



OPEN

The entropy production for thermal operations

H. Dolatkhan¹, S. Salimi¹, A. S. Khorashad¹✉ & S. Haseli²

According to the first and second laws of thermodynamics and the definitions of work and heat, microscopic expressions for the non-equilibrium entropy production have been achieved. Recently, a redefinition of heat has been presented in [Nature Communications volume 8, Article number: 2180 (2017)]. Since thermal operations play an important role in the resource theory of thermodynamics, it would be very interesting to find out the effect of the above-mentioned definition on the expression of the entropy production for these kind of operations. This is one of the aims of the present paper. Using the new definition of heat, it is shown that the entropy production is the same as the mutual information between a system and a bath both for thermal operations and, if the system-bath initial state is factorized, for entropy-preserving operations. It is also discussed that how one can recognize the type of the correlation between a system and a bath through knowledge of the initial state of the system only. It is shown that if the initial state of a system is diagonal in the energy basis, the thermal operations cannot create a quantum correlation between the system and the bath, however, if the system initial state is coherent Gibbs state, there cannot be classical correlation due to the thermal operations.

Recently, study on thermodynamic behavior of quantum mechanical systems has attracted much attention. In fact, providing a clear understanding about the fundamental concepts such as work and heat, and obtaining a deep knowledge of thermodynamics laws in quantum world, have been the main topic of many researches^{1–11}. To understand the foundations of quantum thermodynamics, one can consider it as a resource theory. There are different models for the resource theories of thermodynamics^{12–14}, which vary mostly on the set of allowed operations. One of the most important models is the resource theory of thermal operations (TOs). TOs were introduced in ref. ¹⁵ and applied later in refs. ^{16–19}.

The set of TOs, $\{\varepsilon_T\}$, consists of all maps acting on the state of a system as^{15–17}:

$$\rho'_S = \varepsilon_T(\rho_S) = Tr_B(\rho'_{SB}), \quad (1)$$

in which Tr_B is partial trace over the bath, and ρ'_{SB} is the state of the composite system after the evolution, i.e.,

$$\rho'_{SB} = U_{SB}(\rho_S \otimes \rho_B^{eq})U_{SB}^\dagger$$

where

1. U_{SB} is an energy-preserving unitary operator applied to the system and the bath satisfying

$$[U_{SB}, H_S + H_B] = 0, \quad (2)$$

here, H_S and H_B are Hamiltonians of the system and the bath, respectively.

2. ρ_B^{eq} is a thermal state of the bath at some fixed temperature,

$$\rho_B^{eq} = \frac{e^{-\beta H_B}}{Z_B}, \quad (3)$$

where $\beta = \frac{1}{k_B T}$ (throughout the paper it is assumed that $k_B = 1$), and $Z_B = tr(e^{-\beta H_B})$ is known as the partition function.

¹Department of Physics, University of Kurdistan, P. O. Box: 66177-15175, Sanandaj, Iran. ²Faculty of Physics, Urmia University of Technology, Urmia, Iran. ✉e-mail: a.sorouri@uok.ac.ir

There are two important properties for TOs which are^{20,21}:

1. They have time translation symmetry,

$$\varepsilon_T(e^{-iH_S t} \rho_S e^{iH_S t}) = e^{-iH_S t} \varepsilon_T(\rho_S) e^{iH_S t}, \quad (4)$$

2. They preserve the thermal state,

$$\varepsilon_T(\rho_S^{eq}) = \rho_S^{eq}. \quad (5)$$

Regarding the first law of thermodynamics and this fact that the thermal bath is an incoherent mixture of energy states, Eq. (4) indicates conservation of energy. Equation (5) expresses that it is impossible to change a thermal state without doing any work. This means that there cannot exist any machine working in a cycle and converting thermal energy into work completely. This is actually the physical meaning of the second law of thermodynamics.

The conservation of energy in thermodynamic systems is the topic of the first law of thermodynamics, which states that every increase in the internal energy of a system is due to the following two ways: (a) the work performed on the system and/or (b) the heat absorbed by the system. Irreversible processes are described by the second law of thermodynamics. According to this law, the entropy production is always non-negative; it is zero only when the system and the environment are in thermal equilibrium. Regarding the first and second laws of thermodynamics, one can derive microscopic expressions for the non-equilibrium entropy production in quantum systems^{22–27,45}.

Recently, a new definition of heat has been provided in which the authors introduced heat by properly referring to the information flow and thereby restoring Landauer's erasure principle²⁸. Here, the effect of the definition on the expression of the entropy production for TOs is determined. Since microscopic expression of the non-equilibrium entropy production depends on the definition of heat, one can expect that any new definition of it might change the expression of the entropy production. It is also shown that TOs cannot generate quantum correlation from incoherent input states, however, if the initial state of a system is a coherent Gibbs state, correlation between the system and the bath is quantum correlation.

In the following, firstly, free energy definition and heat definitions are presented. Secondly, using the heat definitions, the corresponding expressions of non-equilibrium entropy production are obtained. Finally, the role of quantum coherence in the entropy production for TOs is studied.

Preliminary

The non-equilibrium free energy for a system in a state ρ_S with Hamiltonian H_S , which interacts with a thermal bath at temperature T , is defined as:

$$F(\rho_S) = E_S - TS(\rho_S), \quad (6)$$

where $E_S = \text{tr}(H_S \rho_S)$ is internal energy and $S(\rho_S) = -\text{tr}(\rho_S \ln(\rho_S))$ is the von Neumann entropy of the system. If one uses $H_S = -\frac{1}{\beta}(\ln(\rho_S^{eq}) + \ln(Z_S))$, the non-equilibrium free energy can be written as

$$F(\rho_S) = F_{eq} + TS(\rho_S || \rho_S^{eq}), \quad (7)$$

where $F_{eq} = -\frac{1}{\beta} \ln(Z_S)$ is the free energy in thermal equilibrium, and $S(\rho_S || \rho_S^{eq})$ is the relative entropy. It is worth mentioning that $F(\rho_S) \geq F_{eq}$ due to the non-negativity of the relative entropy.

