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Exchange fluctuation theorems for strongly interacting quantum pumps

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ABSTRACT

We derive a general quantum exchange fluctuation theorem for multipartite systems with arbitrary coupling strengths by taking into account the informational contribution of the back-action of the quantum measurements, which contributes to the increase in the von-Neumann entropy of the quantum system. The resulting second law of thermodynamics is tighter than the conventional Clausius inequality. The derived bound is the quantum mutual information of the conditional thermal state, which is a thermal state conditioned on the initial energy measurement. These results elucidate the role of quantum correlations in the heat exchange between multiple subsystems.

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I. INTRODUCTION

The unrivaled success of thermodynamics originates in the very nature of the theory. In contrast to microscopic descriptions, equilibrium thermodynamics formulates universally valid statements based on phenomenological observation. Its central quantity is the entropy, which, in a causal universe, can never decrease. However, in far from equilibrium situations, it is often required to reformulate some statements. This explains the importance and impact of the fluctuation theorems,^{1–5} which can be understood as symmetry relations for the probability distribution of entropy production for any physical scenario in the universe.

Remarkably, these fluctuation theorems can be understood as generalizations of the second law of thermodynamics,⁶ and they can be shown to contain previous extensions of thermodynamics away from equilibrium, such as the linear response theory.^{7,8} Different versions of these theorems have already been experimentally verified in different systems including biomolecular systems,⁹ nuclear magnetic resonance systems,¹⁰ trapped ion systems,^{11–13} and nitrogen-vacancy (NV) centers in diamond.^{14,15}

One of the major conceptual building blocks of *stochastic thermodynamics*, a non-equilibrium reformulation of the classical scenario, is to recognize that thermodynamic quantities such as work, heat,¹⁶ and entropy production¹⁷ can be defined along single trajectories.

Therefore, it is somewhat natural that the first focus was put on thermodynamic work since it depends only on the action of a controllable external agent.^{3,4} Arguably, heat is a more interesting and complicated quantity, which is related to the uncontrolled forms of the energy exchange. Indeed, fluctuation theorems were also unveiled for heat exchanged between systems¹⁸ as well as more general “heat-like” quantities.^{19–21} In the present Letter, we will study the fluctuation theorem for heat, or rather more generally any form of energy, exchanged between interacting quantum systems.

In quantum thermodynamics,²² the major problem is that classical trajectories become ill-defined. Hence, any thermodynamic quantity defined along a classical trajectory needs to be carefully re-defined. One of the most successful paradigms has been dubbed *two-time measurement* (TTM) scheme,^{12,18,23–37} in which thermodynamic quantities are determined from two projective measurements of the energy at the beginning and at the end of a process. While such an approach is more geared toward work in isolated quantum systems, it has also found application when considering heat in open quantum systems.^{18,27,38,39}

However, it has been argued that the TTM scheme is thermodynamically inconsistent since the projective energy measurements inevitably destroy quantum coherences.⁴⁰ To overcome this shortcoming of the TTM scheme, recent works proposed alternative paradigms,

such as dynamic Bayesian networks,⁴¹ the Maggenau–Hill quasiprobability,⁴² and the one-time measurement (OTM) scheme.^{43–47} Particularly, in the OTM scheme, the distribution of changes in internal energy is constructed by considering the expectation value of the energy conditioned on the initial energy measurement outcomes. This formalism avoids the second projective measurement, and, therefore, the thermodynamic contribution of quantum coherence or the correlations generated by the dynamics are naturally contained in the formalism.⁴⁸ Therefore, particularly in the strongly coupled systems, the effect of the quantum correlations is non-negligible, so that the OTM scheme naturally becomes the most appropriate paradigm.

In this letter, we employ the OTM scheme to derive a generalized quantum exchange fluctuation theorem for the multipartite case with arbitrary coupling strengths. As a consequence, we obtain a tighter bound on the net entropy change, which can be characterized by the quantum mutual information of a thermal state conditioned on the initial energy measurement. Our main results elucidate the role of quantum correlations in the heat exchange between arbitrary quantum systems.

