Peer-reviewed version available at *Entropy* **2019**, *21*, 477; doi:10.3390/e21050477

Article

Fluctuation Theorem of Information Exchange within an Ensemble of Paths Conditioned at a Coupled-Microstates

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Received: date; Accepted: date; Published: date

Abstract: Fluctuation theorems are a class of equalities each of which links a thermodynamic path functional such as heat and work to a state function such as entropy and free energy. Jinwoo and Tanaka [L. Jinwoo and H. Tanaka, Sci. Rep. 5, 7832 (2015)] have shown that each microstate of a fluctuating system can be regarded as an ensemble (or a 'macrostate') if we consider trajectories that reach each microstate. They have revealed that local forms of entropy and free energy are true thermodynamic potentials of each microstate, encoding heat, and work, respectively, within an ensemble of paths that reach each state. Here we show that information that is characterized by the local form of mutual information between two subsystems in a heat bath is also a true thermodynamic potential of each coupled state and encodes the entropy production of the subsystems and heat bath during a coupling process. To this end, we extend the fluctuation theorem of information exchange [T. Sagawa and M. Ueda, Phys. Rev. Lett. 109, 180602 (2012)] by showing that the fluctuation theorem holds even within an ensemble of paths that reach a coupled state during dynamic co-evolution of two subsystems.

Keywords: local non-equilibrium thermodynamics, fluctuation theorem, mutual information, entropy production, local mutual information, thermodynamics of information, stochastic thermodynamics

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1. Introduction

Thermal fluctuations play an important role in the functioning of molecular machines: Fluctuations mediate the exchange of energy between molecules and the environment, enabling molecules to overcome free energy barriers and to stabilize in low free energy regions. They make positions and velocities random variables, and thus make path functionals such as heat and work fluctuating quantities. In the past two decades, a class of relations called fluctuation theorems have shown that there are universal laws that regulate fluctuating quantities during a process that drives a system far from equilibrium. The Jarzynski equality, for example, links work to the change of equilibrium free energy [1], and the Crooks fluctuation theorem relates the probability of work to the dissipation of work [2] if we mention a few. There are many variations on these basic relations. Seifert has extended the second-law to the level of individual trajectories [3], and Hatano and Sasa have considered transitions between steady states [4]. Experiments on single molecular levels have verified the fluctuation theorems, providing critical insights on the behavior of bio-molecules [5–10].

Sagawa and Ueda have introduced information to the realm of fluctuation theorems [11]. They have established a fluctuation theorem of information exchange, unifying non-equilibrium processes of measurement and feedback control [12]. They have considered a situation where a system, say X, evolves in such a manner that depends on state y of another system Y the state of which is fixed during the evolution of the state of X. In this setup, they have shown that establishing a correlation between the two subsystems accompanies an entropy production. Very recently, we have released the constraint that

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Sagawa and Ueda have assumed, and proved that the same form of the fluctuation theorem of information exchange holds even when both subsystems X and Y co-evolve in time [13].

In the context of fluctuation theorems, external parameter λ_t defines a macrostate at time t, and one varies the parameter in a predetermined manner during $0 \le t \le \tau$, which defines a process. One repeats the process according to initial probability distribution P_0, and then, a system generates as a response an ensemble of microscopic trajectories $\{x_t\}$. Jinwoo and Tanaka [14,15] have shown that the Jarzynski equality and the Crooks fluctuation theorem hold even within an ensemble of trajectories conditioned at a fixed microstate at final time τ, where the local form of non-equilibrium free energy replaces the role of equilibrium free energy. Considering the subset of trajectories makes it clear that the local free energy at conditioned microstate x_τ encodes the amount of supplied work for reaching x_τ during processes λ_t.

