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RESEARCH ARTICLE

Fluctuation relations for heat exchange in the generalized Gibbs ensemble

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In this work, we investigate the heat exchange between two quantum systems whose initial equilibrium states are described by the generalized Gibbs ensemble. First, we generalize the fluctuation relations for heat exchange discovered by Jarzynski and Wójcik to quantum systems prepared in the equilibrium states described by the generalized Gibbs ensemble at various generalized temperatures. Secondly, we extend the connections between heat exchange and the Rényi divergences to quantum systems under generic initial conditions. These relations are applicable for quantum systems with conserved quantities and universally valid for quantum systems in the integrable and chaotic regimes.

Keywords exchange fluctuation relation, generalized Gibbs ensemble

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1 Introduction

In 2004, Jarzynski and Wójcik found that for two quantum systems initially prepared at their thermodynamic equilibrium states with different temperatures T_A and T_B respectively the heat exchange Q between them satisfies the fluctuation theorem [1]

$$\frac{P(Q)}{P(-Q)} = \mathrm{e}^{\Delta\beta Q}, \tag{1}$$

where $P(Q)$ is the distribution of heat exchange and $\Delta\beta \equiv \beta_B - \beta_A$ with $\beta = 1/T$ being the inverse temperature. Recently, the author found that the heat exchange Q between two quantum systems is related to the Rényi divergences between the initial equilibrium state of the total system and the final non-equilibrium state of the total system by [2]

$$\langle (e^{-\Delta\beta Q})^z \rangle = \mathrm{e}^{(z-1)S_z[\rho(0)||\rho(\tau)]}, \tag{2}$$

where z is an arbitrary real number, $\Delta\beta \equiv \beta_B - \beta_A$ with $\beta = 1/T$ being the inverse temperature and the angular bracket on the left side of Eq. (2) means average over ensemble repetitions of initial equilibrium state and the order-z Rényi divergence between $\rho(0)$ and $\rho(\tau)$, which are respectively the initial equilibrium state of the total system and the final non-equilibrium state of the total system at time τ, is defined by $S_z[\rho(0)||\rho(\tau)] \equiv \frac{1}{z-1}\ln[\mathrm{Tr}[\rho(0)^z\rho(\tau)^{1-z}]]$ [3–6]. Equation (2) relates the heat exchange between two systems and the Rényi divergences between microscopic states and thus various moments of the heat exchange are quantified by the relative entropy and the Rényi divergences between microscopic states [2]. The details of various exchange fluctuation relations could be found in Refs. [7–9].

In the exchange fluctuation relations, Eqs. (1) and (2), one assumes that both systems are initially prepared at their own thermodynamic equilibrium states at different temperatures described by the Gibbs ensemble [1, 9]. However, it is known that the equilibrium state of a number of quantum systems cannot be described by the Gibbs ensemble [10–17]. For example, the quantum integrable systems possess a number of conserved quantities which constraint the quantum dynamics of the integrable system [10–17]. The steady state of a quantum integrable system cannot be described by the Gibbs ensemble but are characterized by the generalized Gibbs ensemble [11, 18, 19]. Recently the generalized Gibbs ensemble has been tested experimentally [20]. The purpose of this work is to investigate the heat exchange between two quantum systems whose initial states are best described by the generalized Gibbs ensemble. We found that the heat exchange between quantum systems described by the generalized Gibbs ensemble satisfies heat

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exchange fluctuation relations of the form in Eq. (1) if the generalized heat exchange are defined. Moreover, the heat exchange in the generalized Gibbs ensemble is determined by the Rényi divergences between microscopic states.

The paper is structured as follows: In Section 2, we review some fundamentals of the generalized Gibbs ensemble. In Section 3, we study heat exchange between quantum systems with conserved quantities and then derive the fluctuation relations for heat exchange between quantum systems whose initial equilibrium states are described by the generalized Gibbs ensemble. In Section 4, the relations between heat exchange and the Rényi divergences are established in the generalized Gibbs ensemble. In Section 5, we make use of a physical model to demonstrate our findings. In Section 6, we make a conclusion.

2 The generalized Gibbs ensemble

Ensemble theory is fundamental to the equilibrium thermodynamics and statistical physics [21]. It is known that the statistical ensembles can be derived by the principle of entropy maximization pioneered by Jaynes [22, 23]. For instance, the Gibbs ensemble theory may be deduced by the maximization of the entropy under the constraint that the average energy of the system is fixed and the grand canonical ensemble theory can be derived by the entropy maximization under the constraints that the average energy and the average number of particles are fixed in the equilibrium. However, an important number of physical systems have additional conserved quantities except the energy and particle number. The equilibrium state for quantum system with conserved quantities may also be formulated by the principle of entropy maximization and it turns out that [11] the generalized Gibbs ensemble is established to describe the equilibrium state of the quantum systems with more conserved quantities. For a quantum system with Hamiltonian H and M additional conserved quantities $\{I_1, I_2, \cdots, I_M\}$, the equilibrium state in the generalized Gibbs ensemble is [11]

$$\rho_{\mathrm{GGE}} = \frac{1}{Z} \exp\left[-\left(\beta H + \sum_{k=1}^{M} \beta_k I_k\right)\right], \tag{3}$$

