Anomalous Heat Transfer in Nonequilibrium Quantum Systems

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Anomalous heat transfer (AHT), a process by which heat spontaneously flows from a cold system into a hot one, superficially contradicts the Clausius statement of the second law of thermodynamics. Here we provide a full classification of mechanisms of the AHT in nonequilibrium quantum systems from a quantum-information perspective. For initial states in local equilibrium, we find that the AHT can arise from three resources: initial correlation, intrasystem interaction, and intrasystem temperature inhomogeneity. In particular, for qubit systems, we prove that initial quantum coherence is necessary for AHT if the intersystem interactions are limited to the two-body type. We explicitly show the AHT dominated by each of the mechanisms in a three-qubit system. Our classification scheme may offer a guideline for developing high-efficiency quantum heat pump.

Introduction. The second law of thermodynamics, as a fundamental physical law of nature, establishes the direction of thermodynamic processes. Its Clausius statement claims that heat can only spontaneously flow from a hot object into a cold one [1], and, entropy, a state function characterizing the randomness of the isolated joint system, must be nondecreasing in the process. This thermodynamic irreversibility has been popularly termed “the arrow of time” [2]. However, in an absolutely isolated and finite-sized quantum system, the second law holds only under certain initial conditions, since the system evolution is unitary and reversible [3, 4].

One commonly discussed restriction is that the hot and cold systems should be weakly correlated [4–8]. This weak-correlation condition faithfully describes the usual circumstance between macroscopic objects in daily life [9, 10], as Boltzmann suggested for classical systems [11, 12]. However, correlation effects can be rather significant in generic quantum systems, and, in particular, there exist quantum correlations such as quantum entanglement [13, 14] and quantum discord [15–17] having no classical counterparts, which play an important role in energy flow [18–20]. It has been proposed that when two quantum systems are strongly correlated, “anomalous” heat transfer (AHT), that is, heat spontaneously flows from the cold system into the hot, can occur, at the cost of consuming the intersystem correlation [5, 6, 21, 22]. More recently, the correlation-induced AHT has been experimentally observed in nuclear spin systems [23] and further investigated in a wide range of systems from trapped ions [24] to wormholes [25].

In spite of enormous progress, a general and systematic framework for analyzing AHT in quantum systems is still lacking. In this Letter, we generically define the heat transfer problem, and develop a quantum-information classification of the AHT mechanisms based on the notion of local-equilibrium states [26–29]. We find that, in addition to the intersystem correlation, the nature of interactions, as well as the intrasystem correlation and temperature inhomogeneity, can give rise to the AHT. We further investigate qubit systems in which the forms of interactions are limited by the so-called heat transfer condition. In particular, we prove that classical correlation is not sufficient to induce AHT if the intersystem interactions are of two-body type. We calculate the heat transfer for a three-qubit model and show explicitly that each of the mechanisms can independently realize the AHT.

Heat transfer Hamiltonian. We consider heat transfer between two quantum systems A and B, while the joint system is isolated. In general, the time-independent Hamiltonian of the joint system reads

$$H = H_A + H_B + H_I,$$

(1)

where $H_X$ with $X \in \{A, B\}$ is the Hamiltonian of the system $X$ and $H_I$ describes the intersystem interactions. In Eq. (1) we impose the heat transfer condition $[H_I, H_A + H_B] = 0$, that is, the total energy of $A$ and $B$ is conserved, which ensures that the energy loss of $A$ equals to the energy gain of $B$ during the evolution of the joint system. Therefore, as the joint system evolving from initial $(t = 0)$ state $\rho$ to finial state $\rho'$, one can unambiguously define the heat transfer $Q = \Delta(H_B) = -\Delta(H_A)$, where $\Delta(O) = \text{tr}[O(\rho' - \rho)]$ denotes the variation of the expectation value of an operator $O$. The two states $\rho$ and $\rho'$ are related by the evolution operation $\rho' = e^{-iH_1t} \rho e^{iH_1t}$, where we have taken $\hbar = 1$. The heat transfer condition has been widely exploited in the study of thermal operations in the context of the resource theory [30–33], and it tremendously constrains the parameters of the Hamiltonians. We note that, two joint systems, described by Hamiltonians $H_{1,2}$ and initial states $\rho_{1,2}$, exhibit identical heat transfer processes, if $UH_1 = H_2U$ and $U\rho_1 = \rho_2U$ with $U$ a time-independent unitary transform.
the heat flow and speed of the heat flow, respectively. We note that \[ Q = \text{function of time. Therefore, two flow functions} \]

\[ A \text{rium, we assume that the system} \]

\[ \text{is composed of interacting subsystems} \]

\[ \text{Hamiltonian in Eq. (1) and the initial local-equilibrium state} \]

\[ \text{is defined by the it-} \]

\[ \text{that the initial state} \]

\[ \text{is in general a non-analytic smooth} \]

\[ \rho_{A_k} = e^{-\beta_{A_k}H_{A_k}} / \mathcal{Z}_{A_k}, \quad \rho_{B} = e^{-\beta_{B}H_{B}} / \mathcal{Z}_{B}, \quad (3) \]

where \(1/\beta_u \equiv T_u \) and \( \mathcal{Z}_u = \text{tr} \{\exp(-\beta_u H_u)\} \) being the effective temperature and the partition function of the subsystem \( u \in \{A_{1,2,\ldots,N}, B\} \), respectively, and we have taken the Boltzmann constant \( k_B = 1 \). We denote the final states of the subsystem \( u \) by \( \rho'_u \). In practice, the local-equilibrium states can be prepared by thermalizing the subsystems with independent baths.

It is convenient to introduce the product states

\[ \rho_0 \equiv \otimes_{k=1}^{N} \rho_{A_k} \otimes \rho_{B}, \quad \rho_{A0} \equiv \otimes_{k=1}^{N} \rho_{A_k}. \quad (4) \]

We note that the initial state \( \rho_0 \) is not necessarily the product state \( \rho_0 \), and the subsystem final state \( \rho'_u \) is general non-thermal. Without loss of generality, we assume that \( A \) and \( B \) systems are the cold and the hot, respectively, that is, \( \beta_A > \beta_B \) where \( \beta_A \equiv \min \{\beta_{A_k}\}_{k=1}^{N} \).

**Classification of AHT mechanisms.** We are able to express the heat transfer \( Q \) in terms of quantum relative entropies and obtain the heat transfer equation

\[ (\beta_B - \beta_A)Q = \sum_{k=1}^{N} S(\rho'_{A_k}||\rho_{A_k}) + S(\rho'_{B}||\rho_{B}) \]

\[ + \Delta I_{A'B} + \Delta \mathcal{S}_A + \Delta \mathcal{J}_A. \quad (5) \]

The derivation of Eq. (5) is presented in Supplemental Material. In Eq. (5), the left-hand side describes the effective entropy flux flowing from \( A \) to \( B \), and \((\beta_B - \beta_A)Q < 0 \) defines the AHT regime. The right-hand side characterizes various origins of the entropy flux. (I) The first two terms describe the quantum relative entropy between the final and initial states of each subsystem. Here \( S(g||c) \equiv -\text{tr}(g \ln c) \) is the quantum relative entropy between states \( g \) and \( c \), with \( S(g) \equiv -\text{tr}(\ln g) \) the von-Neumann entropy of the state \( g \) [34]. (II) \( \Delta I_{A'B} \equiv \Delta I_{A'B}(\rho' - I_{A'B}(\rho) \) is the multipartite mutual information among all the subsystems [35, 36], describes the variation of the subsystem correlation. (III) \( \Delta \mathcal{S}_A \equiv \sum_{k=1}^{N} \langle \beta_k - \beta_{A_k} \rangle \Delta \langle H_{A_k} \rangle \) describes the entropy flux induced by the initial temperature inhomogeneity within the system \( A \). (IV) \( \Delta \mathcal{J}_A \equiv \beta_{A} \Delta \langle H_{A} \rangle \) characterizes the entropy flux generated by the interaction energy variation of the system \( A \).