This letter is organized as follows. In Sec. II, we first summarize the notions and notations which we use in this Letter. Then, in Sec. III, we discuss the heat distribution for the multipartite systems in the two-time measurement scheme, from which we derive the corresponding quantum exchange fluctuation theorem and the second law of thermodynamics and recover the bipartite case studied in Ref. 18. Third, in Sec. IV, we discuss the heat distribution for the multipartite systems in the one-time measurement scheme and derive the corresponding quantum exchange fluctuation theorem and second law of thermodynamics with a tighter lower bound, which is associated with the quantum mutual information of the conditional thermal state. Fourth, in Sec. V, we verify the tighter Clausius bound by employing an example of tripartite XY model. Finally, we conclude in Sec. VI.

II. NOTIONS AND NOTATIONS

For ease of notation and to avoid clutter in the formulas, we work in units for which the Boltzmann constant k_B and the reduced Planck constant \hbar simply are $k_B = \hbar = 1$. We consider a d -dimensional multipartite system described by the composite Hilbert space $\mathcal{H} \equiv \otimes_{j=1}^n \mathcal{H}_j$, where \mathcal{H}_j denotes the Hilbert space of the j th subsystem. The corresponding, time-independent Hamiltonians are H_j and $H = \sum_{j=1}^n H_j$. Here, H_j is precisely defined as $H_j \equiv H_j \otimes \mathbb{I}_{\bar{j}}$, where \bar{j} denotes the complement of \mathcal{H}_j . In the following, we will be particularly interested in situations in which the quantum systems are prepared in thermal states at inverse temperatures $\beta_j = 1/T_j$. Then, the canonical partition functions are $Z_j \equiv \sum_{E_j} e^{-\beta_j E_j}$, where $\{E_j, |E_j\rangle\}$ is the energy eigensystem of the Hamiltonian H_j . It will prove convenient to define the energy vectors as $\mathbf{E} \equiv (E_1, \dots, E_n)^T \in \mathbb{R}^n$, energy eigenvectors of H as $|\mathbf{E}\rangle \equiv |E_1, \dots, E_n\rangle \in \mathbb{C}^d$, the inverse temperature vector as $\boldsymbol{\beta} \equiv (\beta_1, \dots, \beta_n)^T \in \mathbb{R}^n$, and the partition function vector as $\mathbf{Z} \equiv (Z_1, \dots, Z_n)^T \in \mathbb{R}^n$. We also define the product of the partition functions as $|\mathbf{Z}| \equiv \prod_{j=1}^n Z_j$.

Consider a situation in which the total system is initially prepared in the product Gibbs state

$$\rho_0^{\text{eq}} \equiv \frac{1}{|\mathbf{Z}|} \prod_{j=1}^n \frac{e^{-\beta_j H_j}}{Z_j} = \sum_{\mathbf{E}} \frac{e^{-\boldsymbol{\beta} \cdot \mathbf{E}}}{|\mathbf{Z}|} |\mathbf{E}\rangle \langle \mathbf{E}|. \quad (1)$$

At the $t=0$, we turn on an interaction V_t and evolve the total system under the unitary operator U_t , satisfying the following Schrödinger's equation: $\partial_t U_t = -i(H + V_t)U_t$, $U_0 = \mathbb{I}$, where $\partial_t := \partial/\partial t$ (see Fig. 1).

In the present analysis, we are interested in describing the thermodynamics of the energy that is “pumped” between the subsystems \mathcal{H}_j , and, hence, we require the total energy to be conserved, $[U_t, H] = 0$. At time $t = \tau$, we switch off the interaction and as always $\rho_\tau \equiv U_\tau \rho_0^{\text{eq}} U_\tau^\dagger$.

In complete analogy to Ref. 18, we define the average heat absorbed by the j th system as the energy difference in the system due to the evolution,

$$\langle Q_j \rangle \equiv \text{tr}\{(\rho_\tau - \rho_0^{\text{eq}})H_j\}. \quad (2)$$

Note that due to energy conservation, we also have $\sum_{j=1}^n \langle Q_j \rangle = 0$. It will also be convenient to introduce the vector $\mathbf{Q} \equiv (Q_1, \dots, Q_n)^T \in \mathbb{R}^n$ as a set of the “stochastic amounts of heat” in each subsystem (see Fig. 1).

