and information-theory inspired approaches [6–9] represent powerful tools to carry out this task. These new paradigms, which refer to systems that start in a nonequilibrium state or that undergo a nonequilibrium dynamics, have led to some generalizations of the second law beyond the scope of standard thermodynamics [10–13]. They also establish new connections between thermodynamics and information theory [14,15], enabling a formal treatment of Maxwell's demon and related subjects [16–19]. On the experimental side, crucial advances have been achieved to access and characterize energy fluctuations in microscopic systems [20–30].

Among the plethora of results obtained on quantum thermodynamics, many of them center on the concept of work [31,32], and its interplay with other thermodynamic variables such as entropy production [33]. The process of heat exchange between two finite-size systems is a less studied phenomenon. While for two quantum systems in an initially uncorrelated state the Clausius statement holds [34], the same may not be true for initially correlated bodies [34,35]. This assertion has been corroborated in a recent experiment using a two-spin system embedded in a nuclear magnetic resonance setup [36]. However, a comprehensive description of such a behavior is lacking. Of particular interest is to unveil the role played by quantum properties, e.g., coherence or entanglement, in the reversion of the thermodynamic arrow of time. In this respect, a fluctuation relation for heat exchange in the presence of classical correlations was derived and discussed in Ref. [37]. The performance of quantum coherence has been analyzed in the context of work extraction [38–42], entropy production [43,44], and Landauer's erasure [45]. Other investigations focus on how coherence transforms under thermodynamic operations [46–48], without intending to assign it some operational meaning.

In this paper, we investigate the physical process of energy exchange between two microscopic systems, consistently with the first law of thermodynamics [49]. To this aim, we present in Sec. II three theorems that describe the transfer of average energy induced by unitary and energy-conserving evolutions. These theorems are valid for arbitrary bipartite states, allowing to incorporate heat exchange (i.e., when each system starts at thermal equilibrium) as a particular case. Two fundamental consequences are derived from such theorems. First, we establish in Sec. III that quantum coherence (in the

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eigenbasis of the free joint Hamiltonian) potentially enhances the energy transfer, under an optimal evolution. Specifically, it is shown that the maximum energy transfer for an incoherent initial state is upper bounded by the obtained one when coherence of certain type is included. In Sec. IV we deduce a class of states for which the energy flow occurs in a single direction. This set contains all the tensor products between thermal states, according to the Clausius statement of the second law, but is not restricted to them. To illustrate our findings, Sec. V provides a characterization of the energy exchange between two qubits. We verify that, for an optimal dynamics, the energy transfer is maximized only if enough initial "useful" coherence is available. This quantum feature is further responsible for reverting the heat flow between thermal qubits, which constitutes a comprehensive framework for the experimental results reported in [36]. We also obtain a linear relation between the maximum energy transfer and the concurrence, for entangled Bell-diagonal states [50,51]. It is shown that a quantum enhancement results from a subset of separable states within this class. Section VI presents the conclusions and some possible paths for future research.

## II. ENERGY EXCHANGE UNDER STRONG ENERGY-CONSERVING (SEC) UNITARIES

Let us consider two quantum systems $A$ and $B$, with nondegenerate and discrete Hamiltonians $H_A$ and $H_B$, respectively. We adopt "energy conservation" according to the condition $[U,H]=0$, where $H=H_A+H_B$ is the total *free* Hamiltonian and $U$ is a unitary map generated by some interaction Hamiltonian $H_I$. This is equivalent to demand that $U$ preserves the sum of the local energies for any initial joint state $\rho$: $\mathrm{Tr}(HU\rho U^\dagger)=\mathrm{Tr}(H\rho)$. Hence, we say that $U$ is "strong energy conserving" (SEC). For small systems, the strength of the interaction energy may be of the same order of the local energies. Therefore, it is not evident how to physically implement $U$, as even for $H_I$ constant we can only guarantee that the total energy (including the contribution from $H_I$) is preserved. A sufficient condition for $U$ to be SEC comes from the relation $[H,H_I]=0$ [52]. The resonant Jaynes-Cummings model [53] exemplifies a well known system that fulfills this requirement. If, in addition, we assume that the total Hamiltonian at the beginning and at the end of the energy exchange process is $H$, the local energies become well defined quantities. It is worth remarking that the adopted definition constitutes a paradigmatic approach to the first law of thermodynamics in microscopic systems (see, e.g., [15,31] and references therein).

Without loss of generality, the state $\rho$ can be written as

$$\rho=\rho_{\mathrm{Diag}}+\chi, \tag{1}$$

where $\rho_{\mathrm{Diag}}$ and $\chi$ are the diagonal part and the coherent (off-diagonal) part of $\rho$ in the eigenbasis of $H$, respectively. Each eigenstate of $H$ with eigenvalue $E$ has the form $|i_E\rangle_A|j_E\rangle_B$, where $|i_E\rangle_A$ and $|j_E\rangle_B$ are local energy eigenstates satisfying $H_A|i_E\rangle_A=\varepsilon_{i_E}|i_E\rangle_A$, $H_B|j_E\rangle_B=\bar{\varepsilon}_{j_E}|j_E\rangle_B$, and $\varepsilon_{i_E}+\bar{\varepsilon}_{j_E}=E$. For $E$ fixed, the relation $\varepsilon_{i_E}+\bar{\varepsilon}_{j_E}=E$ and the nondegeneracy of the local Hamiltonians imply a one-to-one correspondence between $i_E$ and $j_E$. This means that for each $i_E$ there is only one $j_E$ that fulfills this equation and vice versa. In this way, we can completely characterize the spectrum of $H$ by using the total energy index $(E)$ and a single local energy index. Choosing by convention the index $i_E$, the resulting set is denoted as $\{|i_E,E\rangle\}_{i_E,E}$, where $H|i_E,E\rangle=E|i_E,E\rangle$ and $H_A|i_E,E\rangle=\varepsilon_{i_E}|i_E,E\rangle$. This notation provides a natural decomposition into subspaces of fixed energy $E$, very suitable for the analysis of SEC unitaries.

Now, we explicitly write $\rho_{\mathrm{Diag}}$ and $\chi$ in the eigenbasis $\{|i_E,E\rangle\}$. For $\rho_{\mathrm{Diag}}$ we have

$$\rho_{\mathrm{Diag}}=\sum_E p_E\rho_{\mathrm{Diag}}(E), \tag{2}$$

where $\rho_{\mathrm{Diag}}(E)\equiv\sum_{i_E}\frac{p(\varepsilon_{i_E},E)}{p_E}\Pi_{i_E}^{(E)}$ and $\Pi_{i_E}^{(E)}\equiv|i_E,E\rangle\langle i_E,E|$. The joint probability to measure energy $\varepsilon_{i_E}$ for system $A$ and total energy $E$ is given by $p(\varepsilon_{i_E},E)$. Accordingly, $p_E=\sum_{i_E}p(\varepsilon_{i_E},E)$ is the total probability to measure joint energy equal to $E$. On the other hand,

$$\chi=\sum_{E,E'}\chi(E,E'), \tag{3}$$

where $\chi(E,E')\equiv\sum_{i_E,j_{E'}:i_E\neq j_{E'}\text{ or }E\neq E'}\alpha_{i_E,j_{E'}}^{(E,E')}\Pi_{i_E,j_{E'}}^{(E,E')}$ and $\Pi_{i_E,j_{E'}}^{(E,E')}\equiv|i_E,E\rangle\langle j_{E'},E'|$ [54].

The energy transfer to the system $\gamma$ ($\gamma=A,B$) is denoted as $\Delta\langle H_\gamma\rangle$ and represents the average energy variation undergone by this system, through the application of a SEC unitary $U$. If the initial joint state is $\rho$, then $\Delta\langle H_\gamma\rangle=\mathrm{Tr}(H_\gamma U\rho U^\dagger)-\mathrm{Tr}(H_\gamma\rho)$. Taking into account Eq. (1), this quantity is given by

$$\Delta\langle H_\gamma\rangle=\Delta_{\mathrm{Diag}}\langle H_\gamma\rangle+\Delta_{\mathrm{Coh}}\langle H_\gamma\rangle, \tag{4}$$

where $\Delta_{\mathrm{Diag}}\langle H_\gamma\rangle\equiv\mathrm{Tr}(H_\gamma U\rho_{\mathrm{Diag}}U^\dagger)-\mathrm{Tr}(H_\gamma\rho_{\mathrm{Diag}})$ and $\Delta_{\mathrm{Coh}}\langle H_\gamma\rangle\equiv\mathrm{Tr}(H_\gamma U\chi U^\dagger)-\mathrm{Tr}(H_\gamma\chi)$ are the "diagonal energy transfer" and the "coherent energy transfer," respectively.