An immediate observation for Eq. (5) is that the Clausius statement of the second law is recovered, when

An instantaneou state \( g(t) \) satisfies the Liouville-von Neumann equation \( dq(t)/dt = i[g,H] \). In consequence, the \( n \text{th} \) time derivative of the heat transfer can be written as

\[ \frac{d^n Q}{dt^n} = i^n \langle [H_I, H_{B}]_n \rangle \psi, \quad (2) \]

where the operator \([H_I, H_{B}]_n \) is defined by the iteration relation \([H_I, H_{B}]_n \equiv [H_I, [H_I, H_{B}]_{n-1}] \] with \([H_I, H_{B}]_1 \equiv [H_I, H_{B}] \), and \( \langle O \rangle \equiv \text{tr}(\rho O) \) (see Supplemental Material). Equation (2) characterizes the instantaneous heat transfer process of the model (1). Especially, the sign and amplitude of the leading-order non-vanishing derivative indicates the instantaneous direction and speed of the heat flow, respectively. We note that the heat flow \( Q(t) \) is in general a non-analytic smooth function of time. Therefore, two flow functions \( Q_{1,2}(t) \) are not necessarily identical, even if their instantaneous characteristics at a special time \( t_0 \) are identical, that is, \[ d^n Q_1/dt^n |_{t=t_0} = d^n Q_2/dt^n |_{t=t_0} \] for any \( n \geq 0 \).

For revealing the effect of the intrasystem nonequilibrium, we assume that the system \( A \) is composed of \( N \) interacting subsystems \( A_{1,2,\ldots,N} \) [See Fig. 1(a)]. The Hamiltonian reads \( H_A = H_{A0} + H_{AI} \), where \( H_{A0} = \sum_{k=1}^{N} H_{A_k} \) with \( H_{A_k} \) the Hamiltonian of the subsystem \( A_k \). \( H_{AI} \) describes the intra-subsystem interactions, and \( H_{A0} \) and \( H_{AI} \) do not necessarily commute.

**Local-equilibrium states.** We employ the concept of the local-equilibrium states to characterize the initial hotness/coldness of the systems, in which “temperatures” are locally defined parameters. For the Hamiltonian in Eq. (1), a local-equilibrium state \( \rho \) requires that the reduced density matrices of the subsystems \( A_{1,2,\ldots,N} \) and \( B \) take the Gibbs states [See Fig. 1(a)]

\[ \rho_{A_k} = e^{-\beta_{A_k}H_{A_k}} / \mathcal{Z}_{A_k}, \quad \rho_{B} = e^{-\beta_{B}H_{B}} / \mathcal{Z}_{B}, \quad (3) \]
A is interaction-free ($\Delta I_A = 0$), and, initially, A is temperature-homogenous ($\Delta T_A = 0$) and quantum correlation is absent ($\Delta I_{AB} = 0$). Since the remaining relative entropy terms are non-negative, one obtains the normal heat transfer $(\beta_B - \beta_A)Q \geq 0$.

Most importantly, one can readily identify three types of AHT mechanisms by Eq. (5). (I) Correlation-dominated AHT if $\Delta I_{AB}$ negative enough. Since the evolution of the joint system is unitary, the mutual information variation can be further decomposed into the intra- and intersystem components: $\Delta I_{AB} = \Delta I_A + \Delta I_{A:B}$. Here $\Delta I_A = I_A(\rho'_A) - I_A(\rho_A)$, with $I_A(\rho_A) = S(\rho_A) - S(\rho_{A:0})$ the multipartite mutual information within A, gives the mutual information variation in A, and $\Delta I_{A:B} = I_{A:B}(\rho') - I_{A:B}(\rho)$, with $I_{A:B}(\rho) = S(\rho_A) + S(\rho_B) - S(\rho)$ the bipartite mutual information [34], captures the variation of the total correlation between A and B [17]. The AHT dominated by consuming the initial intersystem mutual information, i.e., $\Delta I_{A:B} < 0$, has been widely discussed in previous studies [5, 6, 8, 22–24, 37]. On the other hand, consuming the intrasystem correlation, i.e., $\Delta I_A < 0$, can also give rise to AHT [38]. Note that the entropy production [39, 40] $\Delta I_{A:B} = S(\rho_B') - S(\rho_B)$ can be still positive even if $\Delta I_{A:B} < 0$, which likely produces a normal heat flow [39, 41]. (II) Temperature-inhomogeneity-dominated AHT if $\Delta T_A$ negative enough. (III) Interaction-dominated AHT if $\Delta I_A$ negative enough.

Heat transfer in multi-qubit systems. We develop heat transfer models in multi-qubit systems under constraint of the heat transfer condition, and identify the dominant AHT mechanisms in these models. Consider the system $X \in \{A, B\}$ composed of $N_X$ qubits. The interaction-free Hamiltonian reads

$$H_{X0} = \sum_{i=1}^{N_X} H_{X_i}, \quad H_{X_i} = -\frac{1}{2} \omega_{X_i} \sigma_{X_i}^X,$$  \hspace{1cm} (6)

where $\omega_{X_i} \geq 0$ and $\sigma_{X_i}^x, y, z$ are the frequency and the Pauli operators of the qubit $X_i$, respectively. A qubit model with arbitrary Zeeman fields is identical to that in Eq. (6) up to local qubit rotations. The interaction Hamiltonian between A and B takes the general form

$$H_I = H_{AB}^I + H_{AAB}^I + H_{ABB}^I + \cdots,$$ \hspace{1cm} (7)

where $H_{AB}^I, H_{AAB}^I, H_{ABB}^I$, and $\cdots$, denote two-body, three-body, and higher order many-body interactions, respectively. Here we focus on two- and three-body interactions, which are usually the dominant interactions in experimental systems. Clearly, the heat transfer models for qubit systems take relatively simple forms due to the constraint of the heat transfer condition. The derivation of the Hamiltonians is presented in Supplemental Material.