Before we continue, it is important to realize that strictly speaking, Eq. (2) can be understood as the amounts of exchange thermodynamic heat only as long as the interacting V_t is essentially time-independent. In this case, V_t is suddenly turned on at $t=0$ and suddenly switched off at $t=\tau$. In cases, for which V_t has a more complicated time-dependence, $\{Q_j\}_{j=1}^n$ is strictly speaking the changes of internal energy which may comprise heat and work. In these cases, our scenario describes a quantum energy pump. We stress that the following mathematical analysis remains identical for either case. However, to keep the conceptual arguments as accessible as possible and in close analogy to Ref. 18, we will be calling Q_j heat.

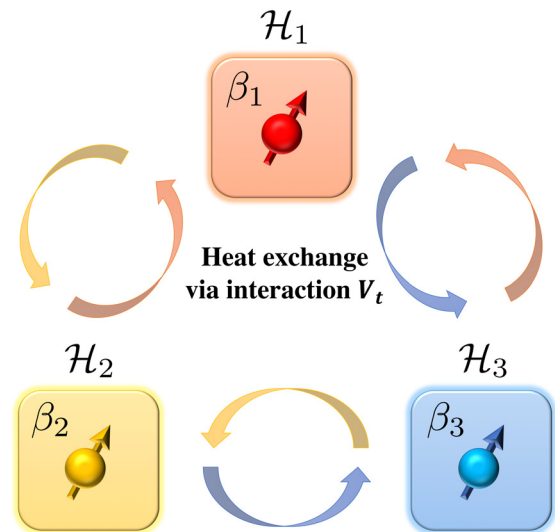


Fig. 1. Setup: We illustrate our setup with tripartite systems. The subsystems \mathcal{H}_1 , \mathcal{H}_2 , and \mathcal{H}_3 are initially prepared in the Gibbs states defined by their inverse temperature and bare Hamiltonians $\{\beta_1, H_1\}$, $\{\beta_2, H_2\}$, and $\{\beta_3, H_3\}$. Then, at time $t=0$, we suddenly turn on the interaction V_t between the tripartite systems, which evolves under the Schrödinger's equation. Then, at time $t = \tau$, we suddenly turn off the interaction. The energy is pumped between the subsystems, so that we require the total energy to be conserved.

III. TWO-TIME MEASUREMENT SCHEME

We first discuss the derivation of the quantum exchange fluctuation theorem for multipartite systems in the two-time measurement (TTM) scheme. At time $t = 0$, we measure the energy of the total system with the Hamiltonian H . Suppose we obtain a set of energy values $E = (E_1, \dots, E_n)^T$, so that the state is projected onto the eigenbases of H , $|E\rangle \equiv |E_1, \dots, E_n\rangle$. Then, we evolve the system under the unitary operator U_τ before we measure H again at $t = \tau$. The outcome of the measurement is $E' = (E'_1, \dots, E'_n)^T$, and the system's state is projected onto $|E'\rangle \equiv |E'_1, \dots, E'_n\rangle$. Then, the heat of the j th system along the trajectory is simply given by the difference in the energy measurement outcomes $E'_j - E_j$. Following Ref. 18, we only focus on the weak coupling regime, where the total energy along this trajectory is approximately conserved $\sum_{j=1}^n (E'_j - E_j) \approx 0$. Note that the quantum exchange fluctuation theorem of the TTM scheme also holds for the arbitrary coupling strengths, which can be obtained by applying the characteristic function approach.⁴⁹

Accordingly, the heat distribution becomes

$$P(\mathbf{Q}) \equiv \sum_{E, E'} \frac{e^{-\beta E}}{|\mathbf{Z}|} |\langle E' | U_\tau | E \rangle|^2 \delta(\mathbf{Q} - (E' - E)), \quad (3)$$

where we defined

$$\delta(\mathbf{Q} - (E' - E)) \equiv \prod_{j=1}^n \delta(Q_j - (E'_j - E_j)). \quad (4)$$

Then, the average heat increments are determined from (see Appendix A)

$$\langle Q_j \rangle_P = \int d\mathbf{Q} P(\mathbf{Q}) Q_j = \text{tr}\{(\rho_\tau - \rho_0^{\text{eq}}) H_j\}. \quad (5)$$