Definitions 1–3 set the framework for the presentation of Theorems 1–3. These theorems characterize the energy transfer for arbitrary initial states and are pivotal in the derivation of subsequent results. The corresponding proofs are given Appendix A, in order to focus on their physical aspect.

*Definition 1.* From the eigenspace $\mathcal{H}_E\equiv\mathrm{span}\{|i_E,E\rangle\}_{i_E}$, spanned by all the joint eigenstates with eigenenergy $E$, we introduce the $E$-local subspace of system $A$, $\mathcal{H}_E^A\equiv\mathrm{span}\{|i_E\rangle_A\}$. A state $\varrho^A(E)$ with eigenvectors $|\varphi_i^E\rangle_A\in\mathcal{H}_E^A$ is called an $E$-local state of system $A$. In addition, an $E$-local unitary $U_E^A$ is a unitary that maps the subspace $\mathcal{H}_E^A$ into itself, and is exclusively defined on this subspace.

*Definition 2.* The requirement that a SEC $U$ preserves the total energy for any state $\rho$ is equivalent to demand that it does so for any joint energy eigenstate $|i_E,E\rangle$. That is, $U$ must transform $|i_E,E\rangle$ into a superposition of eigenstates having equal total energies: $U|i_E,E\rangle\equiv\sum_{j_E}c_{i_E,j_E}^{(E)}|j_E,E\rangle$. Taking into account that the action of $U$ is arbitrary within each eigenspace $\mathcal{H}_E$, for any $E$ the coefficients $\{c_{i_E,j_E}^{(E)}\}$ allow to construct an arbitrary $E$-local unitary: $U_E^A|i_E\rangle_A\equiv\sum_{j_E}c_{i_E,j_E}^{(E)}|j_E\rangle_A$.

*Definition 3. (Restricted passivity).* Any $E$-local state $\varrho^A(E)=\sum_i q_i|\varphi_i^E\rangle_A\langle\varphi_i^E|$ can be transformed by an $E$-local unitary in the state $\varrho_P^A(E)=\sum_{i_E}q_{i_E}|i_E\rangle_A\langle i_E|$, where $q_{i_E}\geqslant q_{i'_E}$ implies that $\varepsilon_{i_E}<\varepsilon_{i'_E}$, for any $i_E,i'_E$. We say that $\varrho_P^A(E)$ is $E$ passive, or passive *within* $\mathcal{H}_E^A$. Physically, this means that

$\varrho_P^A(E)$ is the state of minimum energy, that can be attained from $\varrho^A(E)$ through an $E$-local unitary. Analogously, the maximum energy state that results from applying an $E$-local unitary on $\varrho^A(E)$ is $\varrho_M^A(E) = \sum_{i_E} q_{i_E} |i_E\rangle_A\langle i_E|$, such that $q_{i_E} \geqslant q_{i'_E}$ implies $\varepsilon_{i_E} > \varepsilon_{i'_E}$, for any $i_E, i'_E$ [55].

*Theorem 1*. Let $\rho^A_{\mathrm{Diag}}(E) \equiv \mathrm{Tr}_B \rho_{\mathrm{Diag}}(E)$ be an $E$-local state defined through Eq. (2). Under the effect of a SEC unitary $U$, the diagonal energy transfer to system $A$ is given by $\Delta_{\mathrm{Diag}}\langle H_A\rangle = \sum_E p_E \mathrm{Tr}_A(H_A U_E^A \rho^A_{\mathrm{Diag}}(E) U_E^{A\dagger} - H_A \rho^A_{\mathrm{Diag}}(E))$.

*Physical relevance*. This theorem allows us to straightforwardly establish the possible values for the diagonal energy transfer. Since any $E$-local unitary $U_E^A$ is arbitrary on $\mathcal{H}_E^A$, according to Definition 2, the minimum (maximum) of $\Delta_{\mathrm{Diag}}\langle H_A\rangle$ is determined by separately minimizing (maximizing) each term $\mathrm{Tr}_A(H_A U_E^A \rho^A_{\mathrm{Diag}}(E) U_E^{A\dagger})$ with respect to $U_E^A$. From Definition 3, these extremal values are attained when $U_E^A \rho^A_{\mathrm{Diag}}(E) U_E^{A\dagger}$ is an $E$-passive state (minimum), or a maximum energy $E$-local state (maximum). The corresponding optimal SEC $U$ is readily obtained by means of Definition 2. Theorem 1 is also fundamental for the proof of Theorem 3 (see Appendix A).

*Theorem 2*. Under the effect of a SEC unitary $U$, the coherent energy transfer to system $A$ is given by $\Delta_{\mathrm{Coh}}\langle H_A\rangle = \sum_k \eta_k \varepsilon_k$, where $\{\varepsilon_k\}$ are the eigenvalues of $H_A$ and $\eta_k \equiv 2\sum'_E \sum_{i_E<j_E} \mathrm{Re}(\alpha^{(E,E)}_{i_E,j_E} c^{(E)}_{i_E,k} c^{(E)*}_{j_E,k})$. For $k$ fixed, the sum $\sum'_E$ is restricted to values of $E$ satisfying $E = \varepsilon_k + \bar{\varepsilon}_{l_E}$, where $\bar{\varepsilon}_{l_E}$ is an eigenvalue of $H_B$ (this implies $k \in \{k_E\}$).

*Physical relevance*. The coefficients $\eta_k$ embody an interplay between the coefficients of coherence $\alpha^{(E,E)}_{i_E,j_E}$ and the $c^{(E)}_{i_E,k_E}$, which describe the action of $U$. In particular, they are independent of $\alpha^{(E,E')}_{i_E,j_{E'}}$, for $E \neq E'$. In this way, this theorem singles out the kind of coherence that may contribute to the energy transfer, corresponding to those terms $\chi(E,E')$ with $E = E'$ in Eq. (3). The corollary below states a necessary condition on $U$ to get a non-null coherent energy transfer.

*Corollary 2.1*. Any SEC unitary with the potential to yield $\Delta_{\mathrm{Coh}}\langle H_A\rangle \neq 0$ must belong to the following set: $\{\mathcal{U}\} \equiv \{U$: there exists $c^{(E)}_{i_E,k_E} c^{(E)*}_{j_E,k_E} \neq 0$, for $i_E \neq j_E\}$. If $c^{(E)}_{i_E,k_E} c^{(E)*}_{j_E,k_E} \neq 0$, Definition 2 implies that $\mathcal{U}$ must transform $|i_E,E\rangle$ and $|j_E,E\rangle$ in superpositions of energy eigenstates (there also exist $c^{(E)}_{i_E,l_E} \neq 0$ and $c^{(E)}_{j_E,l_E} \neq 0$, for $l_E \neq k_E$). Otherwise, $\langle j_E,E|\mathcal{U}^\dagger\mathcal{U}|i_E,E\rangle = c^{(E)}_{i_E,k_E} c^{(E)*}_{j_E,k_E} \neq 0$ and $\mathcal{U}$ would not be unitary.

*Theorem 3*. For $\rho$ arbitrary, the SEC unitary $\tilde{U}$ that maximizes $\Delta_{\mathrm{Diag}}\langle H_\gamma\rangle$ is such that $\Delta_{\mathrm{Coh}}\langle H_\gamma\rangle = 0$ [56].

## III. ROLE OF QUANTUM COHERENCE IN THE ENERGY-TRANSFER OPTIMIZATION

The physical impact of Theorem 3 will now become apparent. We start by pointing out that the coherences in $\rho$ do not contribute to the initial local energies, namely, $\mathrm{Tr}(H_\gamma \chi) = \mathrm{Tr}_\gamma(H_\gamma \mathrm{Tr}_{\gamma'}\chi) = 0$ for any $\rho$, where $\gamma' = B$ if $\gamma = A$ and vice versa (the reason for this equality being that $\mathrm{Tr}_{\gamma'}\chi$ can not yield diagonal elements in the eigenbasis of $H_\gamma$). Therefore, the same amount of energy, $\mathrm{Tr}(H_\gamma \rho_{\mathrm{Diag}})$, is initially available in the states $\rho$ and $\rho_{\mathrm{Diag}}$ to be exchanged. Such a property allows us to perform an unbiased comparison between these states, in order to assess the role that coherence plays in this task. We find that indeed coherence is a potential resource to optimize the energy transfer. This is expressed by means of the inequality

$$\max_{\{U\}} \Delta\langle H_\gamma\rangle \geqslant \max_{\{U\}} \Delta_{\mathrm{Diag}}\langle H_\gamma\rangle, \tag{5}$$

where $\{U\}$ is the full set of SEC unitaries.