where $Z(\beta, \beta_1, \cdots, \beta_M) = \mathrm{Tr}[\exp(-\beta H - \sum_{k=1}^{M} \beta_k I_k)]$ is the partition function of the generalized Gibbs ensemble. We assume all conserved quantities commute with the Hamiltonian and the conserved quantities also commute with each other in order that they can be measured simultaneously. The generalized inverse temperatures $\{\beta, \beta_1, \cdots, \beta_M\}$ may be determined by imposing that the generalized Gibbs ensemble averages give the known initial values of the energy $\bar{E}$ and other conserved quantities $\bar{I}_1, \bar{I}_2, \cdots, \bar{I}_M$,

$$\langle H\rangle = \mathrm{Tr}[\rho_{GGE} H] = \bar{E}, \tag{4}$$

$$\langle I_k\rangle = \mathrm{Tr}[\rho_{GGE} I_k] = \bar{I}_k, k = 1, 2, \cdots, M. \tag{5}$$

Recently, the generalized Gibbs ensemble has been tested in experiments [20]. In the present work, we investigate the heat exchange between quantum systems whose initial states are described by the generalized Gibbs ensemble (GGE).

3 Heat exchange in the generalized Gibbs ensemble

In this section, we investigate the fluctuation relations for heat exchange between quantum systems which are initialized in the generalized Gibbs ensemble (GGE).

3.1 Distribution of heat exchange between quantum systems described by GGE

The heat exchange process between two quantum systems A and B which are initialized in the generalized Gibbs ensemble can be described by the following steps:

1) Consider the two systems A and B and we assume both of them are integrable systems and thus their equilibrium states are described by GGE. We assume the system A has the following conserved quantities

$$H_A, I_1^A, I_2^A, \cdots I_M^A, J_1, J_2, \cdots, J_{M'}. \tag{6}$$

Here H_A is the Hamiltonian of the system A and the total number of conserved quantities in system A is $M+M'+1$. While the system B has conserved quantities,

$$H_B, I_1^B, I_2^B, \cdots I_M^B, K_1, K_2, K_3, \cdots, K_N. \tag{7}$$

Here H_B is the Hamiltonian of the system B and the number of conserved quantities in system B is $M+N+1$. Note that the conserved quantities $I_1, \cdots, I_M$ are common to both systems while $J_1, J_2, \cdots, J_{M'}$ are conserved quantities only in system A and $K_1, K_2, \cdots, K_N$ are conserved quantities only in system B. The two systems are initialized in their thermodynamics equilibrium states and the initial state of the total system is given by

$$\rho(0) = \frac{\mathrm{e}^{-(\mathcal{H}_A + \mathcal{H}_B)}}{Z_A Z_B}, \tag{8}$$

where we define $\mathcal{H}_A \equiv \beta_0^A H_A + \sum_{i=1}^{M} \beta_i^A I_i^A + \sum_{i=1}^{M'} \lambda_i J_i$ and $\mathcal{H}_B \equiv \beta_0^B H_B + \sum_{i=1}^{M} \beta_i^B I_i^B + \sum_{i=1}^{N} \alpha_i K_i$, $Z_A = \mathrm{Tr}[\mathrm{e}^{-\mathcal{H}_A}]$ and $Z_B = \mathrm{Tr}[\mathrm{e}^{-\mathcal{H}_B}]$ are respectively the partition functions in the GGE for systems A and B respectively. The equilibrium state of system A is characterized by the generalized temperatures $\boldsymbol{\beta}_A = (\beta_0^A, \beta_1^A, \cdots, \beta_M^A)$ and $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, \cdots, \lambda_{M'})$. The GGE state of B is captured by the generalized temperatures $\boldsymbol{\beta}_B = (\beta_0^B, \beta_1^B, \cdots, \beta_M^B)$ and $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \cdots, \alpha_N)$. Here we make use of the vector notation to simplify the expressions.

2) At $t = 0$, we measure the energy and other conserved quantities of the system A, $H_A, I_1^A, I_2^A, \cdots I_M^A, J_1, J_2, J_3, \cdots, J_{M'}$ and that of the system B, $H_B, I_1^B, I_2^B, \cdots I_M^B, K_1, K_2, K_3, \cdots, K_N$ respectively and the outcomes of the first projective measurement are $E_n^A, I_{1,n}^A, I_{2,n}^A, \cdots, J_{1,n}, J_{2,n}, \cdots J_{M',n}$ in system A and $E_n^B, I_{1,n}^B, I_{2,n}^B, \cdots, K_{1,n}, K_{2,n}, \cdots K_{N,n}$ in system B respectively. The measurement results are the eigenvalues of the corresponding operators

$$H_A|n\rangle = E_n^A|n\rangle, \tag{9}$$

$$I_i^A|n\rangle = I_{i,n}^A|n\rangle, i = 1, 2, \cdots, M, \tag{10}$$

$$J_i|n\rangle = J_{i,n}|n\rangle, i = 1, 2, \cdots, M', \tag{11}$$

$$H_B|n\rangle = E_n^B|n\rangle, \tag{12}$$

$$I_i^B|n\rangle = I_{i,n}^B|n\rangle, i = 1, 2, \cdots, M, \tag{13}$$

$$K_i|n\rangle = K_{i,n}|n\rangle, i = 1, 2, \cdots, N. \tag{14}$$

To simplify the notation, we define the following vectors,

$$\boldsymbol{\mathcal{E}}_n^A = (E_n^A, I_{1,n}^A, I_{2,n}^A, \cdots, I_{M,n}^A), \tag{15}$$