Usually, heat is defined as the change in the internal energy of the bath^{29,31},

$$\Delta \bar{Q} = -\Delta E_B. \quad (8)$$

Although many researchers have used this definition in their works^{24,29,31}, it has been recently shown that it is not a perfect definition for heat²⁸. To provide a more proper definition, one can assume that there is a thermal bath whose state is initially given by a thermal state ρ_B^{eq} and it is subject to Hamiltonian H_B at temperature T . In a process, where the bath state ρ_B^{eq} transforms to ρ_B under the condition that the Hamiltonian H_B is remained unchanged, heat is defined as²⁸

$$\Delta Q = -(\Delta E_B - \Delta F_B) = \frac{-1}{\beta} \Delta S_B, \quad (9)$$

where $\Delta F_B = F(\rho_B') - F(\rho_B^{eq})$ is the change in the free energy of the bath which is stored in the bath as the extractable work. $\Delta S_B = S(\rho_B') - S(\rho_B^{eq})$ is the change in the von Neumann entropy of the bath due to the state transformation. Since in this approach heat is expressed in terms of the entropy difference of the bath, one can say that there is an explicit relation between heat and information flow to or from the bath. This is consistent with Landauer's erasure principle³⁰. According to Eq. (9), heat is also responsible for the change in the internal energy of the bath. However, the bath internal energy can be varied through other form of energy flow on the condition that entropy is preserved. This form of energy flow is stored as extractable work. Comparing Eq. (8) with Eq. (9), one has

$$\Delta Q = \Delta \bar{Q} + \Delta F_B. \quad (10)$$

Since ΔF_B is always non-negative (due to this fact that the initial state of the bath is thermal and the free energy for this state has its minimum value), one comes to

$$\Delta Q \geq \Delta \bar{Q}. \quad (11)$$

If the bath deviates from thermal equilibrium by small variation through a TO, $\rho_B' \sim \rho_B^{eq} + \varepsilon$, one will have $\Delta F_B = TS(\rho_B' || \rho_B^{eq}) \sim \varepsilon^2$ which goes to zero in the limit of large bath. Therefore, both definitions are consistent.

New entropy production for thermal operations

When a system experiences a dynamical process, the change in its entropy, ΔS_S , includes a reversible and an irreversible contribution. The reversible contribution is due to the heat flow, which can be addressed as the entropy flow $\Delta S^{rev} = \beta \Delta Q$, and the irreversible one is called entropy production ΔS^{irr} . Therefore, one can write

$$\Delta S_S = \Delta S^{irr} + \Delta S^{rev}. \quad (12)$$

Regarding the usual definition of heat, Eq. (8), and the total change in the entropy of a system, Eq. (12), one can obtain the entropy production for TOs,

$$\Delta S^{irr} = -\beta \Delta F_S = S(\rho_S || \rho_S^{eq}) - S(\rho_S' || \rho_S^{eq}), \quad (13)$$

which is the familiar form of the entropy production for TOs^{23,35} (see Methods for more detail). ΔS^{irr} is always non-negative due to the contraction of the quantum relative entropy³². As a result

$$\Delta F_S \leq 0, \quad (14)$$

meaning that free energy of the system is decreasing under TOs^{18,20}. According to the definition of TO, Eq. (13) can be written as^{24,25}:

$$\Delta S^{irr} = S(\rho_B' || \rho_B^{eq}) + I(\rho_{SB}'), \quad (15)$$

where $I(\rho_{SB}') = S(\rho_S') - S(\rho_B') - S(\rho_{SB}')$ is the mutual information between the system and the bath. Equation (15) shows that the change in the state of the bath along with the mutual information is responsible for the entropy production variation.

Now, let us obtain an expression for the entropy production for TOs based on the new definition of heat presented in the previous section. If one uses Eq. (9) in Eq. (12), one obtains

$$\Delta S^{irr} = -\beta(\Delta F_S + \Delta F_B) = S(\rho_S || \rho_S^{eq}) - S(\rho_S' || \rho_S^{eq}) - S(\rho_B' || \rho_B^{eq}), \quad (16)$$

which is the new form of the entropy production for TOs, more detail can be found in Methods. Considering the definition of TO, Eq. (16) can be rewritten as

$$\Delta S^{irr} = I(\rho_{SB}'). \quad (17)$$

Since $I(\rho_{SB}')$ is always non-negative, one comes to $\Delta S^{irr} \geq 0$. As can be seen in Eq. (17), it is just the mutual information which determines the entropy production; there is no term showing the change of bath state. It is important to note that for entropy-preserving operations²⁸ if the initial state of the composite system SB is factorized, Eq. (17) is also true (see Methods).

Regarding the non-negativity of ΔS^{irr} together with Eq. (16), one obtains

$$\Delta F_S + \Delta F_B \leq 0, \quad (18)$$

which means that sum of the system and the bath free energies is decreasing under TOs. Equation (18) can be rewritten as

$$\Delta F_S \leq -\Delta F_B, \quad (19)$$

which introduces an upper bound for ΔF_S . As can be seen, unlike Eq. (14), this upper bound depends on the change in the free energy of the bath. Also, it is tighter than Eq. (14), due to the positivity of ΔF_B .