From Eq. (4) and Theorem 3 it follows that, for $U = \tilde{U}$, $\Delta\langle H_\gamma\rangle = \max_{\{U\}}\Delta_{\mathrm{Diag}}\langle H_\gamma\rangle$, which immediately implies Eq. (5). It is worth remarking that the right hand side of this inequality can be readily computed by means of Theorem 1. To apply it, we just need to decompose the local state $\rho^\gamma_{\mathrm{Diag}} = \mathrm{Tr}_{\gamma'}(\rho_{\mathrm{Diag}})$ into $E$-local states: $\rho^\gamma_{\mathrm{Diag}} = \sum_E p_E \rho^\gamma_{\mathrm{Diag}}(E) = \sum_E p_E \mathrm{Tr}_{\gamma'}\rho_{\mathrm{Diag}}(E)$. Theorem 2 provides a necessary condition on the initial coherence, to obtain an enhancement in the energy transfer [corresponding to the strict inequality in Eq. (5)]. Moreover, Corollary 2.1 tells us that such a resource can only be exploited by some unitary in the set $\{\mathcal{U}\}$. We shall later corroborate this quantum thermodynamic signature in the special case of two interacting qubits.

## IV. STATES THAT ONLY ALLOW ENERGY FLOW IN ONE DIRECTION

Let us introduce the following set of states:

$$\{\sigma^{(A\leftarrow B)}\} = \big\{\rho\text{: } \rho^A_{\mathrm{Diag}}(E) \text{ is passive within } \mathcal{H}_E^A \text{ and } \chi(E,E) = 0, \text{ for all } E\big\}. \tag{6}$$

If $\rho \in \{\sigma^{(A\leftarrow B)}\}$, the energy flow for any SEC unitary occurs from system $B$ to system $A$ (hence the notation $A \leftarrow B$). The condition of $E$ passivity for any $\rho^A_{\mathrm{Diag}}(E)$ is necessary and sufficient to have a unidirectional diagonal energy transfer. In this case, Theorem 1 implies that the energy associated to each term in the sum for $\Delta_{\mathrm{Diag}}\langle H_A\rangle$ can never decrease. Conversely, if $\rho^A_{\mathrm{Diag}}(E')$ is not $E'$ passive on the $E$-local subspace $\mathcal{H}^A_{E'}$, we can choose a set of $E$-local unitaries $\{U_E^A\}$ such that $U^A_{E'}$ reduces the energy of $\rho^A_{\mathrm{Diag}}(E')$ while the remaining unitaries are the identity in the corresponding subspaces (for $E \neq E'$). Theorem 2 guarantees that, for a state $\rho$ containing only coherences of the form $\chi(E,E')$, with $E \neq E'$, $\Delta\langle H_A\rangle = \Delta_{\mathrm{Diag}}\langle H_A\rangle$. Therefore, the total energy transfer to system $A$ is always positive for the states defined in Eq. (6). On the other hand, we can not assert that this equation encompasses all the states manifesting unidirectional energy flow. If coherences $\chi(E,E) \neq 0$ are present in $\rho$, answering this question requires the more involved task of determining the sign of $\Delta\langle H_A\rangle$.

The Clausius statement of the second law of thermodynamics applies to uncorrelated states $\rho^A_{\beta_A} \otimes \rho^B_{\beta_B}$, where $\rho^\gamma_{\beta_\gamma}$ is a thermal equilibrium state at inverse temperature $\beta_\gamma$ [34]. For the sake of consistency, we prove in Appendix B that, for $\beta_A > \beta_B$, any such state belongs to $\{\sigma^{(A\leftarrow B)}\}$. However, Eq. (6) evidently extends the scope of this statement, as it includes states with coherences of the type $\chi(E,E')$. To further support this generality, we show in the aforementioned appendix that any tensor product between a passive state [57,58] of system $A$ and a maximally active state [59] of system $B$ also belongs to $\{\sigma^{(A\leftarrow B)}\}$.

## V. CHARACTERIZATION OF THE ENERGY EXCHANGE BETWEEN TWO QUBITS

We consider here two qubits with identical Hamiltonians $H_\gamma = \hbar\omega|1\rangle_\gamma\langle 1| = |1\rangle_\gamma\langle 1|$, where we set $\hbar\omega = 1$ for simplicity and $|1\rangle_\gamma$ ($|0\rangle_\gamma$) represents the excited (ground) state of qubit $\gamma$. This condition ensures that a SEC unitary acts nontrivially on the energy eigenspace $\mathcal{H}_{E=1}$. From Theorem 2, only the coherences $\chi(1,1)$ may contribute to the energy transfer. Therefore, a potential quantum advantage results from states $\rho = \rho_{\text{Diag}} + \chi(1,1)$, where $|\alpha^{(1)}_{0,1}|^2 \equiv |\alpha^{(1,1)}_{0,1}|^2 \leqslant p_{0,1}p_{1,0}$ [54] and $p_{i,j} = \text{Tr}(|i\rangle_A\langle i| \otimes |j\rangle_B\langle j|\rho)$ [cf. Eqs. (2) and (3)]. The description of $\Delta_{\text{Diag}}\langle H_\gamma\rangle$ and $\Delta_{\text{Coh}}\langle H_\gamma\rangle$ is embodied by two real parameters, $0 \leqslant r \leqslant 1$ and $0 \leqslant \phi \leqslant 2\pi$, associated to an arbitrary SEC unitary. These quantities are obtained (without loss of generality) for system $A$ in Appendix C, yielding

$$\Delta_{\text{Diag}}\langle H_A\rangle = (p_{0,1} - p_{1,0})r^2 = \left(p_1^B - p_1^A\right)r^2, \tag{7}$$

$$\Delta_{\text{Coh}}\langle H_A\rangle = 2\,\text{Re}\left(\alpha^{(1)}_{0,1}e^{i\phi}\right)r\sqrt{1-r^2}, \tag{8}$$

where $p_1^\gamma = \text{Tr}(|1\rangle_\gamma\langle 1|\rho)$ is the excited population for qubit $\gamma$.

The optimization of $\Delta\langle H_\gamma\rangle$ is carried out in Appendix D. We find that

$$\Delta\langle H_\gamma\rangle_{\max} = \max_{\{U;\alpha^{(1)}_{0,1}\}}\Delta\langle H_\gamma\rangle = \mu_\gamma, \tag{9}$$

where $\mu_A = p_{0,1}$, $\mu_B = p_{1,0}$, and the maximum corresponds to a state of maximum coherence, given by $|\alpha^{(1)}_{0,1}| = \sqrt{p_{0,1}p_{1,0}}$. In particular, Eq. (9) shows that $\Delta\langle H_A\rangle_{\max} > \max_{\{U\}}\Delta_{\text{Diag}}\langle H_A\rangle = p_{0,1} - p_{1,0}$ [for $r = 1$ in Eq. (7)]. This represents an enhancement of the energy transfer to system $A$, due to coherence, and corroborates for two qubits the quantum advantage suggested by Eq. (5). The exclusive dependence on the local populations $p_i^\gamma$, expressed by Eq. (7), also means that $\Delta_{\text{Diag}}\langle H_A\rangle$ is not affected by classical correlations in $\rho_{\text{Diag}}$. Therefore, for locally thermal qubits the reversion of the thermodynamic arrow of time is only possible through the coherent contribution to the energy transfer. If the qubit $A$ has the larger temperature, such a reversion is implied by the positive value of $\Delta\langle H_A\rangle_{\max}$ in Eq. (9). We can also interpret this "anomalous" heat flow as necessarily owed to quantum correlations. A classically correlated state $\rho$, with both marginals $\rho^\gamma = \text{Tr}_{\gamma'}\rho$ being diagonal in $H_\gamma$ (as is the case for local thermality), is a state without coherence in the eigenbasis of $H_A + H_B$ [60]. Hence, the absence of local coherence implies that $\rho$ must have quantum correlations to produce $\Delta_{\text{Coh}}\langle H_A\rangle \neq 0$.