(I) Two-body intersystem interactions. Specifying the intersystem interactions of the two-body form

$$H^I_{AB} = \sum_{k,l} \sum_{a,b} c_{a,b}^{k,l} \sigma_{A_k}^a \sigma_{B_l}^b$$  \hspace{1cm} and the intrasystem interactions of the general multi-body form $H_{X1} = \sum_{i,j,\ldots,k} \sum_{a,b,\ldots,c} J_{X_i,j-k}^{a,b,c} \sigma_{X_i}^a \sigma_{X_j}^b \cdots \sigma_{X_k}^c$, we find that the heat transfer condition leads to two independent commutation relations $[H_{A0} + H_{B0}, H_{AB}^I] = 0$ and $[H_{X1}, H_{AB}^I] = 0$. The former relation reduces the intersystem interactions for effective heat transfer to

$$H_{AB}^I = \sum_{k,l} \left( c_{A_k B_l} \sigma_{A_k}^a \sigma_{B_l}^b + h.c. \right),$$  \hspace{1cm} (8)

where $\sigma_{X_i}^{\pm} = (\sigma_{X_i}^x \pm i\sigma_{X_i}^y)/2$ and the coupling constant $c_{A_k B_l}$ is non-zero only if the two qubits $A_k$ and $B_l$ are of equal frequency $\omega_{A_k} = \omega_{B_l}$. The latter commutation relation should lead to constraints on $H_{AB}^I$ in Eq. (8) and $H_{X1}$. However, we neglect $H_{X1}$ since we find it does not contribute to the heat transfer. Deriving the instantaneous heat transfer equations for the model defined by Eqs. (6) and (8), we obtain a no-go theorem:

**Theorem 1.** In the presence of only two-body intersystem interactions, instantaneous AHT is impossible if all the qubit triplets $X_a X_k Y_l$, where $(X,Y) \in \{(A,B), (B,A)\}$, have no initial quantum coherence.

The proof of Theorem 1 can be found in Supplemental Material. For clarifying the implications of Theorem 1, we formally decompose the initial state $\rho$ into three components, $\rho = \otimes X_k \rho_{X_k} + D + \chi$, where $\rho_{X_k}$ is the Gibbs state of the qubit $X_k$ as defined in Eq. (3), and $D$ and $\chi$ encode the classical correlation (diagonal) and quantum correlation (off-diagonal) among the qubits, respectively. Theorem 1 implies that, if intersystem interactions are limited to the two-body type, the initial classical correlation $D$ alone ($\chi = 0$) cannot induce AHT. Furthermore, not any initial quantum coherence can induce AHT. For example, an initial state with the coherence component $\chi = ((\otimes X_k \sigma_{X_k}^x + h.c.) \rho)$ does not exhibit AHT. The AHT requires additional quantum coherence at least among one triplet of the particular configurations as demonstrated in Theorem 1.

In general, the quantum coherence among a triplet $X_m X_k Y_l$ can be decomposed into doublet contributions and triplet collective contributions that does not exist in any doublet [42, 43]. In correspondence, we find that the intersystem coherence in doublets $X_m Y_l$ and $X_k Y_l$ only contributes to the heat transfer rate $dQ/dt$, while the intrasystem coherence in doublet $X_m X_k$ as well as the triplet collective coherence contribute to the instantaneous heat transfer convexity $d^2Q/dt^2$ (See Supplemental Material). The intersystem-coherence AHT has been realized in nuclear spin systems [23]. However, when the intersystem coherence vanishes, i.e., $dQ/dt = 0$, AHT occurs for $(\beta_B - \beta_A)2dQ/dt^2 < 0$. This intrasystem-coherence AHT might be interesting for experimental verification.

(II) Three-body intersystem interactions. We further investigate the qubit systems in which the inter-
system interactions are of the three-body form \( H_I = H_{\text{ABB}}^I + H_{\text{BBB}}^I \) and the intrasystem interactions are of two-body form for simplicity. The heat transfer condition leads to three independent commutation relations \( [H_{AB}, H_{B0}, H_{\text{ABB}}^I] = [H_{AB}, H_{B0}, H_{\text{ABB}}^I] = [H_{AB}, H_{B1}, H_I] = 0 \), which impose constraints on the interaction parameters.

The first commutator leads to three types of interactions depending on the frequencies of the qubits involved. For any three qubits \( A_k, l \) and \( B_m \), the interaction denoted by \( H_{A_k, A_l, B_m}^I \) takes the forms as follow. For \( \omega_u = \omega_v + \omega_w \) or \( \omega_v = \omega_w \), where \( \{u, v, w\} \in \{(A_k, A_l, B_m), (A_k, B_m, B_m), (B_m, A_k, A_l)\} \), we obtain \( H_{A_k, A_l, B_m}^I = c_{uvw}\sigma_u^+\sigma_v^+\sigma_w^- + \text{h.c.} \) or \( H_{A_k, A_l, B_m}^I = c_{uvw}\sigma_u^+\sigma_v^-\sigma_w^+ + \text{h.c.} \), respectively, where \( c_{uvw} \) and \( \bar{c}_{uvw} \) are arbitrary complex constants. For unconstrained frequencies, we obtain \( H_{A_k, A_l, B_m}^I = \epsilon_{klm}\sigma_{A_k}^+\sigma_{A_l}^-\sigma_{B_m}^- + \text{h.c.} \), where \( \epsilon_{klm} \) is an arbitrary real constant. The second commutator gives \( H_{\text{ABB}}^I \) of the similar form as \( H_{\text{ABB}}^I \). The third commutator introduces further constraints to interaction parameters. We note that, unlike the two-body interaction case, the intrasystem interaction terms \( \sigma_{A_k}^+\sigma_{A_l}^-\sigma_{B_m}^- \) as well as the intrasystem interactions \( H_{XI} \) cannot be omitted since they can contribute to instantaneous heat transfer.

We note that, exploiting three-body intersystem interactions, all the three types of AHT can be realized. In particular, AHT may occur even if the initial state is the product state \( \rho_0 \) in Eq. (4).

**AHT in three-qubit systems.** We study a three-qubit system \( \{A_{1,2}, B\} \) with a combination of two-body and three-body intersystem interactions. The derivation of the Hamiltonians can be found in Supplemental Material.

(I) In Fig. 1(b), we show an example of temperature-inhomogeneity-dominant AHT. We take \( H_{AI} = 0 \) and the intersystem three-body interaction take the simple expression

\[
H_{AI, A_{1,2}B}^I = c\sigma_{A_1}^+\sigma_{A_2}^-\sigma_B^- + \text{h.c.},
\]

where \( c \) is the coupling strength. We choose the initial state as the product state \( \rho_0 \) in Eq. (4). Therefore, the mutual information variation \( \Delta I_{AB} \geq 0 \), and the intrasystem interaction contribution \( \Delta I_A = 0 \). When \( \Delta I_A \) is negative enough, AHT occurs.

For this model the initial heat transfer rate vanishes \( \dot{Q}/dt = 0 \). Phase transition between the AHT and the normal heat transfer is shown in Fig. 2(a), which we obtained by calculating the initial heat transfer convexity,

\[
\frac{d^2Q}{dt^2} = 2|\varepsilon|^2\omega_B \left[ e^{|\beta_{A_1}\omega_{A_1} + \beta_B\omega_B |} - e^{\beta_{A_1}\omega_{A_1}} \right],
\]

and further parametrizing the qubit frequencies as \( \omega_{A_1} = (1 + a)\omega_B \) and \( \omega_{A_2} = a\omega_B \) with \( a \in (0, \infty) \) (see Supplemental Material). The phase boundary is defined by \( \frac{d^2Q}{dt^2} = 0 \), which gives \( (1 + a)\beta_{A_1}/\beta_B = 1 + a\beta_{A_2}/\beta_B \) [the red lines in Fig. 2(a)]. As \( a \) varies from 0 to \( \infty \), the slope of the phase boundary varies from 0 to 1 correspondingly. Note that, in the top-right region where \( \beta_{A_2} > \beta_{A_1} > \beta_B \), for a fixed \( \beta_{A_1} \), \( \Delta I_A \) gets negative enough to realize AHT when \( \beta_{A_2} \) is large enough to cross the phase boundary.

