Relations between heat exchange and Rényi divergences

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In this work, we establish an exact relation which connects the heat exchange between two systems initialized in their thermodynamic equilibrium states at different temperatures and the Rényi divergences between the initial thermodynamic equilibrium state and the final nonequilibrium state of the total system. The relation tells us that the various moments of the heat statistics are determined by the Renyi divergences between the initial equilibrium state and the final nonequilibrium state of the global system. In particular the average heat exchange is quantified by the relative entropy between the initial equilibrium state and the final nonequilibrium state of the global system. The relation is applicable to both finite classical systems and finite quantum systems.

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I. INTRODUCTION

Work and heat are two central themes of equilibrium thermodynamics [1]. However, for finite systems, the work and the heat exchange are random numbers and both of them have a distribution. In an intriguing development Jarzynski [2] found that for a finite classical system prepared in the thermodynamic equilibrium state the work in a nonequilibrium process is related to the equilibrium free energy differences between the thermodynamic equilibrium states for the final and initial control parameters. The Jarzynski equality establishes deep connections between the equilibrium free energy differences and the work in a nonequilibrium process [3–9]. Afterward, the Jarzynski equality has been demonstrated to hold in finite quantum mechanical systems based on the two projective measurements [10–14]. Since the discovery of the Jarzynski equality, the investigation of various fluctuation relations in nonequilibrium thermodynamics has become an active research field [15–17]. Recently we found [18–20] that the dissipated work which is defined as the work minus the free energy difference is related to the Rényi divergences between two microscopic states in the forward and reversed dynamics. This relation links the dissipation in nonequilibrium thermodynamics to the Rényi divergences in information theory and has recently been verified experimentally in a superconducting qubit system [21].

In 2004, Jarzynski and Wójcik discovered that the heat exchange between two systems A and B which are initialized in the thermodynamic equilibrium states at different temperatures T_A and T_B respectively satisfies the following fluctuation relation [22]:

$$\langle e^{-\Delta\beta Q}\rangle = 1. \tag{1}$$

Here $\Delta\beta = \beta_B - \beta_A$ with $\beta = 1/T$ being the inverse temperature. For more developments on the exchange fluctuation relations, one may refer to [17]. The central result of this paper is the following exact relation about the heat exchange between two systems A and B:

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

where z is an arbitrary real number, Q is the heat exchange between A and B, the angular bracket on the left side denotes an ensemble average over all realizations of the heat exchange process, and $S_z[\rho(0)||\rho(\tau)] \equiv \frac{1}{z-1}\ln\{\mathrm{Tr}[\rho(0)^z\rho(\tau)^{1-z}]\}$ is the order-z Rényi divergence [23–26] between the initial equilibrium state of the total system $\rho(0)$ and the final nonequilibrium state of the total system at time τ, $\rho(\tau)$. Equation (2) is applicable for both finite classical mechanical systems and finite quantum mechanical systems. For classical systems, the $\rho(0)$ and $\rho(\tau)$ that appeared in Eq. (2) should be understood as the corresponding phase-space density, and the trace is replaced by an integral over the entire phase space of the total system. While for quantum mechanical system, $\rho(0)$ and $\rho(\tau)$ in Eq. (2) should be understood as the quantum density matrices of the total system. Equation (2) connects a macroscopic quantity, the heat exchange between two systems, and a microscopic quantity, the Rényi divergences of two microscopic states.

Because the definitions of heat exchange in classical systems and in quantum systems are different [17], we shall discuss the derivation of Eq. (2) for classical systems and quantum systems individually.

II. HEAT EXCHANGE FOR CLASSICAL SYSTEMS

First of all, we discuss the heat exchange between two classical systems which are initialized in their thermodynamic equilibrium state at different temperatures.

A. Distribution of heat exchange in classical systems

Consider two classical systems A and B and their Hamiltonians are given by $H_A(X^A)$ and $H_B(X^B)$, respectively. Here X^A denotes a phase-space point in system A, X^B denotes a phase-space point in system B, and $X = (X^A,X^B)$ labels a point in the phase space of the global system. Now let us describe the heat-exchange process in the classical system.