We complement the discussion about the role of quantum correlations for energy transfer, analyzing this process for Bell-diagonal states [50,51]. The condition of maximally mixed marginals implies that $p_{0,1} = p_{1,0}$. Therefore, $\Delta\langle H_A\rangle = \Delta_{\text{Coh}}\langle H_A\rangle$ [cf. Eq. (7)] and $\Delta\langle H_\gamma\rangle_{\max} = p_{0,1}$, according to Eq. (9). If we specialize to a subset of entangled states [red line in Fig. 1(b)], Eq. (9) simplifies to (see Appendix E)

$$\Delta\langle H_\gamma\rangle_{\max} = \frac{1 + C(\rho)}{4}, \tag{10}$$

where $C(\rho) = \max(0, 4p_{0,1} - 1)$ is the concurrence. We note a linear increase of $\Delta\langle H_\gamma\rangle_{\max}$ with respect to $C(\rho)$, which is monotonically associated to the entanglement of formation [61]. Figure 1 also depicts separable states that yield $|\Delta\langle H_\gamma\rangle| = |\Delta_{\text{Coh}}\langle H_\gamma\rangle| > 0$, thereby outperforming classically correlated states.

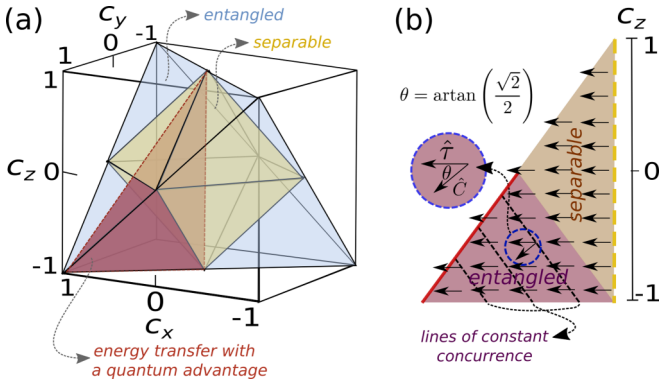


FIG. 1. (a) Energy transfer between two qubits, for initial Bell-diagonal states. This class can be depicted in terms of the parameters $c_i = \text{Tr}(\sigma_i^A \otimes \sigma_i^B\rho)$, where $\{\sigma_i^\gamma\}_{i=x,y,z}$ are the Pauli matrices for the qubit $\gamma$. Separable states lie in the inner yellow octahedron, while entangled ones lie inside the blue region and outside the yellow octahedron. The dark red triangle (see Appendix E) inside the tetrahedron represents a subset of states that produce a non-null energy transfer $\Delta\langle H_\gamma\rangle$ under a suitable SEC $U$. (b) Frontal view of the aforementioned subset. On this plane, the maximum energy transfer $\max_{\{U\}}\Delta\langle H_\gamma\rangle$ is zero only for classically correlated states (yellow dashed line), and its gradient has constant projection with direction $\hat{\tau} = 1/\sqrt{2}(1,1,0)$. Within the entangled triangle $\max_{\{U\}}\Delta\langle H_\gamma\rangle$ increases monotonically with the concurrence $C$ (i.e., $\partial\max_{\{U\}}\Delta\langle H_\gamma\rangle/\partial C > 0$), whose projected gradient possesses constant direction $\hat{C} = 1/\sqrt{3}(1,1,-1)$. The left side (continuous red line) contains maximum coherence states that satisfy Eq. (10) in the main text.

## VI. CONCLUSIONS AND PERSPECTIVES

We have derived three theorems that constitute a theoretical framework to characterize the energy transfer in bipartite quantum systems. Theorem 1 describes this process for "classical" (incoherent) states, allowing to obtain the corresponding values for the energy transfer. Theorem 2 singles out the class of coherence that may have a non-null contribution, as well as the subset of SEC unitaries that could exploit its potential. Employing Theorem 3 (which follows from Theorems 1 and 2), we showed that the maximum energy transfer (optimized over the set of SEC unitaries) for a general state is bounded from below by that of the state dephased in the joint eigenenergy basis. This implies in particular that, for optimal evolutions, coherence never worsens the energy exchange. The type of coherence that does have an impact on this task is also useful for extracting work in a multipartite scenario, under "thermal processes" [62]. Further investigations on such connection are pertinent. On the other hand, we employed Theorems 1 and 2 to deduce a class of states that only allow unidirectional energy flow. An open question is whether this set includes all bipartite states satisfying the mentioned constraint.

We illustrated our results describing the energy transfer between two qubits. In this case, coherence provides a genuine

quantum advantage over incoherent states. It is also the fundamental resource for reverting the thermodynamic arrow of time, in connection with the experimental findings reported in [36]. For Bell-diagonal states, we found that entanglement is not necessary to outperform classically correlated states. Moreover, both entangled and separable states provide a quantum enhancement only if the state contains "useful" coherence, characterized by Theorem 2. For a suitable subset of entangled states, the maximum energy transfer increases monotonically with the concurrence. In particular, Eq. (10) exemplifies this behavior for entangled states of maximum coherence. Searching for a similar relation in systems of higher dimension could be an interesting extension to this analysis.

*Note added*. Recently, we noticed two related (but fundamentally different) works about the role of coherence and correlations in energy transfer [49].

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## APPENDIX A: PROOFS OF THEOREMS 1–3

*Proof of Theorem 1*. Replacing Eq. (2) in the expression for $\Delta_{\mathrm{Diag}}\langle H_A\rangle$ [cf. Eq. (4)] we obtain the equation $\Delta_{\mathrm{Diag}}\langle H_A\rangle = \sum_E p_E \mathrm{Tr}_A(H_A \mathrm{Tr}_B(U\rho_{\mathrm{Diag}}(E)U^\dagger) - H_A\rho^A_{\mathrm{Diag}}(E))$, where $\rho^A_{\mathrm{Diag}}(E) = \mathrm{Tr}_B\rho_{\mathrm{Diag}}(E)$. From Definition 2 and Eq. (2), $U\rho_{\mathrm{Diag}}(E)U^\dagger = \sum_{i_E;j_E,k_E} c^{(E)}_{i_E,j_E} c^{(E)*}_{i_E,k_E} \frac{p(\varepsilon_{i_E},E)}{p_E} \Pi^{(E)}_{j_E,k_E}$, where $\Pi^{(E)}_{j_E,k_E} = \Pi^{(E,E)}_{j_E,k_E}$ is defined through Eq. (3). Using Definition 2 we find a similar expression for $U^A_E\rho^A_{\mathrm{Diag}}(E)U^{A\dagger}_E$: $U^A_E\rho^A_{\mathrm{Diag}}(E)U^{A\dagger}_E = \sum_{i_E;j_E,k_E} c^{(E)}_{i_E,j_E} c^{(E)*}_{i_E,k_E} \frac{p(\varepsilon_{i_E},E)}{p_E} |j_E\rangle_A\langle k_E|$.

The expressions for $U\rho_{\mathrm{Diag}}(E)U^\dagger$ and $U^A_E\rho^A_{\mathrm{Diag}}(E)U^{A\dagger}_E$ are further related by the identity $\mathrm{Tr}_B(U\rho_{\mathrm{Diag}}(E)U^\dagger) = \mathcal{D}_{H_A}(U^A_E\rho^A_{\mathrm{Diag}}(E)U^{A\dagger}_E)$, where $\mathcal{D}_{H_A}(\cdot)$ is the map that eliminates all coherences in the eigenbasis of $H_A$, while leaving unmodified the populations (dephasing with respect to $H_A$). To derive this equality we must compute the operators $\mathrm{Tr}_B\Pi^{(E)}_{j_E,k_E}$, appearing in $\mathrm{Tr}_B(U\rho_{\mathrm{Diag}}(E)U^\dagger)$. Instead of using the notation of the main text, $\Pi^{(E)}_{j_E,k_E} = |j_E,E\rangle_A\langle k_E,E|$, it is convenient to write $\Pi^{(E)}_{j_E,k_E}$ as $\Pi^{(E)}_{j_E,k_E} = |j_E\rangle_A\langle k_E| \otimes |j'_E\rangle_B\langle k'_E|$ [recall that for any $j_E$ ($k_E$) the corresponding $j'_E$ ($k'_E$) has a unique value due to the nondegeneracy of $H_B$]. In this way, $\mathrm{Tr}_B\Pi^{(E)}_{j_E,k_E} = |j_E\rangle_A\langle k_E|\delta_{j'_E,k'_E}$. Now, we show that, *under the constraint of nondegeneracy for $H_A$ and $H_B$*, $\delta_{j'_E,k'_E} = \delta_{j_E,k_E}$. By definition, the eigenenergies of $|j_E\rangle_A$ and $|k_E\rangle_A$ are related to those of $|j'_E\rangle_A$ and $|k'_E\rangle_A$ through the equations $\varepsilon_{j_E} = E - \bar{\varepsilon}_{j'_E}$ and $\varepsilon_{k_E} = E - \bar{\varepsilon}_{k'_E}$. Hence, if $j'_E = k'_E$, the nondegeneracy of $H_A$ implies that $j_E = k_E$. Conversely, for $j_E = k_E$, the nondegeneracy of $H_B$ implies that $j'_E = k'_E$. Therefore, $\delta_{j'_E,k'_E} = \delta_{j_E,k_E}$ and $\mathrm{Tr}_B\Pi^{(E)}_{j_E,k_E} = |j_E\rangle_A\langle k_E|\delta_{j_E,k_E}$, which, after substitution in $\mathrm{Tr}_B(U\rho_{\mathrm{Diag}}(E)U^\dagger)$, yields

$$\mathrm{Tr}_B(U\rho_{\mathrm{Diag}}(E)U^\dagger) = \sum_{i_E,j_E} \left|c^{(E)}_{i_E,j_E}\right|^2 \frac{p(\varepsilon_{i_E},E)}{p_E} |j_E\rangle_A\langle j_E| = \mathcal{D}_{H_A}\left(U^A_E\rho^A_{\mathrm{Diag}}(E)U^{A\dagger}_E\right).$$