$$\boldsymbol{\mathcal{E}}_n^B = (E_n^B, I_{1,n}^B, I_{2,n}^B, \cdots, I_{M,n}^B), \tag{16}$$

$$\boldsymbol{\mathcal{J}}_n = (J_{1,n}, J_{2,n}, \cdots J_{M',n}), \tag{17}$$

$$\boldsymbol{\mathcal{K}}_n = (K_{1,n}, K_{2,n}, \cdots K_{N,n}). \tag{18}$$

With this shorthand notation, the outcome of the first projective measurement is $\{\boldsymbol{\mathcal{E}}_n^A, \boldsymbol{\mathcal{E}}_n^B, \boldsymbol{\mathcal{J}}_n, \boldsymbol{\mathcal{K}}_n\}$ with the corresponding probability

$$p_n(0) = \frac{\mathrm{e}^{-(\boldsymbol{\beta}_A \cdot \boldsymbol{\mathcal{E}}_n^A + \boldsymbol{\lambda} \cdot \boldsymbol{\mathcal{J}}_n + \boldsymbol{\beta}_B \cdot \boldsymbol{\mathcal{E}}_n^B + \boldsymbol{\alpha} \cdot \boldsymbol{\mathcal{K}}_n)}}{Z_A Z_B}. \tag{19}$$

Simultaneously, the quantum state of the total system becomes $|n\rangle = |n_A, n_B\rangle$.

3) We then let the systems A and B contact and interact for a time duration τ. We assume the total Hamiltonian describing the interaction between A and B is

$$\mathcal{H} = H_A + H_B + H_{AB}. \tag{20}$$

Then the quantum state of the total system at $t = \tau$ is $\mathcal{U}_{0,\tau}|n\rangle$ with the time evolution operator being $\mathcal{U}_{0,t} = \exp(-\mathrm{i}t\mathcal{H}) = \exp(-\mathrm{i}t(H_A + H_B + H_{AB}))$.

4) At time τ, we separate the systems A and B apart and then perform the second projective measurement of the conserved quantities of system A and B respectively. The results of the second measurement are $\{\boldsymbol{\mathcal{E}}_m^A, \boldsymbol{\mathcal{E}}_m^B, \boldsymbol{\mathcal{J}}_m, \boldsymbol{\mathcal{K}}_m\}$ and the corresponding conditional probability is given by

$$p_{n\to m} = |\langle m|\mathcal{U}_{0,\tau}|n\rangle|^2. \tag{21}$$

Due to the weak interact between the systems A and B, we then have

$$E_n^A + E_n^B \approx E_m^A + E_m^B, \tag{22}$$

$$I_{k,n}^A + I_{k,n}^B \approx I_{k,m}^A + I_{k,m}^B, \quad k = 1, 2, \cdots, M. \tag{23}$$

With the two systems initialized in the generalized Gibbs ensemble, the generalized heat exchange between the two systems may be defined as

$$\begin{aligned}\mathcal{Q} &= (\boldsymbol{\beta}_B - \boldsymbol{\beta}_A) \cdot (\boldsymbol{\mathcal{E}}_n^A - \boldsymbol{\mathcal{E}}_m^A) - \boldsymbol{\lambda} \cdot (\boldsymbol{\mathcal{J}}_n - \boldsymbol{\mathcal{J}}_m) - \boldsymbol{\alpha} \cdot (\boldsymbol{\mathcal{K}}_n - \boldsymbol{\mathcal{K}}_m) \\ &= \Delta\boldsymbol{\beta} \cdot (\boldsymbol{\mathcal{E}}_n^A - \boldsymbol{\mathcal{E}}_m^A) - \boldsymbol{\lambda} \cdot (\boldsymbol{\mathcal{J}}_n - \boldsymbol{\mathcal{J}}_m) - \boldsymbol{\alpha} \cdot (\boldsymbol{\mathcal{K}}_n - \boldsymbol{\mathcal{K}}_m).\end{aligned} \tag{24}$$

Thus the quantum heat exchange distribution in the GGE is

$$P(Q) = \sum_{m,n} p_n(0) p_{n\to m} \delta[Q - \Delta\boldsymbol{\beta} \cdot (\boldsymbol{\mathcal{E}}_n^A - \boldsymbol{\mathcal{E}}_m^A) + \boldsymbol{\lambda} \cdot (\boldsymbol{\mathcal{J}}_n - \boldsymbol{\mathcal{J}}_m) + \boldsymbol{\alpha} \cdot (\boldsymbol{\mathcal{K}}_n - \boldsymbol{\mathcal{K}}_m)] \tag{25}$$

$$= \sum_{m,n} \frac{\mathrm{e}^{-(\boldsymbol{\beta}_A \cdot \boldsymbol{\mathcal{E}}_n^A + \boldsymbol{\lambda} \cdot \boldsymbol{\mathcal{J}}_n + \boldsymbol{\beta}_B \cdot \boldsymbol{\mathcal{E}}_n^B + \boldsymbol{\alpha} \cdot \boldsymbol{\mathcal{K}}_n)}}{Z_A Z_B} |\langle m|\mathcal{U}_{0,\tau}|n\rangle|^2 \delta[Q - \Delta\boldsymbol{\beta} \cdot (\boldsymbol{\mathcal{E}}_n^A - \boldsymbol{\mathcal{E}}_m^A) + \boldsymbol{\lambda} \cdot (\boldsymbol{\mathcal{J}}_n - \boldsymbol{\mathcal{J}}_m) + \boldsymbol{\alpha} \cdot (\boldsymbol{\mathcal{K}}_n - \boldsymbol{\mathcal{K}}_m)]. \tag{26}$$