In this paper, we apply this conceptual framework of considering a single microstate as an ensemble of trajectories to the fluctuation theorem of information exchange (see Figure 1a). We show that mutual information is a true thermodynamic potential or a state function of a coupled-microstates, and encodes the amount of entropy production within the ensemble of paths that reach the coupled-states. This local version of fluctuation theorem of information exchange provides much more detailed information for each coupled-microstates compared to the results in [12,13]. In the existing approaches that considers the ensemble of all paths, each point-wise mutual information does not provide specific information on a coupled-microstates, but in this new approach of considering a subset of the ensemble, local mutual information provides detailed knowledge about specific coupled-states.

We organize the paper as follows: In section 2, we briefly review some fluctuation theorems that we have mentioned. In section 3, we prove the main theorem and its corollary. In section 4, we provide an illustrative example, and in section 5, we discuss the implication of the results.

2. Brief Overview of Fluctuation Theorems

We consider a system in contact with a heat bath of inverse temperate $\beta := 1/(k_B T)$ where k_B is the Boltzmann constant, and T is the temperature of the heat bath. External parameter λ_t drives the system away from equilibrium during $0 \le t \le \tau$. We assume that the initial probability distribution is equilibrium one at macrostate λ_0. Let Γ be the set of all microscopic trajectories, and Γ_{x_τ} be that of paths conditioned at x_τ at time τ. Then, Jarzynski equality [1] and end-point conditioned version [14,15] of it read as follows:

$$F_{eq}(\lambda_\tau) = F_{eq}(\lambda_0) - \frac{1}{\beta} \ln \left\langle e^{-\beta W} \right\rangle_\Gamma \quad \text{and} \tag{1}$$

$$\mathcal{F}(x_\tau, \tau) = F_{eq}(\lambda_0) - \frac{1}{\beta} \ln \left\langle e^{-\beta W} \right\rangle_{\Gamma_{x_\tau}}, \tag{2}$$

respectively, where brackets $\langle \cdot \rangle_\Gamma$ indicates the average over all trajectories in Γ and $\langle \cdot \rangle_{\Gamma_{x_\tau}}$ indicates the average over trajectories reaching x_τ at time τ. Here W indicates work done on the system through λ_t, $F_{eq}(\lambda_t)$ is equilibrium free energy at macrostate λ_t, and $\mathcal{F}(x_\tau, \tau)$ is local non-equilibrium free energy of x_τ at time τ. Work measurement over a specific ensemble of paths gives us equilibrium free energy as a macro-state function of λ_τ through Eq. (1) and local non-equilibrium free energy as a micro-state function of x_τ at time τ through Eq. (2). The following fluctuation theorem links Eq. (1) and Eq. (2):

$$\left\langle e^{-\beta \mathcal{F}(x_\tau, \tau)} \right\rangle_{x_\tau} = e^{-\beta F_{eq}(\lambda_\tau)}, \tag{3}$$

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where brackets $\langle\cdot\rangle_{x_\tau}$ indicates the average over all microstates x_τ at time τ [14,15]. Defining the reverse process by $\lambda'_t := \lambda_{\tau-t}$ for $0 \le t \le \tau$, the Crooks fluctuation theorem [2] and end-point conditioned version [14,15] of it read as follows:

$$\frac{P_\Gamma(W)}{P'_\Gamma(-W)} = \exp\left(\frac{W - \Delta F_{eq}}{k_B T}\right) \quad \text{and} \tag{4}$$

$$\frac{P_{\Gamma_{x_\tau}}(W)}{P'_{\Gamma_{x_\tau}}(-W)} = \exp\left(\frac{W - \Delta\mathcal{F}}{k_B T}\right), \tag{5}$$

respectively, where $P_\Gamma(W)$ and $P_{\Gamma_{x_\tau}}(W)$ are probability distributions of work W normalized over all paths in Γ and Γ_{x_τ}, respectively. Here P' indicates corresponding probabilities for the reverse process. For Eq. (4), initial probability distribution of the reverse process is equilibrium one at macrostate λ_τ. On the other hand, for Eq. (5), initiail probability distribution for the reverse process should be the final probability distribution of the forward process at macrostate λ_τ. By identifying such W that $P_\Gamma(W) = P'_\Gamma(-W)$, one obtains $\Delta F_{eq} := F_{eq}(\lambda_\tau) - F_{eq}(\lambda_0)$, the difference in equilibrium free energy between macrostates λ_0 and λ_τ, through Eq. (4) [9]. Similar identification may provide $\Delta\mathcal{F} := \mathcal{F}(x_\tau, \tau) - F_{eq}(\lambda_0)$ through Eq. (5).