The proof is concluded by noticing that $\mathcal{D}_{H_A}(\cdot)$ does not modify the average energy of system $A$. ■

*Proof of Theorem 2*. According to Eq. (4), $\Delta_{\mathrm{Coh}}\langle H_A\rangle = \mathrm{Tr}(H_AU\chi U^\dagger) - \mathrm{Tr}(H_A\chi)$. Employing again the notation $\Pi^{(E,E')}_{i_E,j_{E'}} = |i_E\rangle_A\langle j_{E'}| \otimes |k_E\rangle_B\langle l_{E'}|$, used in the previous proof, it is easily shown that $\mathrm{Tr}(H_A\chi) = 0$: For any $\Pi^{(E,E')}_{i_E,j_{E'}}$ we have that $\mathrm{Tr}_A(H_A\mathrm{Tr}_B\Pi^{(E,E')}_{i_E,j_{E'}}) = \mathrm{Tr}_A(H_A|i_E\rangle_A\langle j_{E'}|\delta_{k_E,l_{E'}})$. This expression equals zero if either $i_E \neq j_{E'}$ or $k_E \neq l_{E'}$. Therefore, $\mathrm{Tr}(H_A\chi) = 0$.

On the other hand,

$$U\Pi^{(E,E')}_{i_E,j_{E'}}U^\dagger = \sum_{k_E,l_{E'}} c^{(E)}_{i_E,k_E} c^{(E')*}_{j_{E'},l_{E'}} \Pi^{(E,E')}_{k_E,l_{E'}},$$

applying Definition 2. Since for $E \neq E'$ all the $\Pi^{(E,E')}_{k_E,l_{E'}}$ are global coherent elements, $\sum_{E,E':E\neq E'} \mathrm{Tr}(H_AU\chi(E,E')U^\dagger) = 0$. For coherences of the type $\chi(E,E) = \sum_{i_E,j_E:i_E\neq j_E} \alpha^{(E,E)}_{i_E,j_E}\Pi^{(E,E)}_{i_E,j_E}$, given in Eq. (3), we obtain

$$\mathrm{Tr}_B\sum_E U\chi(E,E)U^\dagger = \sum_E\sum_{i_E\neq j_E} \alpha^{(E,E)}_{i_E,j_E}\mathrm{Tr}_BU\Pi^{(E,E)}_{i_E,j_E}U^\dagger.$$

From the relation $\mathrm{Tr}_B\Pi^{(E,E)}_{k_E,l_E} = |k_E\rangle_A\langle l_E|\delta_{k_E,l_E}$, derived in the previous proof,

$$\mathrm{Tr}_BU\Pi^{(E,E)}_{i_E,j_E}U^\dagger = \sum_{k_E} c^{(E)}_{i_E,k_E}c^{(E)*}_{j_E,k_E}|k_E\rangle_A\langle k_E|.$$

Therefore, $\mathrm{Tr}_B\sum_E U\chi(E,E)U^\dagger$ equals $\sum_E\sum_{k_E}\sum_{i_E<j_E} 2\,\mathrm{Re}(\alpha^{(E,E)}_{i_E,j_E}c^{(E)}_{i_E,k_E}c^{(E)*}_{j_E,k_E})|k_E\rangle_A\langle k_E|$, after inverting the order of the sums $\sum_{i_E\neq j_E}$ and $\sum_{k_E}$. In this expression, the index $E$ runs freely over the eigenvalues of $H$ and the sum $\sum_{k_E}$ runs over values of $k_E$ such that the state $|k_E,E\rangle$ (with eigenenergies $\varepsilon_{k_E}$ and $E$) exists. We can also invert the order for the sums $\sum_E$ and $\sum_{k_E}$ keeping in mind this constraint. The resulting expression is $\mathrm{Tr}_B\sum_E U\chi(E,E)U^\dagger = \sum_k \eta_k|k\rangle_A\langle k|$, where $\eta_k \equiv \sum'_E\sum_{i_E<j_E} 2\,\mathrm{Re}(\alpha^{(E,E)}_{i_E,j_E}c^{(E)}_{i_E,k}c^{(E)*}_{j_E,k})$. Now, the index $k$ runs freely over the eigenvalues of $H_A$ and the aforementioned constraint results from restricting the sum over $E$: for any $k$, $\sum'_E$ is restricted to values of $E$ such that the state $|k,E\rangle$ (with eigenenergies $\varepsilon_k$ and $E$) exists. In this way, we ensure that the sums $\sum_E\sum_{k_E}$ and $\sum_k\sum'_E$ cover exactly the same terms. Therefore, it is concluded that $\Delta_{\mathrm{Coh}}\langle H_A\rangle = \mathrm{Tr}_AH_A(\mathrm{Tr}_B\sum_E U\chi(E,E)U^\dagger) = \sum_k\eta_k\varepsilon_k$. ■

*Proof of Theorem 3*. From Theorem 1 and Definitions 1 and 2, $\Delta_{\mathrm{Diag}}\langle H_A\rangle$ can be maximized by independently maximizing each term $\mathrm{Tr}_A(H_AU^A_E\rho^A_{\mathrm{Diag}}(E)U^{A\dagger}_E)$, with respect to $U^A_E$. The solution corresponds to $\tilde{U}^A_E$ such that $\tilde{U}^A_E\rho^A_{\mathrm{Diag}}(E)\tilde{U}^{A\dagger}_E$ is the $E$-local state of maximum energy, obtained from $\rho^A_{\mathrm{Diag}}(E)$ through an $E$-local unitary (Definition 3). Since both $\rho^A_{\mathrm{Diag}}(E) = \mathrm{Tr}_B\rho_{\mathrm{Diag}}(E)$ and $\tilde{U}^A_E\rho^A_{\mathrm{Diag}}(E)\tilde{U}^{A\dagger}_E$ are diagonal in

the eigenbasis of $H_A$, $\tilde{U}_E^A|i_E\rangle_A = |\tilde{k}_E\rangle_A$. The corresponding coefficients $\tilde{c}^{(E)}_{i_E,k_E}$ (see Definition 2) satisfy the simple relation $\tilde{c}^{(E)}_{i_E,k_E} = \delta_{k_E,\tilde{k}_E}$. This implies that $\tilde{c}^{(E)}_{i_E,k_E}\tilde{c}^{(E)*}_{i'_E,k_E} = \delta_{k_E,\tilde{k}_E}\delta_{k_E,\tilde{k}'_E} = \delta_{\tilde{k}_E,\tilde{k}'_E} = 0$ for any pair $(\tilde{c}^{(E)}_{i_E,k_E},\tilde{c}^{(E)}_{i'_E,k_E})$, given the unitary character of $\tilde{U}_E^A$ (otherwise, $\tilde{U}_E^A|i_E\rangle_A = \tilde{U}_E^A|i'_E\rangle_A = |\tilde{k}_E\rangle_A$, resulting in a nonunitary map). Therefore, $\tilde{U} \notin \{\mathcal{U}\}$ and according to Corollary 2.1, $\Delta_{\mathrm{Coh}}\langle H_A\rangle = 0$. ■

## APPENDIX B: DIRECTION OF ENERGY FLOW FOR TENSOR PRODUCTS BETWEEN THERMAL STATES AND BETWEEN A PASSIVE STATE AND A MAXIMALLY ACTIVE ONE