The characteristic function for the distribution of heat exchange is given by its Fourier transform,

$$G(u) = \int \mathrm{d}\mathcal{Q} P(\mathcal{Q}) \mathrm{e}^{\mathrm{i}u\mathcal{Q}} \tag{27}$$

$$= \frac{\mathrm{Tr}[\mathrm{e}^{-(\mathcal{H}_A + \mathcal{H}_B)} \mathrm{e}^{-\mathrm{i}u(\mathcal{H}_A + \mathcal{H}_B)} \mathcal{U}_{0,\tau}^\dagger \mathrm{e}^{\mathrm{i}u(\mathcal{H}_A + \mathcal{H}_B)} \mathcal{U}_{0,\tau}]}{\mathrm{Tr}[\mathrm{e}^{-(\mathcal{H}_A + \mathcal{H}_B)}]}. \tag{28}$$

Note that the characteristic function for the distribution of heat exchange has similar expression to the quantum decoherence of a single spin coupled to an environment [24], which has been deeply related to the partition function of the environment [25–30] and quantum phase transitions in the environments [31–33].

3.2 Fluctuation relations for heat exchange in the generalized Gibbs ensemble

To derive the fluctuation relations for heat exchange. we assume the Hamiltonian $\mathcal{H} = H_A + H_B + H_{AB}$ is time reversal invariant,

$$\Theta^{-1}\mathcal{H}\Theta = \mathcal{H}, \tag{29}$$

where Θ is the time reversal operator. Then we have

$$p_n(0)p_{n\to m} = \frac{\mathrm{e}^{-(\boldsymbol{\beta}_A\cdot\boldsymbol{\mathcal{E}}_n^A+\boldsymbol{\lambda}\cdot\boldsymbol{\mathcal{J}}_n+\boldsymbol{\beta}_B\cdot\boldsymbol{\mathcal{E}}_n^B+\boldsymbol{\alpha}\cdot\boldsymbol{\mathcal{K}}_n)}}{Z_A Z_B}|\langle m|\mathcal{U}_{0,\tau}|n\rangle|^2. \tag{30}$$

Then the probability for the time reversed transitions is

$$p_{\Theta m}(0)p_{\Theta m\to\Theta n} = \frac{\mathrm{e}^{-(\boldsymbol{\beta}_A\cdot\boldsymbol{\mathcal{E}}_m^A+\boldsymbol{\lambda}\cdot\boldsymbol{\mathcal{J}}_m+\boldsymbol{\beta}_B\cdot\boldsymbol{\mathcal{E}}_m^B+\boldsymbol{\alpha}\cdot\boldsymbol{\mathcal{K}}_m)}}{Z_A Z_B}|\langle n|\Theta^{-1}\mathcal{U}_{0,\tau}\Theta|m\rangle|^2 \tag{31}$$

$$= \frac{\mathrm{e}^{-(\boldsymbol{\beta}_A\cdot\boldsymbol{\mathcal{E}}_m^A+\boldsymbol{\lambda}\cdot\boldsymbol{\mathcal{J}}_m+\boldsymbol{\beta}_B\cdot\boldsymbol{\mathcal{E}}_m^B+\boldsymbol{\alpha}\cdot\boldsymbol{\mathcal{K}}_m)}}{Z_A Z_B}|\langle n|\mathcal{U}_{0,\tau}^{\dagger}|m\rangle|^2 \tag{32}$$

$$= \frac{\mathrm{e}^{-(\boldsymbol{\beta}_A\cdot\boldsymbol{\mathcal{E}}_m^A+\boldsymbol{\lambda}\cdot\boldsymbol{\mathcal{J}}_m+\boldsymbol{\beta}_B\cdot\boldsymbol{\mathcal{E}}_m^B+\boldsymbol{\alpha}\cdot\boldsymbol{\mathcal{K}}_m)}}{Z_A Z_B}|\langle m|\mathcal{U}_{0,\tau}|n\rangle|^2. \tag{33}$$

From Eqs. (32) to (33), we have made use of the time reversal invariance of the Hamiltonian (29). Dividing $p_n(0)p_{n\to m}$ by $p_{\Theta m}(0)p_{\Theta m\to\Theta n}$, we have

$$\frac{p_n(0)p_{n\to m}}{p_{\Theta m}(0)p_{\Theta m\to\Theta n}} = \mathrm{e}^{-(\boldsymbol{\beta}_A\cdot\boldsymbol{\mathcal{E}}_n^A+\boldsymbol{\lambda}\cdot\boldsymbol{\mathcal{J}}_n+\boldsymbol{\beta}_B\cdot\boldsymbol{\mathcal{E}}_n^B+\boldsymbol{\alpha}\cdot\boldsymbol{\mathcal{K}}_n)}\mathrm{e}^{(\boldsymbol{\beta}_A\cdot\boldsymbol{\mathcal{E}}_m^A+\boldsymbol{\lambda}\cdot\boldsymbol{\mathcal{J}}_m+\boldsymbol{\beta}_B\cdot\boldsymbol{\mathcal{E}}_m^B+\boldsymbol{\alpha}\cdot\boldsymbol{\mathcal{K}}_m)} \tag{34}$$