Now we turn to Sagawa-Ueda fluctuation theorem of information exchange [12]. Specifically, we discuss the generalized version [13] of it. To this end, we consider two subsystems X and Y in the heat bath of inverse temperature β. During process λ_t, they interact and co-evolve with each other. Then, the fluctuation theorem of information exchange reads as follows:

$$\left\langle e^{-\sigma+\Delta I}\right\rangle_\Gamma = 1, \tag{6}$$

where brackets indicate the ensemble average over all paths of the combined subsystems, and σ is the sum of entropy production of system X, system Y, and the heat bath, and ΔI is the change in mutual information between X and Y. We note that in the original version of Sagawa-Ueda fluctuation theorem, only system X is in contact with the heat bath and Y does not evolve during the process [12,13]. In this paper, we prove an end-point conditioned version of Eq. (6):

$$I_\tau(x_\tau, y_\tau) = -\ln\left\langle e^{-(\sigma+I_0)}\right\rangle_{x_\tau, y_\tau}, \tag{7}$$

where brackets indicate the ensemble average over all paths to x_τ and y_τ at time τ, and I_t $(0 \le t \le \tau)$ is local form of mutual information between microstates of X and Y at time t (see Figure 1b). If there is no initial correlation, i.e. $I_0 = 0$, Eq. (7) clearly indicates that local mutual information I_τ as a function of coupled-microstates (x_τ, y_τ) encodes entropy production σ within the end-point conditioned ensemble of paths. In the same vein, we may interpret initial correlation I_0 as encoded entropy production for the preparation of the initial condition.

3. Results

3.1. Theoretical Framework

Let X and Y be finite classical stochastic systems in the heat bath of inverse temperate β. We allow external parameter λ_t drives one or both subsystems away from equilibrium during time $0 \le t \le \tau$ [16–18]. We assume that classical stochastic dynamics describes the time evolution of X and Y during process λ_t along trajectories $\{x_t\}$ and $\{y_t\}$, respectively, where x_t (y_t) denotes a specific microstate of X (Y) at time t for $0 \le t \le \tau$ on each trajectory. Since trajectories fluctuate, we repeat process λ_t with initial joint probability distribution $P_0(x, y)$ over all microstates (x, y) of systems X and Y. Then the

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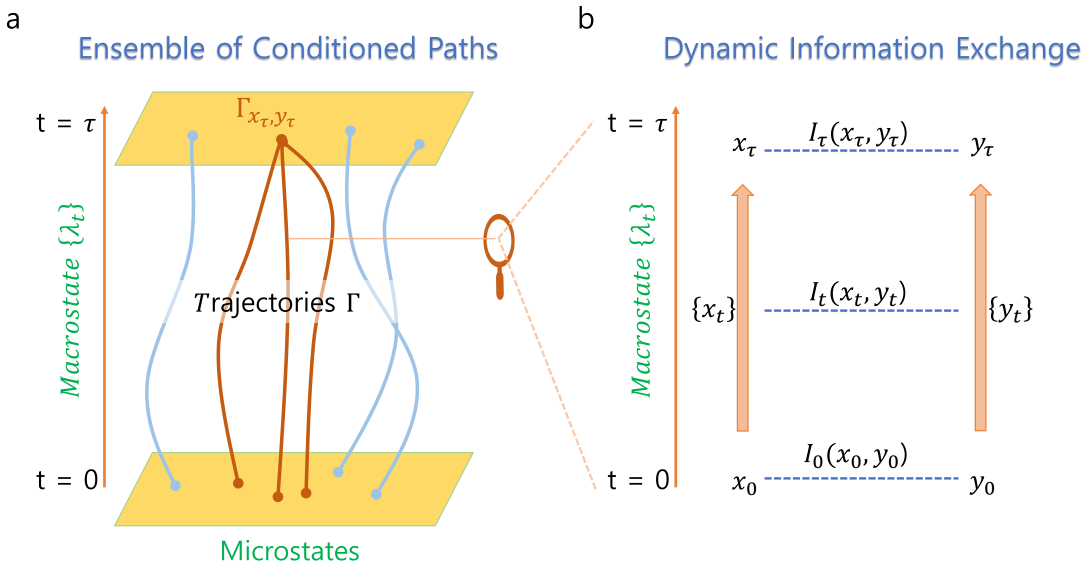