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(1) At $t = 0$, we initialize two classical systems in the thermodynamic equilibrium states at temperatures T_A and T_B. For simplicity, we assume $T_A > T_B$. Then the initial state of the whole system is given by

$$\rho(X_0;0) = \frac{e^{-[\beta_A H_A(X_0^A)+\beta_B H_B(X_0^B)]}}{Z_A Z_B}. \tag{3}$$

Here $X_0 = (X_0^A;X_0^B)$ is a phase-space point in the global system, $\beta_A = 1/T_A$, $\beta_B = 1/T_B$, and $Z_A = \int dX_0^A e^{-\beta_A H_A(X_0^A)}$ is the partition function of the system A and the partition function of system B is $Z_B = \int dX_0^B e^{-\beta_B H_B(X_0^B)}$.

(2) We measure energies of the two systems A and B and the outcomes are $H_A(X_0^A)$ and $H_B(X_0^B)$ with the corresponding probability $\rho(X_0;0)$.

(3) Let the two systems in thermal contact with each other for a time duration τ which is arbitrary and the total Hamiltonian including the interactions is

$$\mathcal{H} = H_A(X^A) + H_B(X^B) + H_{AB}(X^A;X^B). \tag{4}$$

(4) We separate the systems A and B and then measure energies of the two systems respectively and the results are $H_A(X_1^A)$ and $H_B(X_1^B)$. Here $X_1 = (X_1^A,X_1^B)$ is the phase-space point of the global system at time τ under the dynamics governed by the total Hamiltonian $\mathcal{H}$ when the initial phase-space point is $X_0 = (X_0^A,X_0^B)$. We assume the interaction H_{AB} is weak such that the energy of the global system is approximately conserved and thus the heat exchange is given by [22]

$$Q = H_B\big(X_1^B\big) - H_B\big(X_0^B\big) = H_A\big(X_0^A\big) - H_B\big(X_1^B\big). \tag{5}$$

Thus the probability distribution for heat exchange is given by

$$P(Q) = \int dX_0 \rho(X_0;0)\delta\big(Q - H_B\big(X_1^B\big) + H_B\big(X_0^B\big)\big). \tag{6}$$

B. Heat exchange and Rényi divergences in classical systems

Now we are ready to evaluate the generating function of heat exchange,

$$\begin{aligned}
&\langle (e^{-\Delta\beta Q})^z\rangle \\
&= \int dX_0 \rho(X_0;0) e^{-z\Delta\beta[H_B(X_1^B)-H_B(X_0^B)]}, && (7)\\
&= \frac{1}{Z_A Z_B}\int dX_0 e^{-[\beta_A H_A(X_0^A)+\beta_B H_B(X_0^B)]} e^{-z\beta_B[H_B(X_1^B)-H_B(X_0^B)]} \\
&\quad \times e^{-z\beta_A[H_B(X_0^A)-H_B(X_1^A)]}, && (8)\\
&= \frac{1}{Z_A Z_B}\int dX_0 (e^{-[\beta_A H_A(X_0^A)+\beta_B H_B(X_0^B)]})^{1-z} \\
&\quad \times (e^{-[\beta_A H_A(X_1^A)+\beta_B H_B(X_1^B)]})^{z}, && (9)\\
&= \int dX_0 \rho(X_0;0)^{1-z}\rho(X_1;0)^z, && (10)\\
&= \int dX_1 \rho(X_1;\tau)^{1-z}\rho(X_1;0)^z, && (11)\\
&= \exp\{(z-1)S_z[\rho(X;0)||\rho(X;\tau)]\}. && (12)
\end{aligned}$$

Here $\Delta\beta = \beta_B - \beta_A > 0$ and z is an arbitrary real number. From Eq. (10) to (11), we have made use of the Liouville theorem in Hamilton dynamics, which states that the phase-space density along a trajectory of the classical system is invariant, which means that $\rho(X_0,0) = \rho(X_1,\tau)$ and also the phase-space volume is invariant under Hamilton dynamics $dX_0 = dX_1$. From Eq. (11) to (12), we made use of the definition of Rényi divergences or Rényi relative entropy [23–26], $S_z(\rho_1||\rho_2) = \frac{1}{z-1}\ln\int dX\rho_1(X)\rho_2(X)$, which is the order-z Rényi divergence between two probability distributions ρ_1 and ρ_2. We thus derived the relation between heat exchange and the Renyi divergences in classical systems,

$$\langle (e^{-\Delta\beta Q})^z\rangle = \exp\{(z-1)S_z[\rho(X;0)||\rho(X;\tau)]\}. \tag{13}$$