$$= \mathrm{e}^{\Delta\boldsymbol{\beta}\cdot(\boldsymbol{\mathcal{E}}_n^A-\boldsymbol{\mathcal{E}}_m^A)-\boldsymbol{\lambda}\cdot(\boldsymbol{\mathcal{J}}_n-\boldsymbol{\mathcal{J}}_m)-\boldsymbol{\alpha}\cdot(\boldsymbol{\mathcal{K}}_n-\boldsymbol{\mathcal{K}}_m)} \tag{35}$$

$$= \mathrm{e}^{\mathcal{Q}}. \tag{36}$$

So

$$P(\mathcal{Q}) = \sum_{m,n} p_n(0)p_{n\to m}\delta[Q-\Delta\boldsymbol{\beta}\cdot(\boldsymbol{\mathcal{E}}_n^A-\boldsymbol{\mathcal{E}}_m^A)+\boldsymbol{\lambda}\cdot(\boldsymbol{\mathcal{J}}_n-\boldsymbol{\mathcal{J}}_m)+\boldsymbol{\alpha}\cdot(\boldsymbol{\mathcal{K}}_n-\boldsymbol{\mathcal{K}}_m)] \tag{37}$$

$$= \mathrm{e}^{\mathcal{Q}}\sum_{\Theta m,\Theta n} p_{\Theta m}(0)p_{\Theta m\to\Theta n}\delta[Q-\Delta\boldsymbol{\beta}\cdot(\boldsymbol{\mathcal{E}}_n^A-\boldsymbol{\mathcal{E}}_m^A)+\boldsymbol{\lambda}\cdot(\boldsymbol{\mathcal{J}}_n-\boldsymbol{\mathcal{J}}_m)+\boldsymbol{\alpha}\cdot(\boldsymbol{\mathcal{K}}_n-\boldsymbol{\mathcal{K}}_m)] \tag{38}$$

$$= \mathrm{e}^{\mathcal{Q}}\sum_{\Theta m,\Theta n} p_{\Theta m}(0)p_{\Theta m\to\Theta n}\delta[Q+\Delta\boldsymbol{\beta}\cdot(\boldsymbol{\mathcal{E}}_m^A-\boldsymbol{\mathcal{E}}_n^A)+\boldsymbol{\lambda}\cdot(\boldsymbol{\mathcal{J}}_m-\boldsymbol{\mathcal{J}}_n)+\boldsymbol{\alpha}\cdot(\boldsymbol{\mathcal{K}}_m-\boldsymbol{\mathcal{K}}_n)] \tag{39}$$

$$= \mathrm{e}^{\mathcal{Q}}P(-\mathcal{Q}). \tag{40}$$

We thus derived the exchange fluctuation relations in the GGE,

$$\frac{P(\mathcal{Q})}{P(-\mathcal{Q})} = \mathrm{e}^{\mathcal{Q}}. \tag{41}$$

This is a generalization of the heat exchange fluctuation theorem derive by Jarzynksi and Wójcik [1] into very general family of initial conditions. From Eq. (41), we get

$$\langle \mathrm{e}^{-\mathcal{Q}}\rangle = \int \mathrm{d}\mathcal{Q}P(\mathcal{Q})\mathrm{e}^{-\mathcal{Q}} = \int \mathrm{d}\mathcal{Q}P(-\mathcal{Q}) = 1. \tag{42}$$

In terms of characteristic function of the quantum heat distribution, Eq. (41) can be written as

$$G(u) = G(\mathrm{i}-u). \tag{43}$$

Equation (42) can be written as

$$G(\mathrm{i}) = 1. \tag{44}$$

It is clear that Eq. (44) is a consequence of Eq. (43) because we obtain (44) from (43) by setting $u = 0$.

If the two quantum systems A and B have no conserved quantity except the energy of the system, then the generalized heat exchange reduces to

$$\begin{aligned}\mathcal{Q} &= \Delta\beta(E_n^A - E_m^A) \\ &= (\beta_B - \beta_A)(E_n^A - E_m^A) = \Delta\beta Q.\end{aligned} \tag{45}$$

Thus Eq. (41) reduces to Eq. (1).

Note that the exchange fluctuation relations for the quantum systems which are initialized in the grand canonical ensemble have been known before [7, 9]. While our results for the generalized Gibbs ensemble are more general than the grand canonical ensemble because we have considered much more conserved quantities besides the energy, the particle number etc and thus our results may be applicable for more general cases.