As the three-body interaction (9) is perturbed by weak two-body interactions, which violate the heat transfer condition, the AHT is robust. For example, we take the two-body perturbation \( H_{SI} = J \sum_{u,v} \sum_{\sigma_u \sigma_v} \sigma_u^- \sigma_v^+ \) with a uniform coupling constant \( J \). It can be proven that \( H_{SI} \) gives no correction to the initial heat transfer rate, while it gives a correction of the order of \( J^2 \) to the convexity (see Supplemental Material). As shown in Fig. 2(b), when \( J/c = 0 \), we recover the phase diagram of the unperturbed system [Fig. 2(a)]. As \( J/c \) increases, the region of AHT shrinks but remains finite.

(II) In Fig. 1(c), we show an example of intrasystem-interaction-dominated AHT. We take the intersystem interaction \( H_I = 0.005\omega_0 \left( 2i\sigma_A^+\sigma_A^- + \text{h.c.} \right) \sigma_B^+ + (\sigma_{A_1}^- - \sigma_{A_2}^-)\sigma_B^- \) being a combination of two- and three-body types, and the intrasystem interaction \( H_{AI} = 0.5\omega_0(\sigma_{A_1}^+\sigma_{A_1}^- + \text{h.c.}) \). We choose the product state \( \rho_0 \) in Eq. (4) as the initial state with the qubits \( A_{1,2} \) are of the same temperature \( \beta_A = \beta_{A_{1,2}} \). Hence \( \Delta I_{AB} \geq 0 \) and \( \Delta I_A = 0 \) during the evolution. We observe that negative enough \( \Delta I_A \) can induce AHT.

(III) In Fig. 1(d), we show an example of intrasystem-correlation-dominated AHT. The intrasystem interaction is set to be zero \( H_{AI} = 0 \). We prepare the initial state \( \rho = (\rho_{A_1} \otimes \rho_{A_2} + \chi_A) \otimes \rho_B \), where the coherence term \( \chi_A = 0.24 \left( \sigma_{A_1}^+ \otimes \sigma_{A_1}^- + \text{h.c.} \right) \) encodes quantum correlation within \( A \) and \( A_{1,2} \) share the same temperature \( \beta_A = \beta_{A_{1,2}} \). The joint system evolves under the two-body interaction \( H_I = 0.005\omega_0 (\sigma_{A_1}^+\sigma_B^+ + \sigma_{A_2}^-\sigma_B^- + \text{h.c.}) \).
Obviously, we have $\Delta \mathcal{T}_A = \Delta \mathcal{T}_A = 0$ and $\Delta \mathcal{T}_{A,B} \geq 0$ during the evolution. Hence AHT can only be realized by consuming the correlation between the qubits $A_1$ and $A_2$, which is consistent with Theorem 1. This mechanism has been discussed in Ref. 38.

**Discussion.** We have shown that both intrasystem temperature inhomogeneity and intrasystem interactions are able to induce AHT in quantum systems, aside from initial inter- and intrasystem correlation. For qubit systems in which the interactions are limited to the two-body type, we have proven that the AHT occurs only if the initial states contain quantum coherence. Realizing AHT via the other mechanisms requires three-body interactions, which are usually weak and overwhelmed by two-body interactions in nature. However, three- and multi-body interactions have been simulated in laboratory with various quantum techniques from trapped ions to superconducting qubits [44–48]. It would be interesting to simulate the AHT phenomenon dominated by the mechanisms beyond the initial-state correlation.

A quantum system exhibiting AHT is a potential platform for engineering the quantum heat pump. Recently, a two-qubit heat pump driven entirely by quantum correlation as fuel has been proposed theoretically [37]. Our AHT classification offers an atlas for searching the heat pump cycles and optimizing the efficiency performance, which is consistent with Theorem 1. This mechanism requires three-body interactions, which are usually weak and overwhelmed by two-body interactions in nature. However, three- and multi-body interactions have been simulated in laboratory with various quantum techniques from trapped ions to superconducting qubits [44–48]. It would be interesting to simulate the AHT phenomenon dominated by the mechanisms beyond the initial-state correlation.

A quantum system exhibiting AHT is a potential platform for engineering the quantum heat pump. Recently, a two-qubit heat pump driven entirely by quantum correlation as fuel has been proposed theoretically [37]. Our AHT classification offers an atlas for searching the heat pump cycles and optimizing the efficiency performance, in particular, by exploring the intrasystem degrees of freedom. A heat pump based on three-qubit systems we discussed would be an interesting topic for future study.