Let us consider a tensor product of the form $\rho = \rho^A_{\beta_A} \otimes \rho^B_{\beta_B}$, with

$$\rho^A_{\beta_A} = \frac{\exp(-\beta_A H_A)}{Z^A_{\beta_A}}, \quad \rho^B_{\beta_B} = \frac{\exp(-\beta_B H_B)}{Z^B_{\beta_B}}, \tag{B1}$$

thermal equilibrium states at inverse temperatures $\beta_A$ and $\beta_B$, respectively, where $Z^\gamma_{\beta_\gamma} = \mathrm{Tr}[\exp(-\beta_\gamma H_\gamma)]$ is the partition function. Owing to the nondegeneracy condition of the local Hamiltonians ($H_A$ and $H_B$), the eigenvalues of the joint state restricted to the eigenspace of energy $E$ ($\mathcal{H}^E$), $\rho_{\mathrm{Diag}}(E)$, and the eigenvalues of the corresponding $E$-local state, $\rho^A_{\mathrm{Diag}}(E) = \mathrm{Tr}_B\rho_{\mathrm{Diag}}(E)$, are identical [cf. Eq. (2)]. These eigenvalues are explicitly given by

$$\lambda_{i_E} = \frac{\exp(-\beta_B E)}{p_E}\frac{\exp\big[-(\beta_A-\beta_B)\varepsilon_{i_E}\big]}{Z^A_{\beta_A}Z^B_{\beta_B}}. \tag{B2}$$

If the system $A$ has lower temperature than system $B$, then $\beta_A > \beta_B$ and $\lambda_{i_E} < \lambda_{i'_E}$ for $\varepsilon_{i_E} > \varepsilon_{i'_E}$. Therefore, for any value of $E$ the state $\rho^A_{\mathrm{Diag}}(E)$ is passive within $\mathcal{H}^A_E$. Since $\rho^A_{\beta_A}\otimes\rho^B_{\beta_B}$ is diagonal, we conclude from Theorem 1 and Eq. (6) that $\Delta\langle H_A\rangle = \Delta_{\mathrm{Diag}}\langle H_A\rangle > 0$ for any SEC unitary, meaning that heat can only flow from the hotter system ($B$) to the colder one ($A$).

On the other hand, consider now the product $\rho = \rho^A_P \otimes \rho^B_M$, where

$$\rho^A_P = \sum_i \lambda_i|\varepsilon_i\rangle_A\langle\varepsilon_i| \tag{B3}$$

is a passive ($P$) state for system $A$ and

$$\rho^B_M = \sum_j \eta_j|\bar{\varepsilon}_j\rangle_B\langle\bar{\varepsilon}_j| \tag{B4}$$

is a maximally active ($M$) state for system $B$. This formally means that $\lambda_{i+1} \leqslant \lambda_i$ and $\eta_{j+1} \geqslant \eta_j$ for all $i,j$, for eigenenergies put in increasing order: $\varepsilon_{i+1} > \varepsilon_i$ and $\varepsilon_{j+1} > \varepsilon_j$. We immediately note that $\rho = \rho_{\mathrm{Diag}}$ and therefore $\Delta\langle H_A\rangle = \Delta_{\mathrm{Diag}}\langle H_A\rangle$.

Keeping in mind the constraint of nondegeneracy of the local Hamiltonians, we can express the state $\rho_{\mathrm{Diag}}(E)$ as

$$\rho_{\mathrm{Diag}}(E) = \sum_{i_E}\frac{\lambda_{i_E}\eta'_{i_E}}{p_E}\big|\varepsilon_{i_E}\big\rangle_A\big\langle\varepsilon_{i_E}\big| \otimes \big|E-\varepsilon_{i_E}\big\rangle_B\big\langle E-\varepsilon_{i_E}\big|, \tag{B5}$$

where $\eta'_{i_E}$ is the eigenvalue of $\rho^B_M$ corresponding to the eigenstate $|E-\varepsilon_{i_E}\rangle_B$, with eigenenergy $E-\varepsilon_{i_E}$, and $p_E = \sum_{i_E}\lambda_{i_E}\eta'_{i_E}$. The property of passivity implies in particular that $\lambda_{i_E+1} \leqslant \lambda_{i_E}$. Likewise, $E-\varepsilon_{i_E} > E-\varepsilon_{i_E+1}$, by definition, and therefore $\tilde{\eta}_{i_E} \geqslant \tilde{\eta}_{i_E+1}$, given that $\rho^B_M$ is maximally active. In this way, the eigenvalues of $\rho_{\mathrm{Diag}}(E)$, $\{\lambda_{i_E}\eta'_{i_E}/p_E\}$, are monotonically decreasing. This implies that for any $E$ the state $\rho^A_{\mathrm{Diag}}(E) = \mathrm{Tr}_B\rho_{\mathrm{Diag}}(E) = \frac{1}{p_E}\sum_{i_E}\lambda_{i_E}\eta'_{i_E}|\varepsilon_{i_E}\rangle_A\langle\varepsilon_{i_E}|$ is $E$ passive (cf. Definition 3). From Theorem 1 and Eq. (6) of the main text it follows that for this class of states, energy can only be transferred from system $A$ to system $B$.

## APPENDIX C: ENERGY TRANSFER FOR TWO-QUBIT STATES

A general SEC unitary acting on two-qubit states can be parametrized as the nontrivial transformation

$$U|0,0\rangle = e^{i\theta_{0,0}}|0,0\rangle, \tag{C1}$$

$$U|1,1\rangle = e^{i\theta_{1,1}}|1,1\rangle, \tag{C2}$$

$$U|0,1\rangle = e^{i\theta_{0,1}}\big(\sqrt{1-r^2}|0,1\rangle + re^{i\varphi}|1,0\rangle\big), \tag{C3}$$

$$U|1,0\rangle = e^{i\theta_{1,0}}\big(\sqrt{1-r^2}|1,0\rangle - re^{-i\varphi}|0,1\rangle\big), \tag{C4}$$

where $0 \leqslant r \leqslant 1$ and $\{\theta_{i,j},\varphi\}_{0\leqslant i,j\leqslant 1}$ are phases in the interval $(0,2\pi)$. Notice that aside from fulfilling Eqs. (C1)–(C4), the energy gaps of both qubits must coincide for $U$ to be SEC.

By applying Eqs. (C1)–(C4) to the diagonal part of a two-qubit state, a bit of algebra leads to the following expression for the transformed local state $\mathrm{Tr}_B(U\rho_{\mathrm{Diag}}U^\dagger)$:

$$\begin{aligned}\mathrm{Tr}_B(U\rho_{\mathrm{Diag}}U^\dagger) = {}& [p_{0,0} + p_{0,1}(1-r^2) + p_{1,0}r^2]|0\rangle_A\langle 0| \\ & + [p_{1,1} + p_{0,1}r^2 + p_{1,0}(1-r^2)]|1\rangle_A\langle 1|,\end{aligned} \tag{C5}$$

where $p_{i,j} = \mathrm{Tr}(|i\rangle_A\langle i| \otimes |j\rangle_B\langle j|\rho_{\mathrm{Diag}})$. On the other hand, $\mathrm{Tr}_B(\rho_{\mathrm{Diag}}) = (p_{0,0}+p_{0,1})|0\rangle_A\langle 0| + (p_{1,1}+p_{1,0})|1\rangle_A\langle 1|$. Therefore, using the definition of $\Delta_{\mathrm{Diag}}\langle H_A\rangle$, $\Delta_{\mathrm{Diag}}\langle H_A\rangle \equiv \mathrm{Tr}(H_AU\rho_{\mathrm{Diag}}U^\dagger) - \mathrm{Tr}(H_A\rho_{\mathrm{Diag}})$, we get

$$\Delta_{\mathrm{Diag}}\langle H_A\rangle = (p_{0,1}-p_{1,0})r^2\hbar\omega = \big(p_1^B - p_1^A\big)r^2\hbar\omega, \tag{C6}$$

where $p_1^\gamma = \mathrm{Tr}(|1\rangle_\gamma\langle 1|\rho_{\mathrm{Diag}})$ is the population of the excited state for qubit $\gamma$.