Quantum coherence and entropy production

Quantum coherence is one of the most important concepts in quantum physics. Recently, the role of the quantum coherence in determining the behavior of the entropy production has been investigated³⁵. It has been shown that the non-equilibrium free energy of a system can be written as^{20,35,36}:

$$F(\rho_S) = E_{eq} + TS(\Delta_{H_S}(\rho_S) || \rho_S^{eq}) + TC(\rho_S), \quad (20)$$

where $S(\cdot || \cdot)$ is quantum relative entropy and $C(\rho_S)$ is relative entropy of coherence^{33,34},

$$C(\rho_S) = S(\Delta_{H_S}(\rho_S)) - S(\rho_S), \quad (21)$$

where

$$\Delta_{H_S}(\rho_S) = \sum_i \langle E_i | \rho_S | E_i \rangle | E_i \rangle \langle E_i |$$

is a dephasing map acting on density matrix ρ_S and removing all coherences in the energy basis ($\{|E_i\rangle\}$), (see Methods). According to Eq. (20), the entropy production is divided into two parts: classical and quantum^{35,36},

$$\Delta \bar{S}^{irr} = \Delta \bar{S}_C^{irr} + \Delta \bar{S}_Q^{irr}, \quad (22)$$

where

$$\Delta \bar{S}_C^{irr} = S(\Delta_{H_S}(\rho_S) || \rho_S^{eq}) - S(\Delta_{H_S}(\rho'_S) || \rho_S^{eq}) \quad (23)$$

is the classical part, and

$$\Delta \bar{S}_Q^{irr} = C(\rho_S) - C(\rho'_S) \quad (24)$$

is the quantum one. Since the diagonal elements of a density matrix are transformed independently of the off-diagonal ones in state-to-state transformation under TOs, $\Delta \bar{S}_C^{irr}$ is non-negative. Also, $\Delta \bar{S}_Q^{irr}$ is positive because TO is incoherent³³. A quantum operation is coherence-preserving if and only if it is unitary and incoherent³⁷. Therefore, the unitary operator U_{SB} , introduced in the definition of TO, is a coherence-preserving operator. Thus, the total coherence of system+bath remains unchanged under the operation of U_{SB} ,

$$C(\rho'_{SB}) = C(U_{SB}(\rho_S \otimes \rho_B^{eq})U_{SB}^\dagger) = C(\rho_S \otimes \rho_B^{eq}) = C(\rho_S), \quad (25)$$

which is due to this fact that the relative entropy of coherence is additive on tensor product states and ρ_B^{eq} is an incoherent state. Substituting Eq. (25) into Eq. (24), one obtains³⁵

$$\Delta \bar{S}_Q^{irr} = C_{cc}(\rho'_{SB}) + C(\rho'_B), \quad (26)$$

where $C_{cc}(\rho'_{SB}) = C(\rho'_{SB}) - C(\rho'_S) - C(\rho'_B)$ is called correlated coherence^{38,39}.

One can repeat the above procedure to obtain the classical and quantum parts of the entropy production for the new expression, Eq. (16). As was seen before, the entropy production can be divided into two parts,

$$\Delta S^{irr} = \Delta S_C^{irr} + \Delta S_Q^{irr}, \quad (27)$$

where

$$\Delta S_C^{irr} = S(\Delta_{H_S}(\rho_S) || \rho_S^{eq}) - S(\Delta_{H_S}(\rho'_S) || \rho_S^{eq}) - S(\Delta_{H_B}(\rho'_B) || \rho_B^{eq}) \quad (28)$$

is the classical part, and

$$\Delta S_Q^{irr} = C(\rho_S) - C(\rho'_S) - C(\rho'_B) = C_{cc}(\rho'_{SB}) \quad (29)$$

is the quantum one. As can be seen, the new definition of heat results in that only the correlated coherence appears in the entropy production expression with no coherence of subsystems, in spite of what is mentioned in ref. ³⁵.

Using relative entropy of coherence, one obtains³⁹

$$C_{cc}(\rho'_{SB}) = I(\rho'_{SB}) - I(\Delta_{H_S+H_B}(\rho'_{SB})). \quad (30)$$

Regarding Eq. (30), the entropy production in Eq. (17) can be written as

$$\Delta S^{irr} = I(\rho'_{SB}) = [I(\Delta_{H_S+H_B}(\rho'_{SB}))] + [I(\rho'_{SB}) - I(\Delta_{H_S+H_B}(\rho'_{SB}))], \quad (31)$$

hence, the classical and quantum parts of the new entropy production can be written, respectively, as

$$\Delta S_C^{irr} = S(\Delta_{H_S}(\rho_S) || \rho_S^{eq}) - S(\Delta_{H_S}(\rho'_S) || \rho_S^{eq}) - S(\Delta_{H_B}(\rho'_B) || \rho_B^{eq}) = I(\Delta_{H_S+H_B}(\rho'_{SB})), \quad (32)$$

and

$$\Delta S_Q^{irr} = C_{cc}(\rho'_{SB}) = I(\rho'_{SB}) - I(\Delta_{H_S+H_B}(\rho'_{SB})). \quad (33)$$

Since $I(\Delta_{H_S+H_B}(\rho'_{SB}))$ is always non-negative, one comes to $\Delta S_C^{irr} \geq 0$. ΔS_Q^{irr} is also non-negative due to the data-processing inequality related to strong-subadditivity of the von Neumann entropy leading to this fact that mutual information decreases subject to local operations^{40,41}. ΔS_Q^{irr} can be considered as a discord quantifier