Figure 1. Ensemble of Conditioned Paths and Dynamic Information Exchange: (**a**) Orange curves represent trajectories that reach (x_τ, y_τ) at time τ, which are members of Γ_{x_τ,y_τ}. The Γ_{x_τ,y_τ} is a subset of Γ, the set of all trajectories during process λ_t for $0 \leq t \leq \tau$. At each time, λ_t defines a macrostate. (**b**) We magnified a single trajectory in the left panel to represent a detailed view of dynamic coupling during process λ_t for $0 \leq t \leq \tau$. The $I_t(x_t, y_t)$ may vary not necessarily monotonically.

subsystems may generate joint probability distribution $P_t(x, y)$ for $0 \leq t \leq \tau$. Let $P_t(x) := \int P_t(x, y)\, dy$ and $P_t(y) := \int P_t(x, y)\, dx$ be the corresponding marginal probability distributions. We assume

$$P_0(x, y) \neq 0 \text{ for all } (x, y) \tag{8}$$

so that we have $P_t(x, y) \neq 0$, $P_t(x) \neq 0$, and $P_t(y) \neq 0$ for all x and y during $0 \leq t \leq \tau$. Now the entropy production σ during process λ_t for $0 \leq t \leq \tau$ is given by

$$\sigma := \Delta s + \beta Q_b, \tag{9}$$

where Δs is the sum of changes in stochastic entropy along $\{x_t\}$ and $\{y_t\}$, and Q_b is heat dissipated into the heat bath (entropy production in the heat bath) [2,3]. In detail, we have

$$\begin{aligned} \Delta s &:= \Delta s_x + \Delta s_y, \\ \Delta s_x &:= -\ln P_\tau(x_\tau) + \ln P_0(x_0), \\ \Delta s_y &:= -\ln P_\tau(y_\tau) + \ln P_0(y_0). \end{aligned} \tag{10}$$

We note that the stochastic entropy $s[P_t(\circ)] := -\ln P_t(\circ)$ of microstate $\circ$ at time t is uncertainty of $\circ$ at time t: The more uncertain that microstate $\circ$ occurs, the greater the stochastic entropy of $\circ$ is. We also note that in [12], system X is in contact with the heat reservoir, but system Y is not. Nor does system Y evolve. Thus their entropy production reads $\sigma_{\text{su}} := \Delta s_x + \beta Q_b$.