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[1] R. Clausius, *The Mechanical Theory of Heat* (Macmillan, 1879).
[2] A. S. Eddington et al., *The Nature of the Physical World* (Macmillan, London, 1929).
[3] S. Lloyd, *Physical Review A* 39, 5378 (1989).
[4] V. Vedral, “The Arrow of Time and Correlations in Quantum Physics,” (2016), arXiv:1605.00926 [quant-ph].
[5] M. H. Partovi, *Physical Review E: Statistical Physics, Plasmas, Fluids, and Related Interdisciplinary Topics* 77, 021110 (2008).
[6] D. Jennings and T. Rudolph, *Physical Review E* 81, 061130 (2010).
[7] F. Binder, L. A. Correa, C. Gogolin, J. Anders, and G. Adesso, eds., *Thermodynamics in the Quantum Regime: Fundamental Aspects and New Directions*, Fundamental Theories of Physics, Vol. 195 (Springer International Publishing, Cham, 2018).
[8] M. N. Bera, A. Riera, M. Lewenstein, and A. Winter, *Nature Communications* 8, 2180 (2017).
[9] L. Boltzmann, in *The Kinetic Theory of Gases: An Anthology of Classic Papers with Historical Commentary* (World Scientific, 2003) pp. 362–367.
[10] H. D. Zeh, *The Physical Basis of the Direction of Time*, 5th ed., Frontiers Collection (Springer, Berlin ; New York, 2007).
[11] L. Boltzmann, in *Kinetische Theorie II* (Springer, 1970) pp. 115–225.
[12] L. Boltzmann, Annalen der Physik 296, 392 (1897).
[13] V. Vedral, M. B. Plenio, M. A. Rippin, and P. L. Knight, *Physical Review Letters* 78, 2275 (1997).
[14] R. Horodecki, P. Horodecki, M. Horodecki, and K. Horodecki, *Reviews of Modern Physics* 81, 865 (2009).
[15] L. Henderson and V. Vedral, *Journal of Physics A: Mathematical and General* 34, 6899 (2001).
[16] H. Ollivier and W. H. Zurek, *Physical Review Letters* 88, 017901 (2001).
[17] K. Modi, A. Brodutch, H. Cable, T. Paterek, and V. Vedral, *Reviews of Modern Physics* 84, 1655 (2012).
[18] M. Sarovar, A. Ishizaki, G. R. Fleming, and K. B. Whaley, *Nature Physics* 6, 462 (2010).
[19] S. Lloyd, Z.-W. Liu, S. Pirandola, V. Chiloyan, Y. Hu, S. Huberman, and G. Chen, (2017), arXiv:1510.05035 [quant-ph].
[20] T. Ma, M.-J. Zhao, S.-M. Fei, and M.-H. Yung, *Physical Review A* 99, 062303 (2019).
[21] G. Vitagliano, C. Klöckl, M. Huber, and N. Friis (2018) pp. 731–750, arXiv:1803.06884 [quant-ph].
[22] S. Jevtic, D. Jennings, and T. Rudolph, *Physical Review Letters* 108, 110403 (2012).
[23] K. Micadei, J. P. S. Peterson, A. M. Souza, R. S. Sarthour, I. S. Oliveira, G. T. Landi, T. B. Batalhão, R. M. Serra, and E. Lutz, *Nature Communications* 10, 2456 (2019), arXiv:1711.03323 [cond-mat, physics:quant-ph].
[24] P. U. Medina González, I. Ramos-Prieto, and B. M. Rodríguez-Lara, *Physical Review A* 101, 062108 (2020).
[25] Z.-Y. Xian and L. Zhao, *Physical Review Research* 2, 043095 (2020).
[26] G. Lebon, D. Jou, and J. Casas-Vázquez, *Understanding Non-equilibrium Thermodynamics: Foundations, Applications, Frontiers* (Springer Berlin Heidelberg, Berlin, Heidelberg, 2008).
[27] R. Zwanzig, *Nonequilibrium Statistical Mechanics* (Oxford university press, 2001).
[28] F. Intravaia, R. O. Behunin, C. Henkel, K. Busch, and D. A. R. Dalvit, *Physical Review Letters* 117, 100402.
(2016).
[29] A. Levy and R. Kosloff, EPL (Europhysics Letters) 107, 20004 (2014).
[30] P. Ćwikliński, M. Studziński, M. Horodecki, and J. Oppenheim, Physical Review Letters 115, 210403 (2015).
[31] M. Lostaglio, D. Jennings, and T. Rudolph, Nature Communications 6, 1 (2015).
[32] F. G. Brandao, M. Horodecki, J. Oppenheim, J. M. Renes, and R. W. Spekkens, Physical Review Letters 111, 250404 (2013).
[33] E. Chitambar and G. Gour, Reviews of Modern Physics 91, 025001 (2019).
[34] M. A. Nielsen and I. L. Chuang, Quantum Computation and Quantum Information (Cambridge University Press, 2000).
[35] S. Watanabe, IBM Journal of Research and Development 4, 66 (1960).
[36] B. Groisman, S. Popescu, and A. Winter, Physical Review A 72, 032317 (2005).
[37] T. Holdsworth and R. Kawai, “Heat pump driven entirely by quantum correlation,” (2022), arXiv:2208.07440 [quant-ph].
[38] C. L. Latune, I. Sinayskiy, and F. Petruccione, Physical Review Research 1, 033097 (2019).
[39] M. Esposito, K. Lindenberg, and C. Van den Broeck, New Journal of Physics 12, 013013 (2010).
[40] G. T. Landi and M. Paternostro, Reviews of Modern Physics 93, 035008 (2021).
[41] S. Deffner and E. Lutz, Physical Review Letters 107, 140404 (2011).
[42] C. Radhakrishnan, M. Parthasarathy, S. Jambulingam, and T. Byrnes, Physical Review Letters 116, 150504 (2016).
[43] T. Ma, M.-J. Zhao, H.-J. Zhang, S.-M. Fei, and G.-L. Long, Physical Review A 95, 042328 (2017).
[44] G. Maslennikov, S. Ding, R. Hablitzel, J. Gan, A. Roulet, S. Nimmrichter, J. Dai, V. Scarani, and D. Matsukevich, Nature Communications 10, 202 (2019).
[45] H. P. Büchler, A. Micheli, and P. Zoller, Nature Physics 3, 726 (2007).
[46] P. Zhao, X. Tan, H. Yu, S.-L. Zhu, and Y. Yu, Physical Review A 96, 043833 (2017).
[47] A. Mezzacapo, L. Lamata, S. Filipp, and E. Solano, Physical Review Letters 113, 050501 (2014).
[48] N. Chancellor, S. Zohren, and P. A. Warburton, npj Quantum Information 3, 21 (2017).
Anomalous Heat Transfer in Nonequilibrium Quantum Systems

SUPPLEMENTAL MATERIAL

DERIVATION OF EQ. (2)

From the Liouville-von Neumann equation \( d\rho / dt = i[H, \rho] \), we obtain \((-i)^n d^n \rho / dt^n = n[\rho, H] \), where the operator \( n[\rho, H] \) is defined by the iteration relation \( n[\rho, H] = [n-1[\rho, H], H] \) with \( 1[\rho, H] \equiv [\rho, H] \). The \( n \)th derivative of heat transfer reads

\[
(-i)^n \frac{d^n Q}{dt^n} = (-i)^n \text{tr} \left( \frac{d^n \rho}{dt^n} H_B \right) = \text{tr} \left( n[\rho, H] H_B \right) = \text{tr} \left( (n-1[\rho, H], H) H_B \right) = \text{tr} \left( (n-1[\rho, H], H, H_B) \right),
\]

where we have applied the relation \( \text{tr} \left( m[\rho, H][H, H_B] \right) = \text{tr} \left( (m-1[\rho, H], H, H_B) \right) \) in the last equality. Since \( [H, H_B] = [H_I, H_B] \), we obtain Eq. (2).

DERIVATION OF EQ. (5)

We derive the heat transfer equation (5), exploiting the concept of quantum relative entropy of state \( \rho \) with respect to state \( \varsigma \), i.e., \( S(\rho||\varsigma) \equiv -\text{tr}(\rho \ln \varsigma) - S(\rho) \), where \( S(\rho) \equiv -\rho \ln \rho \) is the von-Neumann entropy of the state \( \rho \). Especially, if the reference state \( \varsigma \) is an equilibrium state, \( S(\rho||\varsigma) \) describes the “distance” of the state \( \rho \) to the thermal equilibrium. For a generic system \( X \), described by Hamiltonian \( H_X \) and evolving from the initial state \( \rho_X \) to the final state \( \rho'_X \), we define the relative entropy variation and the energy variation by

\[
\Sigma_X \equiv S(\rho'_X||\rho_X) - S(\rho_X||\rho'_X), \quad \Delta(H_X) \equiv \text{tr}[(\rho'_X - \rho_X) H_X],
\]

respectively, where the reference state \( \rho'_X \) is a Gibbs state \( \rho'_X \equiv e^{-\beta_X H_X}/Z_X \) with \( 1/\beta_X \) the effective temperature and \( Z_X \equiv \text{tr} e^{-\beta_X H_X} \) the partition function. We note that \(-\Sigma_X\) is the entropy production if \( \rho'_X \) is the stationary state of \( X \). Equation (S2) leads to

\[
\beta_X^* \Delta(H_X) = \Delta S_X + \Sigma_X,
\]

where \( \Delta S_X = S(\rho'_X) - S(\rho_X) \) denoting the entropy variation.