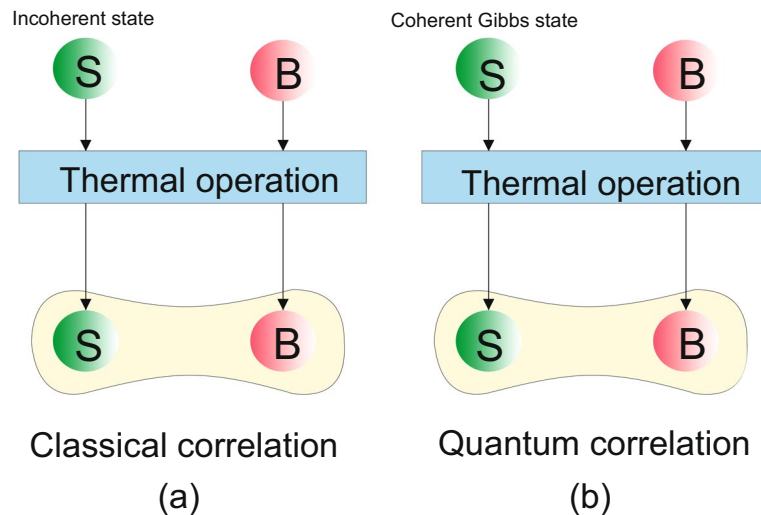


Figure 1. (Color online) (a) TOs cannot generate quantum correlation from incoherent input states. (b) If input state of the system is coherent Gibbs state, correlation between system and bath is quantum correlation.

which depends on the basis and is established on the concept of local projective measurements detecting the quantumness of correlations^{42,43}.

It should be mentioned that if the initial state of the system is diagonal in the energy basis, meaning that $C(\rho_S) = 0$, one comes to

$$C(\rho'_S) = C(\rho'_B) = C_{cc}(\rho'_{SB}) = 0, \tag{34}$$

which indicates that the system and the bath states remain diagonal subject to time evolution. Also

$$\Delta S_Q^{irr} = C_{cc}(\rho'_{SB}) = I(\rho'_{SB}) - I(\Delta_{H_S+H_B}(\rho'_{SB})) = 0, \tag{35}$$

therefore

$$\Delta S^{irr} = \Delta S_C^{irr} = I(\Delta_{H_S+H_B}(\rho'_{SB})), \tag{36}$$

as can be seen, only the classical part appears. Hence, one can say that if the initial state of the system is diagonal in the energy basis, it is impossible to create a quantum correlation between the system and the bath by applying TOs (see Fig. 1). However, if the initial state of the system is the coherent Gibbs state^{20,44},

$$|\lambda\rangle_S := \sum_i \sqrt{\frac{e^{-\beta E_i}}{Z_S}} |E_i\rangle, \tag{37}$$

one comes to $\Delta_{H_S}(|\lambda\rangle_S \langle \lambda|) = \rho_S^{eq}$ and therefore $S(\Delta_{H_S}(|\lambda\rangle_S \langle \lambda|) || \rho_S^{eq}) = 0$. From Eq. (32) and this fact that ΔS_C^{irr} is a non-negative quantity, one can conclude that $\Delta S_C^{irr} = 0$. Hence, for this case, there is no classical part in the entropy production expression,

$$\Delta S^{irr} = \Delta S_Q^{irr} = C_{cc}(\rho'_{SB}), \tag{38}$$

which is in contrast to the previous case, Eq. (36), (see Fig. 1). It should be mentioned that the above results are true for the entropy production introduced in Eq. (22); if the initial state of the system is incoherent, one obtains $\Delta \bar{S}_Q^{irr} = 0$, meaning that only the classical part appears in the entropy production expression, and if the system is initially in a coherent Gibbs state, one arrives at $\Delta \bar{S}_C^{irr} = 0$, meaning that only the quantum part is left.

Example

To illustrate the above-mentioned results, let us consider a two-level system whose Hamiltonian is given by $H_S = \omega_a |a\rangle \langle a| + \omega_b |b\rangle \langle b|$, where $\omega_a > \omega_b$ (Fig. 2). The bath is assumed to be a huge reservoir out of which one can freely and repeatedly, in each run of the protocol, pick one copy of a virtual or ancillary two-level system (qubit) which is on resonance with the system⁴⁵⁻⁴⁷. The bath Hamiltonian is $H_B = \omega_1 |1\rangle \langle 1| + \omega_0 |0\rangle \langle 0| + H_{redu}^B$, where $\omega_1 > \omega_0$, and H_{redu}^B is the Hamiltonian describing the dynamical behavior of the rest of the bath. The initial state of the bath is assumed to be a thermal state, therefore, the state of the virtual qubit can be expressed as