The energy contribution from the "useful" coherences of the joint state, $\chi(\hbar\omega,\hbar\omega)$, is obtained by means of the transformations $U(|0\rangle_A\langle 1|\otimes|1\rangle_B\langle 0|)U^\dagger$ and $U(|1\rangle_A\langle 0|\otimes|0\rangle_B\langle 1|)U^\dagger$. Employing again Eqs. (C1)–(C4) we find that

$$\mathrm{Tr}_B(U\chi(\hbar\omega,\hbar\omega)U^\dagger) = 2\,\mathrm{Re}\big(\alpha^{(1)}_{0,1}e^{i\phi}\big)r\sqrt{1-r^2}\sigma^A_Z, \tag{C7}$$

where $\phi \equiv \theta_{0,1} - \theta_{1,0} + \varphi$. In this way,

$$\begin{aligned}\Delta_{\mathrm{Coh}}\langle H_A\rangle = {}& \mathrm{Tr}(H_AU\chi(\hbar\omega,\hbar\omega)U^\dagger) \\ = {}& 2\,\mathrm{Re}\big(\alpha^{(1)}_{0,1}e^{i\phi}\big)r\sqrt{1-r^2}\hbar\omega.\end{aligned} \tag{C8}$$

## APPENDIX D: ILLUSTRATIVE EXAMPLE: MAXIMUM ENERGY TRANSFER BETWEEN TWO QUBITS

To obtain Eq. (9), we first maximize $\Delta\langle H_\gamma\rangle$ with respect to $\alpha^{(1)}_{0,1}$ and $\phi$, for $r$ fixed. From the condition of energy conservation, $\Delta\langle H_A\rangle = -\Delta\langle H_B\rangle$, and we can maximize

$\Delta\langle H_B\rangle$ by minimizing $\Delta\langle H_A\rangle$. The optimization with respect to $\alpha_{0,1}^{(1)}$ and $\phi$ only encompasses the coherent energy transfer. For $r$ fixed, the maximum and minimum of $\Delta_{\mathrm{Coh}}\langle H_A\rangle$ are given by $2r\sqrt{p_{0,1}p_{1,0}(1-r^2)}\hbar\omega$ and $-2r\sqrt{p_{0,1}p_{1,0}(1-r^2)}\hbar\omega$, respectively. These values are obtained from Eq. (C8), by choosing $\phi=0$ and $\alpha_{0,1}^{(1)}=\pm\sqrt{p_{0,1}p_{1,0}}$. Therefore, $\max_{\{r,\phi;\alpha_{0,1}^{(1)}\}}\Delta\langle H_A\rangle=\max_r\Delta\langle H_A\rangle_+$, where $\Delta\langle H_A\rangle_+/\hbar\omega\equiv(p_{0,1}-p_{1,0})r^2+2r\sqrt{p_{0,1}p_{1,0}(1-r^2)}$. Similarly, $\max_{\{r,\phi;\alpha_{0,1}^{(1)}\}}\Delta\langle H_B\rangle=\min_r\Delta\langle H_A\rangle_-$, with $\Delta\langle H_A\rangle_-/\hbar\omega\equiv(p_{0,1}-p_{1,0})r^2-2r\sqrt{p_{0,1}p_{1,0}(1-r^2)}$.

By employing the chain rule, we find that $\frac{\partial}{\partial r}\Delta\langle H_A\rangle_\pm=2r\frac{\partial}{\partial x}\Delta\langle H_A\rangle_\pm$, being $x\equiv r^2$. Since for $r=0$ we get $\Delta\langle H_A\rangle_\pm=0$, according to Eqs. (C6) and (C8), the values of $r$ that yield the optimization are the solutions of the equation

$$\frac{1}{\hbar\omega}\frac{\partial}{\partial x}\Delta\langle H_A\rangle_\pm=(p_{0,1}-p_{1,0})\pm\frac{\sqrt{p_{0,1}p_{1,0}}}{\sqrt{x(1-x)}}(1-2x)=0. \quad \text{(D1)}$$

This expression can be rewritten as

$$(p_{0,1}+p_{1,0})^2x^2-(p_{0,1}+p_{1,0})^2x+p_{0,1}p_{1,0}=0. \quad \text{(D2)}$$

The solutions of Eq. (D2) are

$$x_+=\frac{p_{0,1}}{p_{0,1}+p_{1,0}}, \quad \text{(D3)}$$

$$x_-=\frac{p_{1,0}}{p_{0,1}+p_{1,0}}, \quad \text{(D4)}$$

where $x_+$ satisfies $\frac{\partial}{\partial x}\Delta\langle H_A\rangle_+=0$ and $\frac{\partial}{\partial x}\Delta\langle H_A\rangle_-=0$ for $x_-$.

Now, we verify that $\Delta\langle H_A\rangle_+(x_+)$ is a maximum and that $\Delta\langle H_A\rangle_-(x_-)$ corresponds to a minimum. The second derivative with respect to $r$ yields

$$\frac{\partial^2}{\partial r^2}\Delta\langle H_A\rangle_\pm=2\frac{\partial\Delta\langle H_A\rangle_\pm}{\partial x}+4x\frac{\partial^2\Delta\langle H_A\rangle_\pm}{\partial x^2}, \quad \text{(D5)}$$

where $\frac{1}{\hbar\omega}\frac{\partial^2\Delta\langle H_A\rangle_\pm}{\partial x^2}=\mp\frac{1}{2}\frac{\sqrt{p_{0,1}p_{1,0}}}{[x(1-x)]^{3/2}}$. Therefore, $\frac{\partial^2\Delta\langle H_A\rangle_+}{\partial r^2}|_{x_+}<0$ and $\frac{\partial^2\Delta\langle H_A\rangle_-}{\partial x^2}|_{x_-}>0$, as expected. By replacing the expressions (D3) and (D4) into $\Delta\langle H_A\rangle_+(x_+)$ and $\Delta\langle H_A\rangle_-(x_-)$, we arrive at Eq. (9).

## APPENDIX E: ENERGY TRANSFER FOR BELL-DIAGONAL STATES

We analyze here Bell-diagonal states that satisfy the equation $\rho=\rho_{\mathrm{Diag}}+\chi(\hbar\omega,\hbar\omega)$ since for these states $\Delta_{\mathrm{Coh}}\langle H_A\rangle>0$ [cf. Eq. (C8)]. For the considered class the marginals of both qubits are maximally mixed states. If we denote as $p_i^\gamma$, $i=0,1$, the local populations for qubit $\gamma$, then $p_0^\gamma=p_1^\gamma=1/2$. Therefore, the diagonal energy transfer is equal to zero, according to Eq. (C6), and any value $\Delta\langle H_A\rangle\neq0$ is associated to a quantum advantage. On the other hand,

$$p_0^A=p_{0,0}+p_{0,1},\quad p_1^A=p_{1,1}+p_{1,0},$$
$$p_0^B=p_{0,0}+p_{1,0},\quad p_1^B=p_{1,1}+p_{0,1},$$

where $p_{i,j}=\mathrm{Tr}(|i\rangle_A\langle i|\otimes|j\rangle_B\langle j|\rho)$. In this way, the condition of maximally mixed marginals implies that

$$p_{0,1}=p_{1,0},\quad p_{0,0}=p_{1,1}. \quad \text{(E1)}$$

Bell-diagonal states have a Bloch representation through the expression $\rho=\frac{1}{4}(\mathbb{I}+\sum_{i=x,y,z}c_i\sigma_i^A\otimes\sigma_i^B)$, where $c_i=\mathrm{Tr}(\sigma_i^A\otimes\sigma_i^B\rho)$ and $\{\sigma_i^\gamma\}_{i=x,y,z}$ are the Pauli matrices for the qubit $\gamma$. For the states of interest we obtain

$$c_x=c_y=\mathrm{Tr}\big(\sigma_x^A\otimes\sigma_x^B\chi\big)=2\,\mathrm{Re}\big(\alpha_{0,1}^{(1)}\big), \quad \text{(E2)}$$

$$c_z=\mathrm{Tr}\big(\sigma_z^A\otimes\sigma_z^B\rho_{\mathrm{Diag}}\big)=1-4p_{0,1}. \quad \text{(E3)}$$

In addition, to demand that such states be Bell diagonal, we require that $\mathrm{Tr}(\sigma_i^A\otimes\sigma_j^B\chi)=0$, for $i\neq j$. By performing a direct computation we verify that this imposes the condition $\mathrm{Im}(\alpha_{0,1}^{(1)})=0$.

Figure 1(a) of the main text shows a graphical depiction of Bell-diagonal states, which is constructed by means of a Cartesian coordinate system with axes $c_i$. In this parameter space, Eqs. (E2) and (E3) describe a plane that intersects the tetrahedron and passes through the points $(c_x,c_y,c_z)=(0,0,1)$, $(1,1,-1)$, and $(-1,-1,-1)$. This whole region contains all the two-qubit states that satisfy the relation $\rho=\rho_{\mathrm{Diag}}+\chi(\hbar\omega,\hbar\omega)$, while simultaneously being Bell diagonal. On the other hand, it is sufficient to focus on half of such a region to describe the associated energy transfer, as we explain next. First, notice that if we choose $\alpha_{0,1}^{(1)}$ not only real but also positive, it is still possible to obtain any value of $\Delta\langle H_A\rangle=\Delta_{\mathrm{Coh}}\langle H_A\rangle$ (and thus of $\Delta\langle H_B\rangle$) as predicted by Eq. (C8). In particular, the maximization over the set of SEC unitaries yields

$$\max_{\{U\}}\Delta\langle H_\gamma\rangle=\max_{\{r,\phi\}}\Delta\langle H_\gamma\rangle=\frac{\hbar\omega c_x}{2}=\frac{\hbar\omega c_y}{2}, \quad \text{(E4)}$$

where Eqs. (C8) and (E2) have been used. To characterize the behavior of $\max_{\{U\}}\Delta\langle H_\gamma\rangle$ with respect to the entanglement of Bell-diagonal states, we shall obtain the lines of constant concurrence on the region of interest.