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Now we assume, during process λ_t, that system X exchanges information with system Y. By this, we mean that trajectory $\{x_t\}$ of system X evolves depending on the trajectory $\{y_t\}$ of system Y (see Figure 1b). Then, local form of mutual information I_t at time t between x_t and y_t is the reduction of uncertainty of x_t due to given y_t [12]:

$$\begin{aligned} I_t(x_t, y_t) &:= s[P_t(x_t)] - s[P_t(x_t|y_t)] \\ &= \ln \frac{P_t(x_t, y_t)}{P_t(x_t)P_t(y_t)}, \end{aligned} \tag{11}$$

where $P_t(x_t|y_t)$ is the conditional probability distribution of x_t given y_t. The more information is being shared between x_t and y_t for their occurrence, the larger the value of $I_t(x_t, y_t)$ is. We note that if x_t and y_t are independent at time t, $I_t(x_t, y_t)$ becomes zero. The average of $I_t(x_t, y_t)$ with respect to $P_t(x_t, y_t)$ over all microstates is the mutual information between the two subsystems, which is greater than or equal to zero [19].

3.2. Proof of Fluctuation Theorem of Information Exchange Conditioned at a Coupled-Microstates

Now we are ready to prove the fluctuation theorem of information exchange conditioned at a coupled-microstates. We define reverse process $\lambda'_t := \lambda_{\tau-t}$ for $0 \le t \le \tau$, where the external parameter is time-reversed [20,21]. The initial probability distribution $P'_0(x, y)$ for the reverse process should be the final probability distribution for the forward process $P_\tau(x, y)$ so that we have

$$\begin{aligned} P'_0(x) &= \int P'_0(x, y)\, dy = \int P_\tau(x, y)\, dy = P_\tau(x), \\ P'_0(y) &= \int P'_0(x, y)\, dx = \int P_\tau(x, y)\, dx = P_\tau(y). \end{aligned} \tag{12}$$

Then, by Eq. (8), we have $P'_t(x, y) \neq 0$, $P'_t(x) \neq 0$, and $P'_t(y) \neq 0$ for all x and y during $0 \le t \le \tau$. For each trajectories $\{x_t\}$ and $\{y_t\}$ for $0 \le t \le \tau$, we define the time-reversed conjugate as follows:

$$\begin{aligned} \{x'_t\} &:= \{x^*_{\tau-t}\}, \\ \{y'_t\} &:= \{y^*_{\tau-t}\}, \end{aligned} \tag{13}$$

where $*$ denotes momentum reversal. Let Γ be the set of all trajectories $\{x_t\}$ and $\{y_t\}$, and Γ_{x_τ, y_τ} be that of trajectories conditioned at coupled-microstates (x_τ, y_τ) at time τ. Due to time-reversal symmetry of the underlying microscopic dynamics, the set Γ' of all time-reversed trajectories is identical to Γ, and the set $\Gamma'_{x'_0, y'_0}$ of time-reversed trajectories conditioned at x'_0 and y'_0 is identical to Γ_{x_τ, y_τ}. Thus we may use the same notation for both forward and backward pairs. We note that the path probabilities P_Γ and $P_{\Gamma_{x_\tau, y_\tau}}$ are normalized over all paths in Γ and Γ_{x_τ, y_τ}, respectively (see Figure 1a). With this notation, the microscopic reversibility condition that enables us to connect the probability of forward and reverse paths to dissipated heat reads as follows [2,22–24]:

$$\frac{P_\Gamma(\{x_t\}, \{y_t\}|x_0, y_0)}{P'_\Gamma(\{x'_t\}, \{y'_t\}|x'_0, y'_0)} = e^{\beta Q_b}, \tag{14}$$

where $P_\Gamma(\{x_t\}, \{y_t\}|x_0, y_0)$ is the conditional joint probability distribution of paths $\{x_t\}$ and $\{y_t\}$ conditioned at initial microstates x_0 and y_0, and $P'_\Gamma(\{x'_t\}, \{y'_t\}|x'_0, y'_0)$ is that for the reverse process. Now we restrict our attention to those paths that are in Γ_{x_τ, y_τ}, and divide both numerator and denominator of