$$\rho_{vir} = q_1 |1\rangle \langle 1| + q_0 |0\rangle \langle 0|, \tag{39}$$

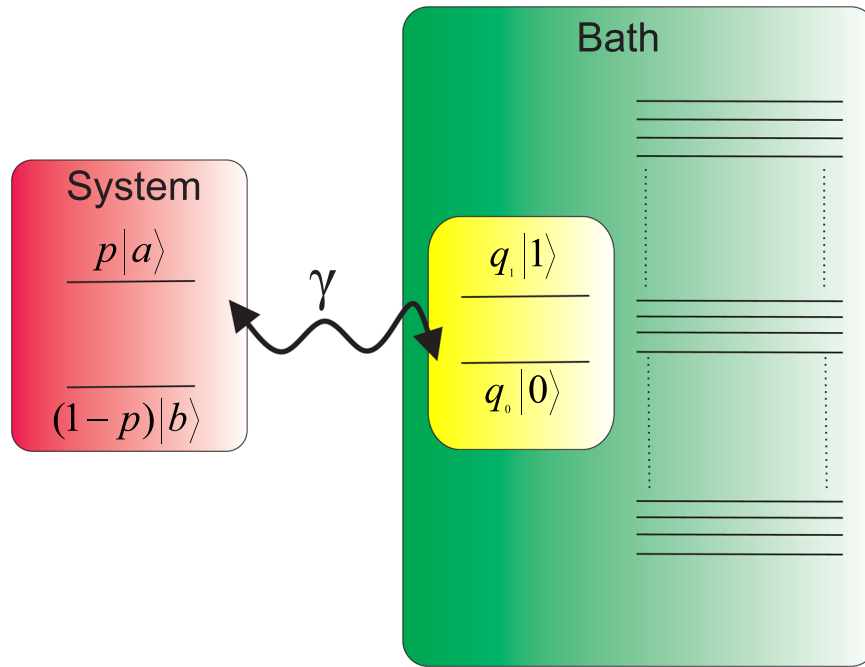


Figure 2. (Color online) Schematic diagram of a bath of virtual qubits. The system is modeled as a two-level system. The bath is in thermal equilibrium at temperature T and one can repeatedly pick one virtual qubit out of the bath in each single run of the protocol.

where $q_i = \frac{e^{-\beta\omega_i}}{Z_B}$. Also, the resonance condition is assumed to be

$$\omega_a - \omega_b = \omega_1 - \omega_0. \tag{40}$$

The “thermal contact” between the system and the bath is described by the interaction Hamiltonian,

$$H_{\text{int}} = \gamma(|b\rangle\langle a| \otimes |1\rangle\langle 0| + |a\rangle\langle b| \otimes |0\rangle\langle 1|), \tag{41}$$

where γ is coupling strength, and it is assumed that $\hbar = 1$. The time evolution of the total system is then governed by the unitary operator $U_t = \exp[-i(H_S + H_B + H_{\text{int}})t]$. After an infinitesimal time δt the state of the total system evolves to

$$\rho_{SB}(\delta t) = U_{\delta t} \rho_{SB}(0) U_{\delta t}^\dagger, \tag{42}$$

where the initial state $\rho_{SB}(0)$ is a direct product of the system and the bath initial states.

Let us examine the above example for two different initial states of the system. Firstly, the initial state of the system is assumed to be an incoherent state,

$$\rho_S(0) = p|a\rangle\langle a| + (1-p)|b\rangle\langle b|, \tag{43}$$

where $0 \leq p \leq 1$. In Fig. 3, entropy production, its classical and quantum parts for this state are plotted versus the parameter p . The plots show that the quantum contribution of the entropy production is zero, hence, the entropy production is the same as the classical part. Secondly, let us assume that the initial state of the system is pure and has coherence in the energy basis,

$$|\psi\rangle_S = \sqrt{p}|a\rangle + \sqrt{1-p}|b\rangle. \tag{44}$$

In Fig. 4, the same three quantities as in Fig. 3 for this state are plotted versus the parameter p . As can be seen, when the initial state of the system is the coherent Gibbs state, $p = 0.35$, the classical contribution of the entropy production is zero, which is consistent to what is mentioned before.

Discussion. In this paper, using the new definition of heat²⁸, the corresponding expression for entropy production was obtained. The difference between this expression and the old one is a term which goes to zero in the limit of large baths, meaning that both expressions come close to each other in this limit.

Furthermore, it was shown that the new definition of heat leads to this fact that the entropy production is the same as mutual information between a system and a bath for TOs; it is also true for entropy-preserving operations provided that the initial state of the system-bath is a tensor product state.

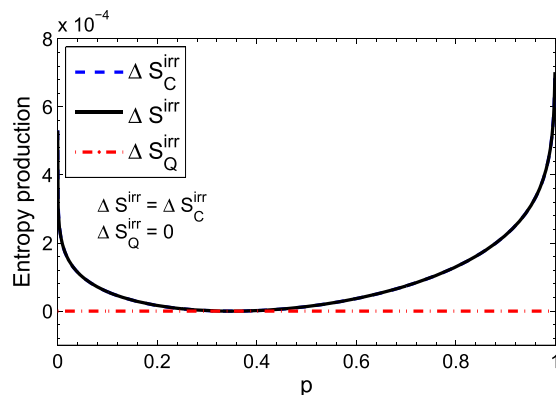


Figure 3. (Color online) (a) Variation of the entropy production, its classical and quantum parts with respect to the parameter p . The initial state of the system is assumed to be an incoherent state. Numerical values are $q_1 = 0.35$, $q_0 = 0.65$ and $\gamma t = 0.01$.

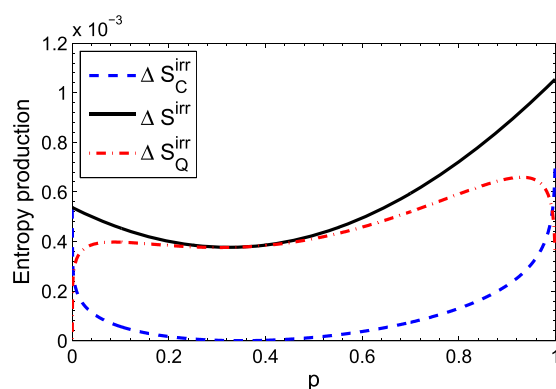


Figure 4. (Color online) The black (solid), the blue (dashed), and the red (dot-dashed) curves represent how entropy production, its classical and quantum parts change over the parameter p , respectively. The initial state of the system is assumed to be $|\psi\rangle_S = \sqrt{p}|a\rangle + \sqrt{1-p}|b\rangle$. Numerical values are $q_1 = 0.35$, $q_0 = 0.65$ and $\gamma t = 0.01$.