Now we make several remarks on the above equality:

(1) In Eq. (13), z is a free parameter and it can take any real values. In the case of $z = 1$, we recover

$$\langle e^{-\Delta\beta Q}\rangle = 1. \tag{14}$$

This is the fluctuation relation for heat exchange first derived by Jarzynski in 2004 [22].

(2) The generating function of heat exchange shall give us the various moments of heat statistics. In particular, the average heat exchange is given by

$$(\beta_B - \beta_A)\langle Q\rangle = D[\rho(X,\tau)||\rho(X,0)], \tag{15}$$

where the right-hand side is the relative entropy [27] between the final nonequilibrium phase-space density of the global system $\rho(X,\tau)$ and the initial equilibrium phase-space density of the global system $\rho(X,0)$. Furthermore, the higher order moments of the heat exchange are given by

$$\langle Q^n\rangle = (\beta_B - \beta_A)^{-n}\int dX\rho(X,\tau)\bigg(\ln\frac{\rho(X,\tau)}{\rho(X,0)}\bigg)^n. \tag{16}$$

Here $n = 1,2,3,\ldots$.

(3) The Renyi divergence is a valid measure of the distinguishability [23–26] and thus the Renyi divergence that appears in Eq. (13) means that heat exchange is a consequence of nonequilibrium dynamics.

(4) Equation (13) is valid for any interaction time τ which is a consequence of the Liouville theorem in Hamilton dynamics.

III. HEAT EXCHANGE FOR QUANTUM SYSTEMS

In this section, we consider the heat exchange between two quantum systems A and B.

A. Distribution of heat exchange in quantum systems

The heat exchange between two systems A and B is defined by the following steps:

(1) The two systems A and B are separately prepared at their own thermodynamic equilibrium states at different temperatures T_A and T_B. For simplicity, we assume that $T_A > T_B$. Then the initial state of the whole system is

$$\rho(0) = \frac{e^{-\beta_A H_A}}{Z_A}\otimes\frac{e^{-\beta_B H_B}}{Z_B}, \tag{17}$$

where $\beta = 1/T$, $Z_A = \mathrm{Tr}[e^{-\beta_A H_A}]$ is the equilibrium partition function of system A, and the partition function of the system B is defined by $Z_B = \mathrm{Tr}[e^{-\beta_B H_B}]$.

(2) We perform the first projective measurement of the energy H_A and H_B and we assume the outcomes are $E_{n,A}$ and $E_{n,B}$, respectively, with the corresponding probability

$$p_n(0) = \frac{e^{-(\beta_A E_{n,A}+\beta_B E_{n,B})}}{Z_A Z_B}. \tag{18}$$

Here $H_A|n,A\rangle = E_{n,A}|n,A\rangle$ and $H_B|n,B\rangle = E_{n,B}|n,B\rangle$. At the same time the states of the two systems are projected into the corresponding eigenstates $|n\rangle = |n_A,n_B\rangle$.

(3) We allow the systems A and B to interact for some time τ and the total Hamiltonian including the interactions is

$$\mathcal{H} = H_A + H_B + H_{AB}. \tag{19}$$

After interactions, the state of the global system is $\mathcal{U}_{0,\tau}|n\rangle$. Here the time development operator is given by

$$\mathcal{U}_{0,\tau} = \exp(-it\mathcal{H}) = \exp[-it(H_A + H_B + H_{AB})]. \tag{20}$$

(4) After interactions for time interval τ, we then separate the systems A and B.