4 Relations between heat exchange and Rényi divergences in the generalized Gibbs ensemble

Recently, the author and its collaborator found that the dissipated work (work minus the free energy difference) in a non-equilibrium process is related to the Rényi divergences between microscopic states in the forward and reversed dynamics under very general family of initial conditions [34–36] and this relation has recently been tested in a superconducting qubit system [37]. In this section, we generalize the relations between heat exchange and the Renyi divergences [2] to quantum systems whose equilibrium states are described by GGE. With the heat distribution function (25), we have the generating function of heat exchange between A and B

$$\langle(\mathrm{e}^{-\mathcal{Q}})^z\rangle = \int \mathrm{d}\mathcal{Q}P(\mathcal{Q})\mathrm{e}^{-z\mathcal{Q}} \tag{46}$$

$$= \sum_{m,n} \frac{\mathrm{e}^{-\left(\boldsymbol{\beta}_A\cdot\boldsymbol{\mathcal{E}}_n^A+\boldsymbol{\lambda}\cdot\boldsymbol{\mathcal{J}}_n+\boldsymbol{\beta}_B\cdot\boldsymbol{\mathcal{E}}_n^B+\boldsymbol{\alpha}\cdot\boldsymbol{\mathcal{K}}_n\right)}}{Z_AZ_B} |\langle m|\mathcal{U}_{0,\tau}|n\rangle|^2\, \mathrm{e}^{-z(\boldsymbol{\beta}_B-\boldsymbol{\beta}_A)\cdot(\boldsymbol{\mathcal{E}}_n^A-\boldsymbol{\mathcal{E}}_m^A)+z\boldsymbol{\lambda}\cdot(\boldsymbol{\mathcal{J}}_n-\boldsymbol{\mathcal{J}}_m)+z\boldsymbol{\alpha}\cdot(\boldsymbol{\mathcal{K}}_n-\boldsymbol{\mathcal{K}}_m)} \tag{47}$$

$$= \frac{1}{Z_AZ_B}\sum_{m,n}\langle m|\mathcal{U}_{0,\tau}|n\rangle\langle n|\mathcal{U}_{0,\tau}^\dagger|m\rangle \mathrm{e}^{-(1-z)\left(\boldsymbol{\beta}_A\cdot\boldsymbol{\mathcal{E}}_n^A+\boldsymbol{\lambda}\cdot\boldsymbol{\mathcal{J}}_n+\boldsymbol{\beta}_B\cdot\boldsymbol{\mathcal{E}}_n^B+\boldsymbol{\alpha}\cdot\boldsymbol{\mathcal{K}}_n\right)}\mathrm{e}^{-z\left(\boldsymbol{\beta}_A\cdot\boldsymbol{\mathcal{E}}_m^A+\boldsymbol{\lambda}\cdot\boldsymbol{\mathcal{J}}_m+\boldsymbol{\beta}_B\cdot\boldsymbol{\mathcal{E}}_m^B+\boldsymbol{\alpha}\cdot\boldsymbol{\mathcal{K}}_m\right)} \tag{48}$$

$$= \frac{1}{Z_AZ_B}\sum_{m,n}\langle m|\mathcal{U}_{0,\tau}\mathrm{e}^{-(1-z)(\mathcal{H}_A+\mathcal{H}_B)}|n\rangle\langle n|\mathcal{U}_{0,\tau}^\dagger\mathrm{e}^{-z(\mathcal{H}_A+\mathcal{H}_B)}|m\rangle \tag{49}$$

$$= \frac{1}{Z_AZ_B}\mathrm{Tr}\left[\mathcal{U}_{0,\tau}\mathrm{e}^{-(1-z)(\mathcal{H}_A+\mathcal{H}_B)}\mathcal{U}_{0,\tau}^\dagger\mathrm{e}^{-z(\mathcal{H}_A+\mathcal{H}_B)}\right] \tag{50}$$

$$= \frac{1}{Z_AZ_B}\mathrm{Tr}\left[\left(\mathcal{U}_{0,\tau}\mathrm{e}^{-(\mathcal{H}_A+\mathcal{H}_B)}\mathcal{U}_{0,\tau}^\dagger\right)^{1-z}\left(\mathrm{e}^{-(\mathcal{H}_A+\mathcal{H}_B)}\right)^z\right] \tag{51}$$

$$= \mathrm{Tr}\left[\left(\mathcal{U}_{0,\tau}\rho(0)\mathcal{U}_{0,\tau}^\dagger\right)^{1-z}\rho(0)^z\right] \tag{52}$$

$$= \mathrm{Tr}\left[\rho(\tau)^{1-z}\rho(0)^z\right] \tag{53}$$

$$= \mathrm{e}^{(z-1)S_z(\rho(0)||\rho(\tau))}. \tag{54}$$

Here we have made use of the shorthand notation $\mathcal{H}_A = \beta_0^A H_A + \sum_{i=1}^M \beta_i^A I_i + \sum_{i=1}^{M'} \lambda_i J_i$ and $\mathcal{H}_B = \beta_0^B H_B + \sum_{i=1}^M \beta_i^B I_i + \sum_{i=1}^N \alpha_i K_i$. We thus proved that the generating function of heat exchange is related to the Rényi divergences between the initial equilibrium state and final out of equilibrium state in the generalized Gibbs ensemble,

$$\langle(\mathrm{e}^{-\mathcal{Q}})^z\rangle = \mathrm{e}^{(z-1)S_z(\rho(0)||\rho(\tau))}. \tag{55}$$

Finally, we make several remarks on Eq. (55):

1) As z is an arbitrary real number in Eq. (55), we set $z = 1$ and yield

$$\langle \mathrm{e}^{-\mathcal{Q}}\rangle = 1. \tag{56}$$

2) From Eq. (55), the average heat exchange in the GGE is

$$\langle\mathcal{Q}\rangle = D\left(\rho(\tau)||\rho(0)\right), \tag{57}$$

where the right hand side is the relative entropy [38] between microscopic states $\rho(\tau)$ and $\rho(0)$, which are the final out of equilibrium state of the total system and the initial equilibrium state of the total system, respectively. Furthermore, the other moments of the heat exchange in the GGE is

$$\langle \mathcal{Q}^n \rangle = \mathrm{Tr}\left[\rho(\tau)\mathcal{T}_n\left(\ln[\rho(\tau)] - \ln[\rho(0)]\right)^n\right], \tag{58}$$

where $n = 1, 2, 3, \cdots$ and $\mathcal{T}_n$ is an ordering operator so that in the binomial expansion of $(\ln[\rho(\tau)] - \ln[\rho(0)])^n$, $\ln[\rho(\tau)]$ always sits on the left of $\ln[\rho(0)]$.