It was also shown that the upper bound of the free energy change of a system under TOs is tighter due to this new definition of heat.

Finally, the role of quantum coherence in the new expression of entropy production was studied and it was realized that if the initial state of a system is diagonal in the energy basis, one cannot create a quantum correlation between the system and its bath, subject to TO. On the other hand, it turned out that the correlation between a system and a bath is quantum correlation if the initial state of the system is a coherent Gibbs state.

Methods

In this section, the derivation of Eqs. (13), (15), (16), (17) and (20) is detailed. The approach is slightly different from the previous methods^{22–25}. First of all, it is necessary to note that the following relations are true for TOs:

$$\Delta E_S + \Delta E_B = 0, \quad (45)$$

$$I(\rho'_{SB}) = \Delta S_S + \Delta S_B, \quad (46)$$

and

$$\Delta F_B = TS(\rho'_B || \rho_B^{eq}). \quad (47)$$

Equation (45) is true because of the energy conservation condition, Eq. (46) comes from this condition that the initial total state is a direct product of the system and bath states and the total state evolves unitarily, $S(\rho'_{SB}) = S(U_{SB}(\rho_S \otimes \rho_B^{eq})U_{SB}^\dagger) = S(\rho_S) + S(\rho_B^{eq})$, and Eq. (47) is due to the fact that the initial state of the bath is a thermal state.

Derivation of Eq. (13). According to Eq. (12), the entropy production is given by

$$\Delta S^{irr} = \Delta S_S - \Delta S^{rev}, \tag{48}$$

in which ΔS_S is the change in the entropy of the system and ΔS^{rev} is equal to $\beta\Delta Q$. Regarding Eq. (8) as the definition of heat, one obtains

$$\Delta \bar{S}^{irr} = \Delta S_S - \Delta S^{rev} = \Delta S_S - \beta\Delta \bar{Q} = \Delta S_S + \beta\Delta E_B, \tag{49}$$

which leads to

$$\Delta \bar{S}^{irr} = \Delta S_S - \beta\Delta E_S = -\beta\Delta F_S, \tag{50}$$

due to Eq. (45) and the definition of the free energy. Since $F(\rho_S) = F_{eq} + TS(\rho_S||\rho_S^{eq})$, one obtains

$$\Delta \bar{S}^{irr} = -\beta\Delta F_S = S(\rho_S||\rho_S^{eq}) - S(\rho_S'||\rho_S^{eq}). \tag{51}$$

Derivation of Eq. (15). Substituting Eqs. (45), (46) and (47) into Eq. (50) and keeping in mind the definition of the free energy, one arrives at

$$\Delta \bar{S}^{irr} = -\beta\Delta F_S = \Delta S_S - \beta\Delta E_S = I(\rho_{SB}') - \Delta S_B + \beta\Delta E_B = I(\rho_{SB}') + \beta\Delta F_B = I(\rho_{SB}') + S(\rho_B'||\rho_B^{eq}), \tag{52}$$

which is Eq. (15).

Derivation of Eq. (16). The approach is similar to the one used to obtain Eq. (13), the only difference is that here Eq. (9) is considered as the definition of heat. Starting with Eq. (12) and considering the definition of heat according to Eq. (9), one comes to

$$\Delta S^{irr} = \Delta S_S - \Delta S^{rev} = \Delta S_S - \beta\Delta Q = \Delta S_S + \Delta S_B = \Delta S_S + \beta\Delta E_B - \beta\Delta F_B, \tag{53}$$

which, together with Eq. (45) and the definition of the free energy, gives

$$\Delta S^{irr} = -\beta(\Delta F_S + \Delta F_B). \tag{54}$$

Now, replacing ΔF_B and ΔF_S from Eqs. (47) and (51), respectively, results in Eq. (16),

$$\Delta S^{irr} = -\beta(\Delta F_S + \Delta F_B) = S(\rho_S||\rho_S^{eq}) - S(\rho_S'||\rho_S^{eq}) - S(\rho_B'||\rho_B^{eq}). \tag{55}$$

Derivation of Eq. (17). To obtain Eq. (17), one can use the definition of the free energy and Eqs. (45) and (46) to rewrite Eq. (54) as

$$\Delta S^{irr} = -\beta(\Delta F_S + \Delta F_B) = \Delta S_S + \Delta S_B - \beta(\Delta E_S + \Delta E_B) = I(\rho_{SB}'). \tag{56}$$

For entropy-preserving operations ($S(\rho_{SB}') = S(\Lambda(\rho_{SB})) = S(\rho_{SB})$), if the initial state of the composite system SB is factorized ($\rho_{SB} = \rho_S \otimes \rho_B$), one will have

$$S(\rho_{SB}') = S(\rho_{SB}) = S(\rho_S) + S(\rho_B). \tag{57}$$

Regarding Eq. (57) and the definition of the mutual information, one obtains $I(\rho_{SB}') = \Delta S_S + \Delta S_B$, therefore

$$\Delta S^{irr} = \Delta S_S - \Delta S^{rev} = \Delta S_S - \beta\Delta Q = \Delta S_S + \Delta S_B = I(\rho_{SB}'), \tag{58}$$

which is the same as Eq. (56).