For the heat transfer model in Eq. (1), we define \( \rho_X \) and \( \rho'_X \) as the reduced density matrix of the system \( X \in \{A, B\} \) for the initial state \( \rho \) and the final state \( \rho' \), respectively. Applying Eq. (S3) to \( A \) and \( B \) systems, we obtain the relation

\[
(\beta_B^* - \beta_A^*) Q = \Delta I_{A:B} + \Sigma_A + \Sigma_B,
\]

where \( \Delta I_{A:B} \equiv I_{A:B}(\rho') - I_{A:B}(\rho) \), with \( I_{A:B}(\rho) \equiv S(\rho_A) + S(\rho_B) - S(\rho) \) the bipartite mutual information, captures the variation of the total correlation between \( A \) and \( B \), and we have used the relation \( S(\rho') = S(\rho) \) since the joint system is isolated. Note that the reference temperatures \( \beta_{A,B}^* \) are arbitrary and need to be specified according to physical circumstances.

As \( A \) is composed of \( N \) subsystems \( A_{1,2,...,N} \) and initially in local equilibrium [Eq. (3)], the relative entropy variation of \( A \) can be further decomposed. From Eq. (S3) we obtain

\[
\Sigma_A = -\Delta S_A + \beta_A^* \sum_{k=1}^N \Delta(H_{A_k}) + \beta_A^* \Delta(H_{A_I})
\]

\[
= \sum_{k=1}^N \left( \beta_{A_k}^* \Delta(H_{A_k}) - \Delta S_{A_k} \right) + \left( \sum_{k=1}^N \Delta S_{A_k} - \Delta S_A \right) + \sum_{k=1}^N (\beta_A^* - \beta_{A_k}^*) \Delta(H_{A_k}) + \beta_A^* \Delta(H_{A_I})
\]

\[
= \sum_{k=1}^N S(\rho'_{A_k}||\rho_{A_k}) + \Delta I_A + \Delta \Sigma_A + \Delta \Sigma_A.
\]
In the last equality of Eq. (S5), we have defined $\Delta I_A \equiv I_A(\rho'_A) - I_A(\rho_A)$, with $I_A(\rho_A) \equiv S(\rho_A||\rho_{A,0}) = \sum_{k=1}^{N} S(\rho_{A_k}) - S(\rho_A)$ the relative entropy among the $N$ subsystems. $\Delta I_A = \sum_{k=1}^{N} (\beta_{A_k} - \beta_{A}) \Delta \langle H_{A_k} \rangle$, and $\Delta I_B \equiv \beta_{A}^* \Delta \langle H_{A_I} \rangle$. For the system $B$, we identify the reference state $\rho_B$ to the Gibbs state $\rho_B$ in Eq. (3) and obtain

$$\Sigma_B = S(\rho_B||\rho_B), \quad \beta_B^* = \beta_B. \quad (S6)$$

Assuming that $A$ and $B$ are the cold and the hot, respectively, i.e., $1/\beta_A < 1/\beta_B$ with $1/\beta_A = \max\{1/\beta_{A_k}\}$, we take the reference temperature $\beta_B = \beta_A$. Combining Eqs. (S4)-(S6), we obtain the heat transfer equation (5).

**HEAT TRANSFER CONDITIONS IN QUBIT SYSTEMS**

(I) **Two-body intersystem interactions.** For qubit systems with the two-body (multi-body) intersystem (intrasystem) interactions $H_{AB}^{I}$ ($H_{XI}$) defined in the main text, the heat transfer condition gives

$$[H_{A0} + H_{B0}, H_{AB}^{I}] + [H_{AI}, H_{AB}^{I}] + [H_{BI}, H_{AB}^{I}] = 0. \quad (S7)$$

We obtain the commutators

$$[H_{A0} + H_{B0}, H_{AB}^{I}] \sim \sigma_A \otimes \sigma_B, \quad [H_{AI}, H_{AB}^{I}] \sim \sigma_A \otimes \cdots \sigma_A \otimes \sigma_B, \quad [H_{BI}, H_{AB}^{I}] \sim \sigma_A \otimes \sigma_B \otimes \cdots \sigma_B, \quad (S8)$$

where “$\sigma_X \otimes \cdots \sigma_Y$" represents a linear combination of the tensor products $\{\sigma_X, \ldots \sigma_Y\}$. Note that the commutators in Eq. (S8) are linearly independent. Combining Eqs. (S7) and (S8), we readily have

$$[H_{A0} + H_{B0}, H_{AB}^{I}] = [H_{XI}, H_{AB}^{I}] = 0. \quad (S9)$$

(II) **Three-body intersystem interactions.** For three-body intersystem interactions $H_{I} = H_{AAB}^{I} + H_{ABB}^{I}$, the heat transfer condition leads to

$$[H_{A0} + H_{B0}, H_{AAB}^{I}] + [H_{A0} + H_{B0}, H_{ABB}^{I}] + [H_{AI}, H_{AAB}^{I}] + [H_{AI}, H_{ABB}^{I}] + [H_{BI}, H_{AAB}^{I}] + [H_{BI}, H_{ABB}^{I}] = 0. \quad (S10)$$

Assuming that the intersystem interactions are of two-body type $H_{XI} = \sum_{i,j} J_{X_{ij}} \sigma_{X_i}^{a} \sigma_{X_j}^{b}$ and the three-body intersystem interactions take the form $H_{XYZ}^{I} = \sum_{k,l,m} J_{X_{klm}} \sigma_{X_k}^{a} \sigma_{X_l}^{b} \sigma_{X_m}^{c}$, where $XYZ \in \{AAB, ABB\}$, we obtain the commutators

$$[H_{A0} + H_{B0}, H_{AAB}^{I}] \sim \sigma_A \otimes \sigma_A \otimes \sigma_B, \quad [H_{A0} + H_{B0}, H_{ABB}^{I}] \sim \sigma_A \otimes \sigma_B \otimes \sigma_B, \quad [H_{AI}, H_{AAB}^{I}] \sim \sigma_A \otimes \sigma_A \otimes \sigma_B \otimes \sigma_B \text{ or } \sigma_A \otimes \sigma_B \otimes \sigma_B \otimes \sigma_B, \quad [H_{AI}, H_{ABB}^{I}] \sim \sigma_A \otimes \sigma_A \otimes \sigma_B \otimes \sigma_B \text{ or } \sigma_A \otimes \sigma_B \otimes \sigma_B \otimes \sigma_B, \quad (S11)$$

From Eq. (S11) we observe that the commutators in Eq. (S10) are linearly independent, and, therefore,

$$[H_{A0} + H_{B0}, H_{AAB}^{I}] = [H_{A0} + H_{B0}, H_{ABB}^{I}] = [H_{AI} + H_{BI}, H_{I}] = 0. \quad (S12)$$

The heat transfer conditions in Eqs. (S9) and (S12) leads to constrain the parameters of the Hamiltonians.