It is then only a simple exercise to show that (see Appendix B)

$$\langle e^{-\beta \cdot \mathbf{Q}} \rangle_P = \int d\mathbf{Q} P(\mathbf{Q}) e^{-\beta \cdot \mathbf{Q}} = 1, \quad (6)$$

where we used the completion relation $\mathbb{I} = \sum_E |E\rangle \langle E|$ and $|\mathbf{Z}| = \sum_{E'} e^{-\beta E'} = \sum_E e^{-\beta E}$. From Jensen's inequality, we immediately also obtain that

$$\sum_{j=1}^n \beta_j \langle Q_j \rangle \geq 0. \quad (7)$$

Equations (6) and (7) readily reduce to the bipartite results of Ref. 18. In this case, we recognize $Q_1 = -Q_2 = Q$, and with $\Delta\beta \equiv \beta_1 - \beta_2$, we have

$$\langle e^{-\beta_1 Q_1 - \beta_2 Q_2} \rangle_P = \langle e^{-\Delta\beta Q} \rangle_P = 1 \quad (8)$$

and

$$\Delta\beta \cdot \langle Q \rangle \geq 0. \quad (9)$$

More interestingly, we will now derive results equivalent to Eqs. (6) and (7) within the OTM scheme.

IV. ONE-TIME MEASUREMENT SCHEME

As before, at time $t = 0$, we measure the energy of the total system with the total bare Hamiltonian H and then evolve the

system under the unitary operator U_τ . In the OTM scheme, we do *not* perform the second measurement. Therefore, we define the stochastic heat of a trajectory as the energy difference between the average energy *conditioned* on the initial energy value $\langle E | U_\tau^\dagger H_j U_\tau | E \rangle$ and initial energy value E_j ,

$$\tilde{Q}_j \equiv \langle E | U_\tau^\dagger H_j U_\tau | E \rangle - E_j. \quad (10)$$

Here, note that $|E\rangle$ is the post-measurement state after the first energy measurement; therefore, it is fixed. As before, the total energy is conserved, and we, hence, have $\sum_{j=1}^n \tilde{Q}_j = 0$.

Following Ref. 44, the heat distribution $P(\mathbf{Q})$ is defined as

$$\tilde{P}(\mathbf{Q}) \equiv \sum_E \frac{e^{-\beta E}}{|\mathbf{Z}|} \delta(\mathbf{Q} - \tilde{\mathbf{Q}}), \quad (11)$$

where $\tilde{\mathbf{Q}} \equiv (\tilde{Q}_1, \dots, \tilde{Q}_n)^T \in \mathbb{R}^n$, and we defined

$$\delta(\mathbf{Q} - \tilde{\mathbf{Q}}) \equiv \prod_{j=1}^n \delta(Q_j - \tilde{Q}_j). \quad (12)$$

It is easy to see that we have (see Appendix C)

$$\langle Q_j \rangle_{\tilde{P}} = \int d\mathbf{Q} \tilde{P}(\mathbf{Q}) Q_j = \text{tr}\{(\rho_\tau - \rho_0^{\text{eq}}) H_j\}, \quad (13)$$

which is identical to what we found for the TTM scheme in Eq. (2).

Deriving the corresponding fluctuation theorem is then again a simple exercise. We obtain

$$\langle e^{-\beta \cdot \mathbf{Q}} \rangle_{\tilde{P}} = \int d\mathbf{Q} \tilde{P}(\mathbf{Q}) e^{-\beta \cdot \mathbf{Q}} = \frac{|\tilde{\mathbf{Z}}|}{|\mathbf{Z}|}, \quad (14)$$

where

$$|\tilde{\mathbf{Z}}| \equiv \sum_E \prod_{j=1}^n e^{-\beta_j \langle E | U_\tau^\dagger H_j U_\tau | E \rangle} \quad (15)$$

is recognized as the normalization of the conditional thermal state^{45,48}

$$\tilde{\rho}_\tau \equiv \sum_E \frac{e^{-\beta \cdot \tilde{E}(E)}}{|\tilde{\mathbf{Z}}|} U_\tau | E \rangle \langle E | U_\tau^\dagger, \quad (16)$$

where $\tilde{E}(E) \equiv (\tilde{E}_1(E), \dots, \tilde{E}_n(E))^T \in \mathbb{R}^n$ with $\tilde{E}_j(E) \equiv \langle E | U_\tau^\dagger H_j U_\tau | E \rangle$. We have already shown that the conditional thermal state is a thermal state conditioned on the initial energy measurement outcome E , which maximizes the von-Neumann entropy given the constraint that the ensemble average of the Hamiltonian is fixed.^{44,50}