Derivation of Eq. (20). The free energy for a system in a state ρ_S is

$$F(\rho_S) = \text{tr}(H_S\rho_S) - TS(\rho_S). \tag{59}$$

Substituting $H_S = -\frac{1}{\beta}(\ln(\rho_S^{eq}) + \ln(Z_S))$ into the above equation, one obtains

$$F(\rho_S) = F_{eq} + TS(\rho_S||\rho_S^{eq}), \tag{60}$$

where $F_{eq} = -\frac{1}{\beta}\ln(Z_S)$ is the free energy in thermal equilibrium and $S(\rho_S||\rho_S^{eq}) = \text{tr}(\rho_S\ln(\rho_S)) - \text{tr}(\rho_S\ln(\rho_S^{eq}))$ is quantum relative entropy. Regarding $\text{tr}(\rho_S\ln(\rho_S^{eq})) = \text{tr}(\Delta_{H_S}(\rho_S)\ln(\rho_S^{eq}))$, one comes to

$$F(\rho_S) = F_{eq} - TS(\rho_S) + TS(\Delta_{H_S}(\rho_S)) + TS(\Delta_{H_S}(\rho_S)||\rho_S^{eq}) = F_{eq} + TS(\Delta_{H_S}(\rho_S)||\rho_S^{eq}) + TC(\rho_S), \tag{61}$$

where $C(\rho_S) = S(\Delta_{H_S}(\rho_S)) - S(\rho_S)$ is relative entropy of coherence.

Received: 5 December 2019; Accepted: 14 May 2020;