First, both Eqs. (S9) and (S12) involve the constraints of the type $[H_{A0} + H_{B0}, H_{I}] = 0$. We can find the solution of $[H_{A0} + H_{B0}, H_{I}] = 0$ for an arbitrary type of $H_{I}$. In general, $H_{I}$ can be formally written as

$$H_{I} = \sum_{S_{+}, S_{-}, S_{z}} c_{S_{+}, S_{-}, S_{z}} \Xi_{S_{+}, S_{-}, S_{z}} \equiv \left( \prod_{u \in S_{+}} \sigma_{u}^{+} \right) \left( \prod_{v \in S_{-}} \sigma_{v}^{-} \right) \left( \prod_{w \in S_{z}} \sigma_{w}^{z} \right), \quad (S13)$$

where $S_{a}$ with $a \in \{\pm, z\}$ denotes a set of the indices of $\sigma^{a}$-type qubits, and $c_{S_{+}, S_{-}, S_{z}} = c_{S_{-}, S_{+}, S_{z}}$ due to Hermiticity. $\Xi_{S_{+}, S_{-}, S_{z}}$ represents a multi-body interaction of $(S_{+}, S_{-}, S_{z})$ type. We can easily calculate the commutator

$$[H_{A0} + H_{B0}, H_{I}] = - \sum_{S_{+}, S_{-}, S_{z}} \Xi_{S_{+}, S_{-}, S_{z}} c_{S_{+}, S_{-}, S_{z}} \sum_{\sigma = \pm} \left( \sum_{A_{k} \in S_{\sigma}} \omega_{A_{k}} + \sum_{B_{k} \in S_{\sigma}} \omega_{B_{k}} \right). \quad (S14)$$
Hence \([H_{A0} + H_{B0}, H_I] = 0\) leads to the constraint

\[
c_{S-,S+,S_+} = 0, \quad \text{or} \quad \sum_{A_k \in S_+} \omega_{A_k} + \sum_{B_k \in S_+} \omega_{B_k} = \sum_{A_k \in S_-} \omega_{A_k} + \sum_{B_k \in S_-} \omega_{B_k}, \tag{S15}
\]

for any configuration \((S_+, S_-, S_+)\), due to the linear independency of the operators \(\Xi_{S_+,S_-,S_+}\). We apply Eq. (S15) to the cases of two- and three-body interactions.

(I) **Two-body intersystem interaction** \(H_{AB}^I\): \([H_{A0} + H_{B0}, H_{AB}^I] = 0\) leads to Eq. (8). We note that we have neglected the interaction terms \(\sum_{k,l} c_{kl}^{22} \sigma_{A_k}^+ \sigma_{B_l}^+\), since these terms do not contribute to the instantaneous heat transfer. This can be readily proved by Eq. (2). The commutator \([H_{XI}, H_{AB}^I] = 0\) in Eq. (S9) should introduce further constraints to interaction parameters. Nevertheless, from Eq. (2) one can prove that \(H_{XI}\) gives no contribution to the instantaneous heat transfer. Therefore, we have neglected the intrasystem interactions, \(H_{XI} = 0\).

(II) **Three-body intersystem interaction** \(H_{AAB}^I\) and \(H_{ABB}^I\). From Eq. (S15), we find that the commutator \([H_{A0} + H_{B0}, H_{AAB}^I] = 0\) in Eq. (S12) leads to the expression of \(H_{ABB}^I\) presented in the main text. \([H_{A0} + H_{B0}, H_{AAB}^I] = 0\) gives \(H_{ABB}^I\) of the similar form as \(H_{AAB}^I\). In addition, the commutator \([H_{A1} + H_{B1}, H_I] = 0\) in Eq. (S12) introduces further constraints to interaction parameters.

**PROOF AND DISCUSSION OF THEOREM 1**

For the qubit Hamiltonian given by Eqs. (6) and (8) and \(H_{XI} = 0\), we obtain

\[
[H_{AB}^I, H_{B0}] = -\sum_{k,l} \omega_{B_l} \left(c_{A_kB_l}\sigma_{A_k}^- \sigma_{B_l}^+ \right) - \text{h.c.}. \tag{S16}
\]

Therefore, by Eq. (2) we conclude that the heat transfer rate \(dQ/dt\) vanishes if there is no intersystem coherence in any doublet \(A_k B_l\), that is, the reduced density matrix \(\rho_{A_kB_l} = \tr_{A_kB_l} \rho\) is diagonal.

From Eq. (2) we obtain the heat transfer convexity

\[
\frac{d^2 Q}{dt^2} = \sum_{k \neq m, l \neq n} \frac{d^2 Q_{mn,kl}}{dt^2} + \sum_{k \neq m} \frac{d^2 Q_{ml,kl}}{dt^2} + \sum_{k, l \neq n} \frac{d^2 Q_{kn,kl}}{dt^2} + \sum_{k, l} \frac{d^2 Q_{kl,kl}}{dt^2}, \tag{S17}
\]

where \(d^2 Q_{mn,kl}/dt^2 = -\left\langle \left[H_{A_{mn}}^I, \left[H_{A_k B_l}, H_{B0}\right]\right]\right\rangle_{\rho}\). We evaluate the commutators

\[
[H_{A_{mn}}^I, \left[H_{A_k B_l}, H_{B0}\right]\right]_{k \neq m} = -\delta_{n,l} \omega_{B_l} \left(c_{A_mB_k}\sigma_{A_m}^- \sigma_{A_k}^+ \right) - \text{h.c.} \sigma_{B_l}^+, \tag{S18}
\]

The first term in Eq. (S17) obviously vanishes. The second term in Eq. (S17) vanishes if there is no coherence among any triplet \(A_m A_k B_l\) (the triplet state is diagonal), since all the diagonal elements of the corresponding commutators in Eq. (S18) are zero. Similarly, the third term in Eq. (S17) vanishes if there is no coherence among any triplet \(A_k B_n B_l\). The last term in Eq. (S17) reads

\[
\frac{d^2 Q_{kl,kl}}{dt^2} = \left|c_{A_kB_l}\right|^2 \omega_{B_l} \left[\tr \left(\rho_{B_l} \sigma_{B_l}^+\right) - \tr \left(\rho_{A_k} \sigma_{A_k}^+\right)\right], \tag{S19}
\]

where \(\rho_{X_k} = \tr_{\setminus X_k} \rho\) is the reduced density matrix of \(X_k\). Considering that all the qubits that initially in local equilibrium, \(\rho_{X_k} = e^{-\beta_{X_k} H_{X_k}} / Z_{X_k}\), we find

\[
(\beta_{B_l} - \beta_{A_k} \left)d^2 Q_{kl,kl}/dt^2\right|_{t=0} \geq 0, \tag{S20}
\]

with the equality holds only if \(\beta_{A_k} = \beta_{B_l}\). Therefore, AHT is prohibited.