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the left-hand side of Eq. (14) by $P_\tau(x_\tau, y_\tau)$. Since $P_\tau(x_\tau, y_\tau)$ is identical to $P'_0(x'_0, y'_0)$, Eq. (14) becomes as follows:

$$\frac{P_{\Gamma_{x_\tau,y_\tau}}(\{x_t\},\{y_t\}|x_0,y_0)}{P'_{\Gamma_{x_\tau,y_\tau}}(\{x'_t\},\{y'_t\}|x'_0,y'_0)} = e^{\beta Q_b} \tag{15}$$

since the probability of paths is now normalized over Γ_{x_τ,y_τ}. Then we have the following:

$$\begin{aligned}
\frac{P'_{\Gamma_{x_\tau,y_\tau}}(\{x'_t\},\{y'_t\})}{P_{\Gamma_{x_\tau,y_\tau}}(\{x_t\},\{y_t\})} &= \frac{P'_{\Gamma_{x_\tau,y_\tau}}(\{x'_t\},\{y'_t\}|x'_0,y'_0)}{P_{\Gamma_{x_\tau,y_\tau}}(\{x_t\},\{y_t\}|x_0,y_0)} \cdot \frac{P'_0(x'_0,y'_0)}{P_0(x_0,y_0)} && (16)\\
&= \frac{P'_{\Gamma_{x_\tau,y_\tau}}(\{x'_t\},\{y'_t\}|x'_0,y'_0)}{P_{\Gamma_{x_\tau,y_\tau}}(\{x_t\},\{y_t\}|x_0,y_0)} \cdot \frac{P'_0(x'_0,y'_0)}{P'_0(x'_0)p'_0(y'_0)} \cdot \frac{P_0(x_0)P_0(y_0)}{P_0(x_0,y_0)} && (17)\\
&\qquad \times \frac{P'_0(x'_0)}{P_0(x_0)} \cdot \frac{P'_0(y'_0)}{P_0(y_0)} \\
&= \exp\{-\beta Q_b + I_\tau(x_\tau,y_\tau) - I_0(x_0,y_0) - \Delta s_x - \Delta s_y\} && (18)\\
&= \exp\{-\sigma + I_\tau(x_\tau,y_\tau) - I_0(x_0,y_0)\}. && (19)
\end{aligned}$$

To obtain Eq. (17) from Eq. (16), we multiply Eq. (16) by $\frac{P'_0(x'_0)P'_0(y'_0)}{P'_0(x'_0)P'_0(y'_0)}$ and $\frac{P_0(x_0)P_0(y_0)}{P_0(x_0)P_0(y_0)}$, which are 1. We obtain Eq. (18) by applying Equations (10)–(12) and (15) to Eq. (17). Finally, we use Eq. (9) to obtain Eq. (19) from Eq. (18). Now we multiply both sides of Eq. (19) by $e^{-I_\tau(x_\tau,y_\tau)}$ and $P_{\Gamma_{x_\tau,y_\tau}}(\{x_t\},\{y_t\})$, and take integral over all paths in Γ_{x_τ,y_τ} to obtain the fluctuation theorem of information exchange conditioned at a coupled-microstates:

$$\begin{aligned}
\left\langle e^{-(\sigma+I_0)} \right\rangle_{x_\tau,y_\tau} &:= \int_{\{x_t\},\{y_t\}\in\Gamma_{\{x_\tau\},\{y_\tau\}}} e^{-(\sigma+I_0)} P_{\Gamma_{x_\tau,y_\tau}}(\{x_t\},\{y_t\})\, d\{x_t\}d\{y_t\} \\
&= \int_{\{x_t\},\{y_t\}\in\Gamma_{\{x_\tau\},\{y_\tau\}}} e^{-I_\tau(x_\tau,y_\tau)} P'_{\Gamma_{x_\tau,y_\tau}}(\{x'_t\},\{y'_t\})\, d\{x'_t\}d\{y'_t\} \\
&= e^{-I_\tau(x_\tau,y_\tau)} \int_{\{x_t\},\{y_t\}\in\Gamma_{\{x_\tau\},\{y_\tau\}}} P'_{\Gamma_{x_\tau,y_\tau}}(\{x'_t\},\{y'_t\})\, d\{x'_t\}d\{y'_t\} \\
&= e^{-I_\tau(x_\tau,y_\tau)}.
\end{aligned} \tag{20}$$