(5) Finally we perform the second projective measurement of the energy H_A and H_B, and we assume the outcomes are $E_{m,A}$ and $E_{m,B}$, respectively, and the conditional probability for obtaining $E_{m,A}$ and $E_{m,B}$ is

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

Here $|m\rangle = |m_A,m_B\rangle$ and they satisfy the Schrödinger equation, $H_A|m_A\rangle = E_{m,A}|m,A\rangle$ and $H_B|m_B\rangle = E_{m,B}|m,B\rangle$. We assume the interactions is so weak that approximately the energy of the total system is conserved. Thus the heat exchange between the two systems A and B is

$$Q = E_{n,A} - E_{m,A} \approx E_{m,B} - E_{n,B}. \tag{22}$$

Thus the quantum heat-exchange distribution is [22]

$$\begin{aligned} P(Q) &= \sum_{m,n} p_n(0) p_{n\to m} \delta(Q - E_{m,B} + E_{n,B}), && (23)\\ &= \sum_{m,n} p_n(0) |\langle m|\mathcal{U}_{0,\tau}|n\rangle|^2 \delta(Q - E_{m,B} + E_{n,B}), && (24)\\ &= \sum_{m,n} \frac{e^{-(\beta_A E_{n,A}+\beta_B E_{n,B})}}{Z_A Z_B} |\langle m|\mathcal{U}_{0,\tau}|n\rangle|^2 \delta\\ &\quad \times (Q - E_{m,B} + E_{n,B}). && (25)\end{aligned}$$

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

$$\begin{aligned} G(u) &= \int dQ P(Q) e^{iuQ},\\ &= \mathrm{Tr}[e^{-(\beta_A H_A+\beta_B H_B)} e^{-iuH_B} \mathcal{U}_{0,\tau}^\dagger e^{iuH_B} \mathcal{U}_{0,\tau}]. && (26)\end{aligned}$$

It should be noted that the characteristic function for heat exchange in Eq. (26) has an expression analogous to the quantum decoherence of a probe spin coupled to a bath [28] which has been demonstrated to connect to the partition function of the bath in the complex plane of physical parameters [29–35].

B. Heat exchange and Rényi divergences in quantum systems

The generating function of heat exchange between A and B are

$$\begin{aligned} \langle (e^{-\Delta\beta Q})^z \rangle &= \int dQ P(Q) e^{-z\Delta\beta Q}, && (27)\\ &= \sum_{m,n} \frac{e^{-(\beta_A E_{n,A}+\beta_B E_{n,B})}}{Z_A Z_B} |\langle m|\mathcal{U}_{0,\tau}|n\rangle|^2 e^{-z(\beta_B-\beta_A)(E_{m,B}-E_{n,B})}, && (28)\\ &= \sum_{m,n} \frac{e^{-(\beta_A E_{n,A}+\beta_B E_{n,B})}}{Z_A Z_B} \langle m|\mathcal{U}_{0,\tau}|n\rangle\langle n|\mathcal{U}_{0,\tau}^\dagger|m\rangle e^{-z(\beta_B-\beta_A)(E_{m,B}-E_{n,B})}, && (29)\\ &= \frac{1}{Z_A Z_B} \sum_{m,n} \langle m|\mathcal{U}_{0,\tau} e^{-(1-z)(\beta_A H_A+\beta_B H_B)}|n\rangle\langle n|\mathcal{U}_{0,\tau}^\dagger e^{-z(\beta_A H_A+\beta_B H_B)}|m\rangle, && (30)\\ &= \frac{1}{Z_A Z_B} \mathrm{Tr}[\mathcal{U}_{0,\tau} e^{-(1-z)(\beta_A H_A+\beta_B H_B)} \mathcal{U}_{0,\tau}^\dagger e^{-z(\beta_A H_A+\beta_B H_B)}], && (31)\\ &= \frac{1}{Z_A Z_B} \mathrm{Tr}[(\mathcal{U}_{0,\tau} e^{-(\beta_A H_A+\beta_B H_B)} \mathcal{U}_{0,\tau}^\dagger)^{1-z} (e^{-(\beta_A H_A+\beta_B H_B)})^z], && (32)\\ &= \mathrm{Tr}[(\mathcal{U}_{0,\tau}\rho(0)\mathcal{U}_{0,\tau}^\dagger)^{1-z}\rho(0)^z], && (33)\\ &= \mathrm{Tr}[\rho(\tau)^{1-z}\rho(0)^z], && (34)\\ &= \exp\{(z-1)S_z[\rho(0)||\rho(\tau)]\}. && (35)\end{aligned}$$