3) It is known in information theory that the Rényi divergences is a measure of the distinguishability between two states [3–6] and therefore the Rényi divergence in Eq. (55) implies that heat exchange is a consequence of out of equilibrium dynamics of two systems.

4) Equation (55) is true for any contact time τ between two systems and this is a result of unitarity in dynamics of quantum systems.

5) If the two quantum systems A and B have no conserved quantity except their energies, then the generalized heat reduces to

$$\begin{aligned}\mathcal{Q} &= \Delta\beta(E_n^A - E_m^A)\\ &= (\beta_B - \beta_A)(E_n^A - E_m^A) = \Delta\beta Q.\end{aligned} \tag{59}$$

Thus Eq. (55) reduces to Eq. (2).

6) The heat exchange in the Gibbs ensemble may be extracted from the Ramsey interference of a single spin [39]. It is conceivable that the same method may be adopted to measure the heat exchange between quantum systems which are described by the generalized Gibbs ensemble. Therefore the central results in this work, the fluctuation relations for heat exchange in the GGE (41) and the relation between heat exchange and the Rényi divergences (55) may be verified experimentally.

5 Physical model study

To demonstrate the above results, we study a physical model which describes the heat exchange between two quantum systems A and B. The system A is a single quantum spin with Hamiltonian

$$H_A = -B_0\sigma_0^z. \tag{60}$$

Here B_0 is the energy splitting of the quantum spin. The system B is a quantum system described by the Jaynes-Cummings (JC) model with Hamiltonian

$$H_B = \omega_0 a^\dagger a + \frac{\Omega}{2}\sigma_1^z + \lambda(\sigma_1^+ a + \sigma_1^- a^\dagger). \tag{61}$$

Here ω_0 is the frequency of the cavity field, Ω is the energy splitting of the atom and λ is the coupling between the atom and the cavity field. The interaction Hamiltonian between A and B is assumed to be

$$H_I = g(\sigma_0^x\sigma_1^x + \sigma_0^y\sigma_1^y). \tag{62}$$

We assume the initial equilibrium state of the system A is the Gibbs state at inverse temperature β_A, $\rho_A = \mathrm{e}^{\beta_A B_0\sigma_0^z}/\mathrm{Tr}[\mathrm{e}^{\beta_A B_0\sigma_0^z}]$. While the initial state of the system B can not be described by the Gibbs ensemble because there is an additional conserved quantity in the system B besides the Hamiltonian H_B, namely $I_1 = a^\dagger a + \sigma_1^z$. In such a case, the equilibrium state of the system B should be described by the generalized Gibbs ensemble with density matrix,

$$\rho_B = \mathrm{e}^{-\beta_B H_B - \beta_1 I_1}/\mathrm{Tr}[\mathrm{e}^{-\beta_B H_B - \beta_1 I_1}]. \tag{63}$$

Here β_B and β_1 are the generalized temperatures in the generalized Gibbs ensemble. After initializations, the two systems interact through H_I for time duration τ. In such a process, the two systems exchange energy. Because system B is described by the generalized Gibbs ensemble, one needs to adopt the concept of generalized heat instead of the heat and the generalized heat distributions satisfy fluctuation relations. To verify our findings, Eq. (43), we need to calculate the characteristic function of the generalized heat distribution, namely,

$$G(u) = \mathrm{Tr}[\mathrm{e}^{-(\mathcal{H}_A+\mathcal{H}_B)}\mathrm{e}^{-\mathrm{i}u(\mathcal{H}_A+\mathcal{H}_B)}\mathcal{U}_{0,\tau}^\dagger \mathrm{e}^{\mathrm{i}u(\mathcal{H}_A+\mathcal{H}_B)}\mathcal{U}_{0,\tau}] \tag{64}$$

$$= \mathrm{Tr}[\mathrm{e}^{-(1+\mathrm{i}u)(\mathcal{H}_A+\mathcal{H}_B)}\mathcal{U}_{0,\tau}^\dagger \mathrm{e}^{\mathrm{i}u(\mathcal{H}_A+\mathcal{H}_B)}\mathcal{U}_{0,\tau}], \tag{65}$$

Here $\mathcal{H}_A = \beta_A H_A$, $\mathcal{H}_B = \beta_B H_B + \beta_1 I_1$ and the evolution operator is $\mathcal{U}_{0,\tau} = \exp[-\mathrm{i}\tau(H_A + H_B + H_I)]$.