Both intra- and intersystem coherence can give rise to the second-order AHT. The initial state of the triplet can be formally written as

\[
\rho_{A_m A_k B_l} = \rho_{A_m A_k} \otimes \rho_{B_l} + \sum_{a=x} \chi^{\alpha}_{A} \otimes \sigma_{B_l}^a, \tag{S21}
\]
where \( \text{tr}(\chi^x_y^z) = 0 \), the terms \( \chi^x_A \otimes \sigma^x_B \) encode intersystem correlation, and \( \rho_B \) is the Gibbs state of \( B \) with temperature \( 1/\beta_B \). We obtain

\[
\frac{d^2Q_{\text{mkl}}}{dt^2} = \omega_B \left[ \tanh \left( \frac{\beta_B \omega_B}{2} \right) \langle c_{A,m}B_\nu^* c_{A,m}B_\nu^* \sigma_{A,m}^\nu \sigma_{A,m}^\nu + \text{h.c.} \rangle \rho_{A,m}^{A,m} + 2 \langle c_{A,m}B_\nu^* c_{A,m}B_\nu^* \sigma_{A,m}^\nu \sigma_{A,m}^\nu + \text{h.c.} \rangle \chi_A \right].
\]  

(S22)

The first term represents the intrasystem coherence in \( A \), and the second term represents the intersystem correlation, where only the collective coherence terms \( \sigma_{A,m}^\nu \sigma_{A,m}^\nu \) can give finite contributions.

HEAT TRANSFER IN THREE-QUBIT SYSTEMS

For three qubit system \( \{A_1, 2, B\} \) with a combination of two-body and three-body intersystem interactions \( H_I = H^{I}_{AB} + H_{AAB}^I \), the heat transfer condition gives

\[
\left[ H^{I}_{AAB}, H_{A0} + H_{B0} \right] + \left[ H^{I}_{AB}, H_{AI} \right] + \left[ H_{AAB}, H_{AI} \right] + \left[ H_{AB}, H_{A0} + H_{B0} \right] = 0.
\]  

(S23)

In general the interaction Hamiltonians take the expressions \( H^{I}_{AAB} = \sum_{a,b,c} c_{a,b}^{c} \sigma^a_{A_1} \sigma^b_{A_2} \sigma^c_{B} \), and \( H_{AB} = \sum_{a,b} \text{J}^{a,b} \sigma^a_{A_1} \sigma^b_{A_2} \). We obtain the commutators,

\[
\left[ H^{I}_{AAB}, H_{A0} + H_{B0} \right] + \left[ H^{I}_{AB}, H_{AI} \right] \sim \sigma_A, \otimes \sigma_A, \otimes \sigma_B, \quad \left[ H_{AAB}, H_{AI} \right] + \left[ H_{AB}, H_{A0} + H_{B0} \right] \sim \sigma_A \otimes \sigma_B.
\]  

(S24)

Therefore, Eq. (S23) leads to

\[
\left[ H^{I}_{AAB}, H_{A0} + H_{B0} \right] + \left[ H^{I}_{AB}, H_{AI} \right] = \left[ H^{I}_{AAB}, H_{AI} \right] + \left[ H^{I}_{AB}, H_{A0} + H_{B0} \right] = 0.
\]  

(S25)

We consider a special parametrization. We take the frequencies and the intrasystem interactions of the forms

\[
\omega_A, r_1 = \omega_B, = \omega, \quad H_{AI} = \omega \left( r_2 \sigma^x_{A_1} \sigma^x_{A_2} + \text{h.c.} \right),
\]  

(S26)

where \( r_1 > 0 \) and \( r_2 \) is a complex number. We find that, for \( r_2 = \pm \frac{1}{2} \sqrt{r_1(2 - r_1)} \), the commutators in Eq. (S25) gives

\[
\begin{align*}
\sigma^{xx} &= c^{yy}, & c^{yy} &= (1 - r_1)c^{xy}, & c^{xy} &= c^{yy}, & c^{yx} &= -c^{xy}, & c^{yx} &= -c^{xy}, \\
\sigma^{yy} &= c^{xy}, & c^{xy} &= (2 - r_1)c^{xy}, & c^{xy} &= -c^{yx}, & c^{yx} &= c^{xy}, & c^{yx} &= -c^{xy},
\end{align*}
\]  

(S27)

and all the other interaction coefficients vanish. From Eq. (S27), we obtain the interactions

\[
H_I = H^{I}_{AAB} + H^{I}_{AB} = 2i \left( \sigma^x_{A_1} \sigma^x_{A_2} - \sigma^+_A \sigma^-_A \right) \left( c^{yy} \sigma^y_B + c^{xy} \sigma^x_B \right) + 2 \left( c^{xy} \sigma^y_B - c^{yy} \sigma^x_B \right),
\]  

(S28)

where the parameters \( r_1 \in \{0, 2\} \), \( r_2 = \pm \frac{1}{2} \sqrt{r_1(2 - r_1)} \in [-1/2, 1/2] \), and \( c^{xy,yx} \) are real. For \( r_1 = 1 \) and \( r_2 = 1/2 \), Eq. (S28) reduces to the intersystem interaction Hamiltonian in Fig. 1(c).

For the model described by \( \omega_A = \omega_A + \omega_B, H_{AI} = 0 \), and Eq. (9), by Eq. (2) we obtain the heat transfer rate and convexity

\[
\frac{dQ}{dt} = i\omega_B \langle \sigma^x_{A_1} \sigma^x_{A_2} \sigma^x_B - \text{h.c.} \rangle \rho, \quad \frac{d^2Q}{dt^2} = -\frac{1}{2} \omega_B |c|^2 \langle \sigma^x_{A_1} \sigma^x_{A_2} \sigma^x_B - \text{h.c.} \rangle \rho.
\]  

(S29)

For a coherence-free initial state, i.e., diagonal \( \rho \) in Eq. (S29), the initial heat transfer rate vanishes. When the initial state is the product state \( \rho_0 = \rho_A \otimes \rho_A \otimes \rho_B \) defined in Eq. (4), we obtain the initial heat transfer convexity in Eq. (10). In addition, at the phase boundary \( \beta_B = \beta_A + \alpha(\beta_A - \beta_A) \), we find that \( dq/dt \mid t=0 = 0 \).

The heat transfer condition \( [H_I, H] = 0 \) is violated by adding the two-body interactions \( H'_I = J \sum_a \sum_{u,v} \sigma^u_a \sigma^v_a \), where \( J \) is a real constant. For the product state \( \rho_0 \), it is obvious that the initial heat transfer rate vanishes. The heat convexity reads

\[
\frac{d^2Q}{dt^2} = \frac{4|c|^2 \omega_B \left( e^{2\omega_B(a \beta_A + \beta_B)} - e^{2(1+a)\omega_B \beta_A} \right)}{(1 + e^{2(1+a)\omega_B \beta_A}) \left( 1 + e^{2\omega_B \beta_B} \right)} - 16J^2 \omega_B \left( \frac{e^{2(1+a)\omega_B \beta_A} - e^{2\omega_B \beta_B}}{(1 + e^{2(1+a)\omega_B \beta_A}) \left( 1 + e^{2\omega_B \beta_B} \right)} \right).
\]  

(S30)

On the right side of Eq. (S30), the first term is identical to Eq. (10) and the second term is induced by \( H'_I \). Therefore, the AHT region survives for sufficiently small \( J \).