In complete analogy to previous results for quantum work,⁴³ the corresponding fluctuation theorem for heat exchange simply becomes (see Appendix D)

$$\langle e^{-\beta \cdot \mathbf{Q}} \rangle_{\tilde{P}} = e^{-S(\tilde{\rho}_\tau || \rho_0^{\text{eq}})}, \quad (17)$$

where $S(\tilde{\rho}_\tau || \rho_0^{\text{eq}}) = \text{tr}\{\tilde{\rho}_\tau \ln(\tilde{\rho}_\tau)\} - \text{tr}\{\tilde{\rho}_\tau \ln(\rho_0^{\text{eq}})\}$ is the quantum relative entropy measuring the “distance” of the conditional thermal state to the corresponding Gibbs state. Then, from Jensen's inequality, we also have

$$\sum_{j=1}^n \beta_j \langle Q_j \rangle \geq S(\tilde{\rho}_\tau || \rho_0^{\text{eq}}). \quad (18)$$

This is a sharpened statement of the second law, which sets a tighter bound on the net energy exchange.

For multipartite systems, the quantum mutual information of $\tilde{\rho}_\tau$ is defined as⁵¹

$$\tilde{I}_\tau(1 : \dots : n) \equiv \sum_{j=1}^n S(\tilde{\rho}_{j,\tau}) - S(\tilde{\rho}_\tau), \quad (19)$$

where $\tilde{\rho}_{j,\tau} \equiv \text{tr}_j\{\tilde{\rho}_\tau\}$ is the reduced state of $\tilde{\rho}_\tau$ of the j th system. Writing γ_τ as the product state of these reduced states,

$$\gamma_\tau \equiv \bigotimes_{j=1}^n \tilde{\rho}_{j,\tau}, \quad (20)$$

we have

$$S(\tilde{\rho}_\tau || \rho_0^{\text{eq}}) = \tilde{I}_\tau(1 : \dots : n) + S(\gamma_\tau || \rho_0^{\text{eq}}). \quad (21)$$

From Eq. (18), we can obtain our second main result

$$\sum_{j=1}^n \beta_j \langle Q_j \rangle \geq \tilde{I}_\tau(1 : \dots : n). \quad (22)$$

Thus, we have found that the net heat exchanged in multipartite systems is lower bounded by the amount of mutual information between the subsystems.

V. EXAMPLE: TRIPARTITE XY MODEL

As an example, we consider a three-qubit system, whose Hamiltonian is given by the XY model,

$$H_t = \omega(\sigma_z^{(1)} + \sigma_z^{(2)} + \sigma_z^{(3)}) + V_t, \quad (23)$$

where we define

$$V_t \equiv \begin{cases} 0 & (t < 0, t > \tau), \\ \sum_{j=1}^3 \sum_{i < j} (\sigma_x^{(i)} \sigma_x^{(j)} + \sigma_y^{(i)} \sigma_y^{(j)}) & (0 \leq t \leq \tau) \end{cases} \quad (24)$$

with $\{\mathbb{I}, \sigma_x, \sigma_y, \sigma_z\}$ the Pauli matrices. Here, the bare Hamiltonian for each system is $H_j = \omega \sigma_z^{(j)}$ ($j = 1, 2, 3$). Then, we plot the net entropy

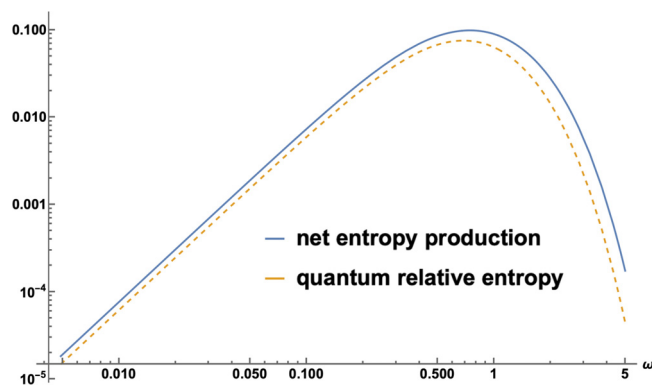


FIG. 2. Three-qubit example: We plot the net entropy production and the quantum relative entropy as a function of the transverse field $\omega \in [0, 5.0]$ with $\beta_1 = 1$, $\beta_2 = 2$, $\beta_3 = 3$, and $\tau = 4.0$. We can verify $\sum_{j=1}^3 \beta_j \langle Q_j \rangle \geq S(\tilde{\rho}_\tau || \rho_0^{\text{eq}})$.