In Fig. 1, we show that the characteristic function of quantum heat distribution between system A (a quantum system) and system B (described by the JC model). The system A is initially prepared at temperature, $\beta_A B_0 = 1$. While the initial equilibrium state of system B is described by the generalized Gibbs ensemble with generalized temperatures, $\beta_B\omega_0 = 2$, $\beta_1\omega_0 = 0.5$. For the JC model, we take the parameters $\lambda/\omega_0 = 1, \Omega/\omega_0 = 3, g/\omega_0 = 2$. One can see that both the real part [Fig. 1(a)] and imaginary part [Fig. 1(b)] of $G(u)$ are respectively equal to that of $G(\mathrm{i} - u)$ for arbitrary u. This equivalently means that the generalized heat distribution satisfies $P(\mathcal{Q}) = \mathrm{e}^{\mathcal{Q}}P(-\mathcal{Q})$.

In Fig. 2, we present the average of the exponentiated generalized heat (blue dot) as a function of interaction time $\omega_0\tau$ in the heat exchange process described above. Also we show the Rényi divergences $\mathrm{e}^{(z-1)S_z(\rho(0)||\rho(\tau))}$ with $z = 1/2$ (red solid line) as a function of interaction time $\omega_0\tau$ for the same heat exchange process. One can see that for a quantum system with additional conserved charges, the concept of the generalized heat is key for validating the relations between heat exchange

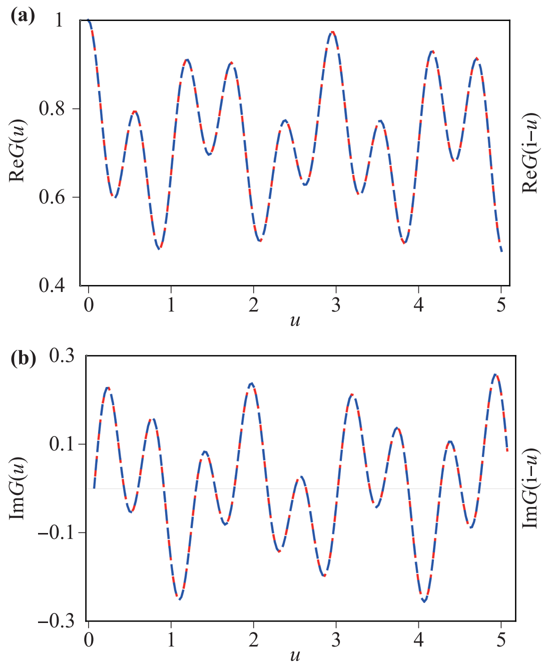

Fig. 1 Comparison of $G(u)$ and $G(\mathrm{i}-u)$, which are the characteristic function of the generalized heat distribution between two quantum systems, one is a quantum spin and the other system is described by JC model. The system A is initialized at temperature, $\beta_A B_0 = 1$ while the initial equilibrium state of system B is described by the generalized Gibbs ensemble with generalized temperatures, $\beta_B\omega_0 = 2$, $\beta_1\omega_0 = 0.5$. In the JC model, we take the parameters $\lambda/\omega_0 = 1$, $\Omega/\omega_0 = 3$, $g/\omega_0 = 2$. **(a)** The real part of the characteristic function, $\mathrm{Re}G(u)$, as a function of u (the red dashed line) and the real part of the characteristic function $\mathrm{Re}G(\mathrm{i}-u)$ as a function of u (the blue dashed line). **(b)** The imaginary part of the characteristic function $\mathrm{Re}G(u)$ as a function of u (the red dashed line) and the imaginary part of the characteristic function $\mathrm{Re}G(\mathrm{i}-u)$ as a function of u (the blue dashed line).

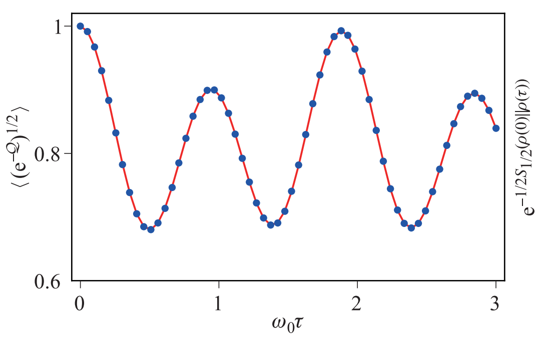

Fig. 2 The exponentiated generalized heat and the Rényi divergences in the generalized Gibbs ensemble. The blue dot shows $\langle (e^{-\mathcal{Q}})^{1/2} \rangle$ as a function of interaction time $\omega_0\tau$ between system A and B. The red solid line shows $e^{(z-1)S_z(\rho(0)||\rho(\tau))}$ with $z = 1/2$ as a function of interaction time τ for the same interaction process. The value of the parameters for system A and B are the same as that in Fig. 1.

and Rényi divergences. For quantum systems without additional conserved charges except the Hamiltonian, the generalized heat reduces to the ordinary heat.

6 Conclusions

We have investigated the heat exchange between two quantum systems initialized in the equilibrium states described by the generalized Gibbs ensemble. We have found that statistics of heat exchange satisfies fluctuation relations for quantum systems initialized in equilibrium states described by the generalized Gibbs ensemble at different generalized temperatures if we adopt the concept of generalized heat exchange. This fluctuation relation is a generalization of the heat exchange fluctuation relation by Jarzynski and Wójcik to quantum systems described by generalized Gibbs ensemble. Moreover, we have extended the connections between heat exchange and Rényi divergences to quantum systems initialized in the generalized Gibbs ensemble. These relations are applicable for quantum systems with conserved quantities and are universally valid for quantum systems in the integrable and chaotic regimes.

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