Published online: 16 June 2020

References

- Weimer, H., Henrich, M. J., Rempp, F., Schröder, H. & Mahler, G. Local effective dynamics of quantum systems: A generalized approach to work and heat. *Europhys. Lett.* **83**, 30008 (2008).
- Jarzynski, C. Equalities and inequalities: Irreversibility and the second law of thermodynamics at the nanoscale. *Annu. Rev. Condens. Matter Phys.* **2**, 329 (2011).
- Gelbwaser-Klimovsky, D., Alicki, R. & Kurizki, G. Minimal universal quantum heat machine. *Phys. Rev. E* **87**, 012140 (2013).
- Salmilehto, J., Solinas, P. & Möttönen, M. Quantum driving and work. *Phys. Rev. E* **89**, 052128 (2014).
- Hossein-Nejad, H., ÓReilly, E. J. & Olaya-Castro, A. Work, heat and entropy production in bipartite quantum systems. *New J. Phys.* **17**, 075014 (2015).
- Gallego, R., Eisert, J. & Wilming, H. Thermodynamic work from operational principles. *New J. Phys.* **18**, 103017 (2016).
- Jarzynski, C., Quan, H. T. & Rahav, S. Quantum-classical correspondence principle for work distributions. *Phys. Rev. X* **5**, 031038 (2015).
- Alipour, S., Benatti, F., Bakhshinezhad, F., Afsary, M., Marcantoni, S. & Rezakhani, A. T. Correlations in quantum thermodynamics: Heat, work, and entropy production. *Sci. Rep.* **6**, 35568 (2016).
- Ahmadi, B., Salimi, S., Khorashad, A. S. & Kheirandish, F. The quantum thermodynamic force responsible for quantum state transformation and the flow and backflow of information. *Sci. Rep.* **9**, 8746 (2019).
- Ahmadi, B., Salimi, S. & Khorashad, A. S. Information and the second law of thermodynamics. Preprint at arXiv:1809.00611 (2018).
- Manzano, G., Galve, F., Zambrini, R. & Parrondo, J. M. R. Entropy production and thermodynamic power of the squeezed thermal reservoir. *Phys. Rev. E* **93**, 052120 (2016).
- Gour, G., Müller, M. P., Narasimhachar, V., Spekkens, R. W. & Halpern, N. Y. The resource theory of informational nonequilibrium in thermodynamics. *Phys. Rep.* **583**, 1 (2015).
- Goold, J., Huber, M., Riera, A., del Rio, L. & Skrzypczyk, P. The role of quantum information in thermodynamics—a topical review. *J. Phys. A: Math. Theor.* **49**, 143001 (2016).
- Ng, N. H. Y. & Woods, M. P. Resource theory of quantum thermodynamics: Thermal operations and second laws. *Thermodynamics in the Quantum Regime* (Springer, Berlin, 2018), pp. 625–650.
- Janzing, D., Wocjan, P., Zeier, R., Geiss, R. & Beth, T. Thermodynamic cost of reliability and low temperatures: Tightening Landauer's principle and the second law. *Int. J. Theor. Phys.* **39**, 2717 (2000).
- Horodecki, M. & Oppenheim, J. Fundamental limitations for quantum and nanoscale thermodynamics. *Nat. Commun.* **4**, 2059 (2013).
- Brandão, F. G. S. L., Horodecki, M., Oppenheim, J., Renes, J. M. & Spekkens, R. W. Resource theory of quantum states out of thermal equilibrium. *Phys. Rev. Lett.* **111**, 250404 (2013).
- Brandão, F. G. S. L., Horodecki, M., Ng, N., Oppenheim, J. & Wehner, S. The second laws of quantum thermodynamics. *Proc. Natl. Acad. Sci. U.S.A.* **112**, 3275 (2015).
- Cwiklinski, P., Studzinski, M., Horodecki, M. & Oppenheim, J. Limitations on the evolution of quantum coherences: Towards fully quantum second laws of thermodynamics. *Phys. Rev. Lett.* **115**, 210403 (2015).
- Lostaglio, M., Jennings, D. & Rudolph, T. Description of quantum coherence in thermodynamic processes requires constraints beyond free energy. *Nat. Commun.* **6**, 6383 (2015).
- Lostaglio, M., Korzekwa, K., Jennings, D. & Rudolph, T. Quantum coherence, time-translation symmetry, and thermodynamics. *Phys. Rev. X* **5**, 021001 (2015).
- Deffner, S. & Lutz, E. Generalized Clausius inequality for nonequilibrium quantum processes. *Phys. Rev. Lett.* **105**, 170402 (2010).
- Deffner, S. & Lutz, E. Nonequilibrium entropy production for open quantum systems. *Phys. Rev. Lett.* **107**, 140404 (2011).
- Esposito, M., Lindenberg, K. & Van den Broeck, C. Entropy production as correlation between system and reservoir. *New J. Phys.* **12**, 013013 (2010).
- Esposito, M. & Van den Broeck, C. Second law and Landauer principle far from equilibrium. *Europhys. Lett.* **95**, 40004 (2011).
- Manzano, G., Horowitz, J. M. & Parrondo, J. M. R. Quantum fluctuation theorems for arbitrary environments: Adiabatic and nonadiabatic entropy production. *Phys. Rev. X* **8**, 031037 (2018).
- Manzano, G., Horowitz, J. M. & Parrondo, J. M. R. Nonequilibrium potential and fluctuation theorems for quantum maps. *Phys. Rev. E* **92**, 032129 (2015).
- Bera, M. N., Riera, A., Lewenstein, M. & Winter, A. Generalized laws of thermodynamics in the presence of correlations. *Nat. Commun.* **8**, 2180 (2017).
- Reeb, D. & Wolf, M. M. An improved Landauer principle with finite-size corrections. *New J. Phys.* **16**, 103011 (2014).
- Landauer, R. Irreversibility and heat generation in the computing process. *IBM J. Res. Dev.* **5**, 183–191 (1961).
- Jennings, D. & Rudolph, T. Entanglement and the thermodynamic arrow of time. *Phys. Rev. E* **81**, 061130 (2010).
- Nielsen, M. L. & Chuang, I. L. *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge, 2000).
- Baumgratz, T., Cramer, M. & Plenio, M. B. Quantifying coherence. *Phys. Rev. Lett.* **113**, 140401 (2014).
- Streltsov, A., Adesso, G. & Plenio, M. B. Colloquium: Quantum coherence as a resource. *Rev. Mod. Phys.* **89**, 041003 (2017).
- Santos, J. P., Celeri, L. C., Landi, G. T. & Paternostro, M. The role of quantum coherence in non-equilibrium entropy production. *npj Quantum Information* **5**, 23 (2019).
- Francica, G., Goold, J. & Plastina, F. Role of coherence in the nonequilibrium thermodynamics of quantum systems. *Phys. Rev. E* **99**, 042105 (2019).
- Peng, Y., Jiang, Y. & Fan, H. Maximally coherent states and coherence-preserving operations. *Phys. Rev. A* **93**, 032326 (2016).
- Tan, K. C., Kwon, H., Park, C. Y. & Jeong, H. Unified view of quantum correlations and quantum coherence. *Phys. Rev. A* **94**, 022329 (2016).
- Kraft, T. & Piani, M. Genuine correlated coherence. *J. Phys. A: Math. Theor.* **51**, 414013 (2018).
- Xi, Z., Li, Y. & Fan, H. Quantum coherence and correlations in quantum system. *Sci. Rep.* **5**, 10922 (2015).
- Wang, X.-L., Yue, Q.-L., Yu, C.-H., Gao, F. & Qin, S.-J. Relating quantum coherence and correlations with entropy-based measures. *Sci. Rep.* **7**, 12122 (2017).
- Ollivier, H. & Zurek, W. H. Quantum discord: A measure of the quantumness of correlations. *Phys. Rev. Lett.* **88**, 017901 (2001).
- Modi, K., Brodutch, A., Cable, H., Paterek, T. & Vedral, V. The classical-quantum boundary for correlations: Discord and related measures. *Rev. Mod. Phys.* **84**, 1655 (2012).
- Kwon, H., Jeong, H., Jennings, D., Yadin, B. & Kim, M. S. Clock-work trade-off relation for coherence in quantum thermodynamics. *Phys. Rev. Lett.* **120**, 150602 (2018).
- Chen, H.-B., Chen, G.-Y. & Chen, Y.-N. Thermodynamic description of non-Markovian information flux of nonequilibrium open quantum systems. *Phys. Rev. A* **96**, 062114 (2017).
- Skrzypczyk, P., Short, A. J. & Popescu, S. Work extraction and thermodynamics for individual quantum systems. *Nat. Commun.* **5**, 4185 (2014).
- Brunner, N., Linden, N., Popescu, S. & Skrzypczyk, P. Virtual qubits, virtual temperatures, and the foundations of thermodynamics. *Phys. Rev. E* **85**, 051117 (2012).

Acknowledgements

We thank G. Manzano for useful discussions and helpful comments.

Author contributions

H. Dolatkah, S. Salimi, A. S. Khorashad, and S. Haseli all contributed to the development and completion of the idea, performing the calculations, analyzing the results, discussions and writing the manuscript. The final draft of the manuscript was revised by A. S. Khorashad and reviewed by all authors.

Competing interests

The authors declare no competing interests.

Additional information

Correspondence and requests for materials should be addressed to A.S.K.

Reprints and permissions information is available at www.nature.com/reprints.

Publisher's note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.



Open Access This article is licensed under a Creative Commons Attribution 4.0 International License, which permits use, sharing, adaptation, distribution and reproduction in any medium or format, as long as you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons license, and indicate if changes were made. The images or other third party material in this article are included in the article's Creative Commons license, unless indicated otherwise in a credit line to the material. If material is not included in the article's Creative Commons license and your intended use is not permitted by statutory regulation or exceeds the permitted use, you will need to obtain permission directly from the copyright holder. To view a copy of this license, visit <http://creativecommons.org/licenses/by/4.0/>.

© The Author(s) 2020