production $\sum_{j=1}^3 \beta_j \langle Q_j \rangle$ and the quantum relative entropy $S(\tilde{\rho}_\tau || \rho_0^{\text{eq}})$ with $\omega \in [0, 5.0]$, $\beta_1 = 1$, $\beta_2 = 2$, $\beta_3 = 3$, and $\tau = 4.0$. Then, we obtain the following result (see Fig. 2), which verifies Eq. (18).

VI. CONCLUSION

In conclusion, we have employed the one-time measurement scheme to derive the generalized quantum exchange fluctuation theorem for multipartite systems, which includes the information about the quantum correlations. From it, we have also obtained a tighter lower bound on the net entropy change, which is set by the quantum mutual information of the thermal state conditioned on the initial energy measurement outcomes. These results elucidate the role of quantum correlations in the heat exchange in a generic scenario, where the effect of the quantum correlation due to the interaction between multiple subsystems is non-negligible.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Akira Sone: Writing – original draft (lead). **Diogo O. Soares-Pinto:** Writing – review & editing (equal). **Sebastian Deffner:** Writing – review & editing (equal).

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

APPENDIX A: PROOF OF EQ. (5)

In this section, we demonstrate the proof of Eq. (5). From Eq. (3), we have

$$\langle Q_j \rangle_P = \int dQ Q_j P(Q) = \frac{1}{|Z|} \sum_{E,E'} (E'_j - E_j) e^{-\beta E} |\langle E' | U_\tau | E \rangle|^2. \quad (A1)$$

Here, note that precisely, because the bare Hamiltonian is time-independent, H_j is

$$H_j \equiv \sum_{E_j} E_j |E_j\rangle \langle E_j| \otimes \mathbb{I}_j = \sum_{E'_j} E'_j |E'_j\rangle \langle E'_j| \otimes \mathbb{I}_j. \quad (A2)$$

Also, we have

$$\sum_{E'} |E'\rangle \langle E'| = \mathbb{I}. \quad (\text{A3})$$

These lead to

$$\langle Q_j \rangle_P = \text{tr}\{(\rho_\tau - \rho_0^{\text{eq}})H_j\} = \langle Q_j \rangle. \quad (\text{A4})$$

APPENDIX B: PROOF OF EQ. (6)

In this section, we demonstrate the proof of Eq. (6). From Eq. (3), we have

$$\langle e^{-\beta \cdot Q} \rangle_P = \int dQ e^{-\beta \cdot Q} P(Q) = \sum_{E, E'} \frac{e^{-\beta \cdot E'}}{|Z|} |\langle E' | U_\tau | E \rangle|^2. \quad (\text{B1})$$

Here, we have

$$\sum_E |E\rangle \langle E| = \mathbb{I} \quad (\text{B2})$$

and

$$|Z| = \sum_{E'} e^{-\beta \cdot E'} = \sum_E e^{-\beta \cdot E} \quad (\text{B3})$$

because of the time-independence of the bare Hamiltonian. Therefore, we can obtain

$$\langle e^{-\beta \cdot Q} \rangle_P = 1. \quad (\text{B4})$$

APPENDIX C: PROOF OF EQ. (13)

In this section, we demonstrate the proof of Eq. (13) in details. From Eqs. (10)–(12), the average conditional heat of the j th system is given by

$$\langle Q_j \rangle_{\tilde{P}} = \int dQ Q_j \tilde{P}(Q) = \sum_E \frac{e^{-\beta \cdot E}}{|Z|} \langle E | U_\tau^\dagger H_j U_\tau | E \rangle - \sum_{E_j} \frac{e^{-\beta_j E_j}}{Z_j} E_j. \quad (\text{C1})$$