The concurrence $C(\rho)$ is an entanglement measure (monotonically related to the entanglement of formation) defined as $C(\rho)\equiv\max(0,\eta_4-\eta_3-\eta_2-\eta_1)$, where $\{\eta_i\}$ are the eigenvalues of the Hermitian matrix $R=\sqrt{\sqrt{\rho}(\sigma_y\otimes\sigma_y)\rho^*(\sigma_y\otimes\sigma_y)\sqrt{\rho}}$, set in increasing order: $\eta_{i+1}\geqslant\eta_i$. $\sigma_y=-i|0\rangle\langle1|+i|1\rangle\langle0|$ is a Pauli matrix and $\rho^*$ is the state defined through complex conjugation of $\rho$ in the standard (computational) basis: $\rho^*_{i,j}=(\rho_{i,j})^*$. Since we choose $\alpha_{0,1}^{(1)}$ real, $\rho^*=\rho$. Moreover, Bell-diagonal states are invariant under the application of $\sigma_y\otimes\sigma_y$. This implies that $R=\sqrt{\sqrt{\rho}\rho\sqrt{\rho}}=\rho$, which allows us to compute the concurrence in terms of the eigenvalues of $\rho$. These eigenvalues are related to the parameters $c_i$ by the equation

$$\lambda_{ab}=\tfrac{1}{4}[1+(-1)^ac_x-(-1)^{a+b}c_y+(-1)^bc_z], \quad \text{(E5)}$$

where $\lambda_{ab}$ is the eigenvalue associated to the Bell state $|\psi_{ab}\rangle=\frac{1}{\sqrt{2}}[|0,b\rangle+(-1)^a|1,1\oplus b\rangle]$, $a,b=0,1$. Taking into account

Eqs. (E2) and (E3), we obtain

$$\lambda_{00} = \lambda_{10} = \tfrac{1}{4}(1 + c_z) = \tfrac{1}{2} - p_{0,1}, \tag{E6}$$

$$\lambda_{11} = \tfrac{1}{4}(1 - 2c_x - c_z) = -\mathrm{Re}\big(\alpha_{0,1}^{(1)}\big) + p_{0,1}, \tag{E7}$$

$$\lambda_{01} = \tfrac{1}{4}(1 + 2c_x - c_z) = \mathrm{Re}\big(\alpha_{0,1}^{(1)}\big) + p_{0,1}. \tag{E8}$$

For the states we are interested in ($c_x \geqslant 0$), Eqs. (E7) and (E8) imply that $\lambda_{01} \geqslant \lambda_{11}$. This leaves us with the three possible chains of inequalities $\lambda_{00} = \lambda_{10} \geqslant \lambda_{01} \geqslant \lambda_{11}$, $\lambda_{01} \geqslant \lambda_{00} = \lambda_{10} \geqslant \lambda_{11}$, and $\lambda_{01} \geqslant \lambda_{11} \geqslant \lambda_{00} = \lambda_{10}$. In the first case, $\max\{\lambda_{ab}\} = \lambda_{00} = \lambda_{10}$ and $C(\rho) = \max(0, -\lambda_{01} - \lambda_{11}) = 0$. For the remaining possibilities, the concurrence yields $C(\rho) = \max(0, \lambda_{01} - \lambda_{11} - 2\lambda_{00}) = \max(0, c_x - (1 + c_z)/2)$. Accordingly, $C(\rho)$ is non-null for states such that $c_x - (1 + c_z)/2 > 0$. The lines where $C(\rho) = C$ is constant correspond to equations of the form $C = c_x - (1 + c_z)/2$. In this way, we obtain the following expression for $c_z$ in terms of $c_x$:

$$c_z = 2(c_x - C) - 1. \tag{E9}$$

This equation represents straight lines that vary in their intersection with the $c_z$ axis, and have constant slope equal to 2. For $C = 0$, $c_z = 2c_x - 1$ determines the boundary between entangled and separable states in Fig. 1(b) of the main text. As $C$ increases, the lines move towards the bottom left vertex of the entangled triangle, along the constant direction $\hat{C}$ [see Fig. 1(b)].

The behavior of $\max_{\{U\}}\Delta\langle H_\gamma\rangle$ with respect to $C$ can now be deduced by using the definition of directional derivative. Employing Eq. (E4), we can calculate the projection of the gradient of $\max_{\{U\}}\Delta\langle H_\gamma\rangle$ onto the plane determined by Eqs. (E2) and (E3). To this end, we just have to compute the components of the gradient on such a plane. Denoting this projection as $\nabla(\max_{\{U\}}\Delta\langle H_\gamma\rangle)$, we obtain

$$\nabla(\max_{\{U\}}\Delta\langle H_\gamma\rangle) = \frac{\hbar\omega}{2}(1,1,0) = \frac{\hbar\omega}{\sqrt{2}}\hat{\tau}, \tag{E10}$$

where $\hat{\tau}$ is the unit vector with coordinates $(c_x, c_y, c_z) = 1/\sqrt{2}(1,1,0)$. The partial derivative of $\max_{\{U\}}\Delta\langle H_\gamma\rangle$ with respect to the concurrence $\frac{\partial}{\partial C}\max_{\{U\}}\Delta\langle H_\gamma\rangle$ is proportional to the directional derivate of $\max_{\{U\}}\Delta\langle H_\gamma\rangle$ along the direction $\hat{C}$, $\hat{C}\cdot\nabla(\max_{\{U\}}\Delta\langle H_\gamma\rangle)$. The proportionality factor is the inverse of the derivative of $C$ along such a direction and is positive by definition. Therefore, the sign of $\frac{\partial}{\partial C}\max_{\{U\}}\Delta\langle H_\gamma\rangle$ is the same of the scalar product $\hat{C}\cdot\hat{\tau}$. Keeping in mind the geometry of the "level surfaces" (within the plane of interest) for the concurrence, expressed by Eq. (E9), the direction of the corresponding projected gradient is $\hat{C} = 1/\sqrt{3}(1,1,-1)$. In this way, $\hat{C}\cdot\hat{\tau} = \sqrt{2/3}$, and we have a monotonic increment of the maximum energy transfer with respect to $C$: $\frac{\partial}{\partial C}\max_{\{U\}}\Delta\langle H_\gamma\rangle > 0$.

Finally, we explicitly compute the value of $\max_{\{U\}}\Delta\langle H_\gamma\rangle$ for states of maximum coherence $\alpha_{0,1}^{(1)} = \sqrt{p_{0,1}p_{1,0}} = p_{0,1}$ [cf. Eq. (E1)]. According to Eqs. (E2) and (E3), $c_x = 2p_{0,1}$ and $c_z = 1 - 4p_{0,1}$ for these states. In this way, Eq. (E9) yields $C = c_x - (1 + c_z)/2 = 4p_{0,1} - 1$. Moreover, $\max_{\{U\}}\Delta\langle H_\gamma\rangle = \hbar\omega p_{0,1}$, using Eq. (E4). This result coincides with Eq. (9) of the main text, obtained for two-qubit states that are not necessarily Bell diagonal, by also optimizing $\Delta\langle H_\gamma\rangle$ with respect to $\alpha_{0,1}^{(1)}$. Therefore, we arrive at the expression

$$\frac{\max_{\{U;\alpha_{0,1}^{(1)}\}}\Delta\langle H_\gamma\rangle}{\hbar\omega} = \frac{\Delta\langle H_\gamma\rangle_{\max}}{\hbar\omega} = \frac{1 + C}{4}, \tag{E11}$$

which constitutes a simple relation between $\Delta\langle H_\gamma\rangle_{\max}$ and the concurrence. It is worth remarking that Eq. (E11) does not mean that the optimal energy transfer only depends on the concurrence. Since it has been computed over a unidimensional region [see the red line in Fig. 1(b) of the main text], a dependence with a single variable is expected. However, we can at least be sure that $\frac{\partial}{\partial C}\max_{\{U\}}\Delta\langle H_\gamma\rangle > 0$, as was concluded by the previous analysis.


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