Here $\rho(\tau) = \mathcal{U}_{0,\tau}\rho(0)\mathcal{U}_{0,\tau}^\dagger$. Thus we have derived the relation between heat exchange and the Renyi divergences in quantum mechanical systems,

$$\langle (e^{-\Delta\beta Q})^z \rangle = \exp\{(z-1)S_z[\rho(0)||\rho(\tau)]\}. \tag{36}$$

We make several remarks on the above relation:

(1) In Eq. (36), z is an arbitrary real number and if $z = 1$ we get

$$\langle e^{-\Delta\beta Q}\rangle = 1. \tag{37}$$

This is the exchange fluctuation theorem in quantum mechanical systems first derived by Jarzynksi in 2004 [22].

(2) The average heat exchange is given by

$$(\beta_B - \beta_A)\langle Q\rangle = D[\rho(\tau)||\rho(0)]. \tag{38}$$

Here the right-hand side is the relative entropy [27] between the final nonequilibrium state $\rho(\tau)$ and the initial equilibrium state of the global system $\rho(0)$. Moveover, the higher order moments of the heat exchange is given by

$$\langle Q^n\rangle = (\beta_B - \beta_A)^{-n}\mathrm{Tr}(\rho(\tau)\mathcal{T}_n\{\ln[\rho(\tau)] - \ln[\rho(0)]\}^n). \tag{39}$$

Here $n = 1,2,3,\ldots,$ and $\mathcal{T}_n$ is an ordering operator which sorts that in each term of the binomial expansion $\{\ln[\rho(\tau)] - \ln[\rho(0)]\}^n$, $\ln[\rho(\tau)]$ always lies on the left of $\ln[\rho(0)]$.

(3) The Renyi divergences is a valid measure of the distinguishability [23–26] and thus the Renyi divergence appearance in Eq. (36) for quantum system means that the heat exchange comes from the nonequilibrium quantum dynamics of the systems due to interactions.

(4) Equation (36) is valid for any interaction time τ which is a consequence of unitarity in quantum dynamics.

(5) It was proposed that the quantum heat exchange could be measured from the Ramsey interference of a single spin [36]. Thus our relation (36) means that we can also measure the family of quantum Rényi divergences between the equilibrium state and an out-of-equilibrium state of a quantum system by the Ramsey interference experiment.

Lastly we would like to stress the difference between the present work and Ref. [18]. In Ref. [18], we considered a system which is initialized in a thermal equilibrium state under nonequilibrium driving. In the driving process, work is performed on the system and we found the dissipated work (work minus the free energy difference) and Rényi divergences between the quantum states in the driving process and its time-reversed process are deeply related. While in the present work we found the heat exchange between two systems initialized in their thermal equilibrium states with different temperatures is also quantified by the Rényi divergences between the initial state of the total system and the final state of the total system. Reference [18] and the present work provide links between the fundamental concepts in nonequilibrium thermodynamics and information theory.

IV. SUMMARY

In summary, we have derived an exact equality which relates the heat exchange between two systems initialized in the thermodynamic equilibrium states at different temperatures and the Rényi divergences between the initial thermodynamic equilibrium state and the final nonequilibrium state of the global system. Because the Renyi divergence is a valid measure of distinguishability, the relation implies that heat exchange comes from the nonequilibrium dynamics of two systems. The relation implies that the various moments of the heat statistics are determined by the Rényi divergences. In particular, the average heat exchange between two systems initially prepared at different temperatures is quantified by the relative entropy of the initial equilibrium state and the final nonequilibrium state of the global system. Our results are consequences of two assumptions, namely, the initial states of the two systems are described by the Gibbs ensemble and the interaction energy in the process of contact is negligible compared to the energy of both systems. The relation is applicable to both finite classical systems and finite quantum systems. Finally it is conceivable that similar relations could be derived for particle exchange between two systems initialized in the thermodynamic equilibrium states with different chemical potentials.

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