Here, we have

$$\text{tr}\{\rho_\tau H_j\} = \text{tr}\{U_\tau \rho_0^{\text{eq}} U_\tau^\dagger H_j\} = \sum_E \frac{e^{-\beta \cdot E}}{|Z|} \langle E | U_\tau^\dagger H_j U_\tau | E \rangle. \quad (\text{C2})$$

Also, from Eq. (1), we have

$$\sum_{E_j} \frac{e^{-\beta_j E_j}}{Z_j} E_j = \text{tr}\{\rho_0^{\text{eq}} H_j\}. \quad (\text{C3})$$

Therefore, we can finally obtain Eq. (13)

$$\langle Q_j \rangle_{\tilde{P}} = \text{tr}\{(\rho_\tau - \rho_0^{\text{eq}})H_j\} = \langle Q_j \rangle. \quad (\text{C4})$$

APPENDIX D: PROOF OF EQ. (17)

In this section, we demonstrate the proof of Eq. (17) in details. From Eq. (14), we have

$$\langle e^{-\beta \cdot Q} \rangle_{\tilde{P}} = \frac{|\tilde{Z}|}{|Z|}, \quad (\text{D1})$$

where $|Z|$ is defined in Eq. (15)

$$|\tilde{Z}| \equiv \sum_E \prod_{j=1}^n e^{-\beta_j \langle E | U_\tau^\dagger H_j U_\tau | E \rangle}. \quad (\text{D2})$$

The conditional thermal state is defined in Eq. (16) as

$$\tilde{\rho}_\tau \equiv \sum_E \frac{e^{-\beta \cdot \tilde{E}(E)}}{|\tilde{Z}|} U_\tau | E \rangle \langle E | U_\tau^\dagger, \quad (\text{D3})$$

and let us compute the quantum relative entropy of $\tilde{\rho}_\tau$ with respect to the initial state ρ_0^{eq} . The quantum relative entropy is given by

$$S(\tilde{\rho}_\tau || \rho_0^{\text{eq}}) = -S(\tilde{\rho}_\tau) - \text{tr}\{\tilde{\rho}_\tau \ln \rho_0^{\text{eq}}\}. \quad (\text{D4})$$

First, the von-Neumann entropy of $\tilde{\rho}_\tau$ is given by

$$\begin{aligned} S(\tilde{\rho}_\tau) &= -\text{tr}\{\tilde{\rho}_\tau \ln \tilde{\rho}_\tau\} \\ &= \sum_E (\beta \cdot \tilde{E}(E)) \text{tr}\{\tilde{\rho}_\tau U_\tau | E \rangle \langle E | U_\tau^\dagger\} + \ln |\tilde{Z}| \\ &= \sum_E \sum_{j=1}^n \beta_j \langle E | U_\tau^\dagger H_j U_\tau | E \rangle \frac{e^{-\beta \cdot \tilde{E}(E)}}{|\tilde{Z}|} + \ln |\tilde{Z}| \\ &= \sum_{j=1}^n \beta_j \text{tr}\{\tilde{\rho}_\tau H_j\} + \ln |\tilde{Z}|. \end{aligned} \quad (\text{D5})$$

Second, the quantum cross entropy $-\text{tr}\{\tilde{\rho}_\tau \ln \rho_0^{\text{eq}}\}$ is given by

$$\begin{aligned} -\text{tr}\{\tilde{\rho}_\tau \ln \rho_0^{\text{eq}}\} &= -\text{tr}\left\{\tilde{\rho}_\tau \ln e^{-\sum_{j=1}^n \beta_j H_j}\right\} \\ &= \sum_{j=1}^n \beta_j \text{tr}\{\tilde{\rho}_\tau H_j\} + \ln |Z|. \end{aligned} \quad (\text{D6})$$

Therefore, we can obtain

$$S(\tilde{\rho}_\tau || \rho_0^{\text{eq}}) = -\ln \frac{|\tilde{Z}|}{|Z|}. \quad (\text{D7})$$

From Eq. (14), we can finally obtain Eq. (17)

$$\langle e^{-\beta \cdot Q} \rangle_{\tilde{P}} = e^{-S(\tilde{\rho}_\tau || \rho_0^{\text{eq}})}. \quad (\text{D8})$$

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