Here we use the fact that $e^{-I_\tau(x_\tau,y_\tau)}$ is constant for all paths in Γ_{x_τ,y_τ}, probability distribution $P'_{\Gamma_{x_\tau,y_\tau}}$ is normalized over all paths in Γ_{x_τ,y_τ}, and $d\{x_t\} = d\{x'_t\}$ and $d\{y_t\} = d\{y'_t\}$ due to the time-reversal symmetry [25]. Eq. (20) clearly shows that just as local free energy encodes work [14], and local entropy encodes heat [15], the local form of mutual information between coupled-microstates (x_τ, y_τ) encodes entropy production, within the ensemble of paths that reach each microstate. The following corollary provides more information on entropy production in terms of energetic costs.

3.3. Corollary

To discuss entropy production in terms of energetic costs, we define local free energy $\mathcal{F}_x$ of x_t and $\mathcal{F}_y$ of y_t at macrostate λ_t as follows:

$$\begin{aligned}
\mathcal{F}_x(x_t,t) &:= E_x(x_t,t) - k_B T s[P_t(x_t)] \\
\mathcal{F}_y(y_t,t) &:= E_y(y_t,t) - k_B T s[P_t(y_t)],
\end{aligned} \tag{21}$$

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Peer-reviewed version available at Entropy 2019, 21, 477; doi:10.3390/e21050477

where T is the temperature of the heat bath, k_B is the Boltzmann constant, E_x and E_y are internal energy of systems X and Y, respectively, and $s[P_t(\circ)] := -\ln P_t(\circ)$ is stochastic entropy [2,3]. Work done on either one or both systems through process λ_t is expressed by the first law of thermodynamics as follows:

$$W := \Delta E + Q_b, \tag{22}$$

where ΔE is the change in internal energy of the total system composed of X and Y. If we assume that systems X and Y are weakly coupled, in that interaction energy between X and Y is negligible compared to the internal energy of X and Y, we may have

$$\Delta E := \Delta E_x + \Delta E_y, \tag{23}$$

where $\Delta E_x := E_x(x_\tau, \tau) - E_x(x_0, 0)$ and $\Delta E_y := E_y(y_\tau, \tau) - E_y(y_0, 0)$ [26]. We rewrite Eq. (18) by adding and subtracting the change of internal energy ΔE_x of X and ΔE_y of Y as follows:

$$\begin{aligned}\frac{P'_{\Gamma_{x_\tau,y_\tau}}(\{x'_t\},\{y'_t\})}{P_{\Gamma_{x_\tau,y_\tau}}(\{x_t\},\{y_t\})} &= \exp\{-\beta(Q_b + \Delta E_x + \Delta E_y) + \beta\Delta E_x - \Delta s_x + \beta\Delta E_y - \Delta s_y\} \qquad (24)\\ &\quad\times \exp\{I_\tau(x_\tau,y_\tau) - I_0(x_0,y_0)\}\\ &= \exp\{-\beta(W - \Delta\mathcal{F}_x - \Delta\mathcal{F}_y) + I_\tau(x_\tau,y_\tau) - I_0(x_0,y_0)\}, \qquad (25)\end{aligned}$$

where we have applied Equations (21)–(23) consecutively to Eq. (24) to obtain Eq. (25). Here $\Delta\mathcal{F}_x := \mathcal{F}_x(x_\tau,\tau) - \mathcal{F}_x(x_0,0)$ and $\Delta\mathcal{F}_y := \mathcal{F}_y(y_\tau,\tau) - \mathcal{F}_y(y_0,0)$. Now we multiply both sides of Eq. (25) by $e^{-I_\tau(x_\tau,y_\tau)}$ and $P_{\Gamma_{x_\tau,y_\tau}}(\{x_t\},\{y_t\})$, and take integral over all paths in Γ_{x_τ,y_τ} to obtain the following:

$$\begin{aligned}\left\langle e^{-\beta(W-\Delta\mathcal{F}_x-\Delta\mathcal{F}_y)-I_0}\right\rangle_{x_\tau,y_\tau} &:= \int_{\{x_t\},\{y_t\}\in\Gamma_{\{x_\tau\},\{y_\tau\}}} e^{-\beta(W-\Delta\mathcal{F}_x-\Delta\mathcal{F}_y)-I_0} P_{\Gamma_{x_\tau,y_\tau}}(\{x_t\},\{y_t\})\, d\{x_t\}d\{y_t\}\\ &= \int_{\{x_t\},\{y_t\}\in\Gamma_{\{x_\tau\},\{y_\tau\}}} e^{-I_\tau(x_\tau,y_\tau)} P'_{\Gamma_{x_\tau,y_\tau}}(\{x'_t\},\{y'_t\})\, d\{x'_t\}d\{y'_t\}\\ &= e^{-I_\tau(x_\tau,y_\tau)},\end{aligned} \tag{26}$$

which generalizes known relations in the literature [11,26–30]. We note that Eq. (26) holds under the weak-coupling assumption between systems X and Y during process λ_t, and $\Delta\mathcal{F}_x + \Delta\mathcal{F}_y$ in Eq. (26) is the difference in non-equilibrium free energy, which is different from the change in equilibrium free energy that appears in similar relations in the literature [11,27–30]. If there is no initial correlation, i.e. $I_0 = 0$, Eq. (26) indicates that local mutual information I_τ as a state function of coupled-microstates (x_τ, y_τ) encodes entropy production, $\beta(W - \Delta\mathcal{F}_x - \Delta\mathcal{F}_y)$, within the ensemble of paths in Γ_{x_τ,y_τ}. In the same vein, we may interpret initial correlation I_0 as encoded entropy-production for the preparation of the initial condition.

4. Example

Let X and Y be two systems that weakly interact with each other, and be in contact with the heat bath of inverse temperature β. We may think of X and Y, for example, be bio-molecules that interact with each other or X as a device which measures the state of other system and Y be a measured system. We consider a dynamic coupling process as follows: Initially, X and Y are separately in equilibrium such that the initial correlation $I_0(x_0, y_0)$ is zero for all x_0 and y_0. At time $t = 0$, system X is put in contact with system Y so that a coupling occurs due to their (weak) interactions until time $t = \tau$. During the coupling process, external parameter λ_t for $0 \le t \le \tau$ may exchange work with either one or both systems (see Figure 1b).

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Since each process fluctuates, we repeat the process many times to obtain probability distribution $P_t(x, y)$ for $0 \leq t \leq \tau$. We allow both systems co-evolve interactively and thus $I_t(x_t, y_t)$ may vary not necessarily monotonically. Let us assume that the final probability distribution $P_\tau(x_\tau, y_\tau)$ is as shown in Table 1.

Table 1. The joint probability distribution of x and y at final time τ: Here we assume that both systems X and Y have three states, 0, 1, and 2.

$X\backslash Y$	**0**	**1**	**2**
0	1/6	1/9	1/18
1	1/18	1/6	1/9
2	1/9	1/18	1/6

Then, a few representative mutual information read as follows:

$$\begin{aligned} I_\tau(x_\tau = 0, y_\tau = 0) &= \ln \frac{1/6}{(1/3)\cdot(1/3)} = \ln(3/2), \\ I_\tau(x_\tau = 0, y_\tau = 1) &= \ln \frac{1/9}{(1/3)\cdot(1/3)} = 0, \\ I_\tau(x_\tau = 0, y_\tau = 2) &= \ln \frac{1/18}{(1/3)\cdot(1/3)} = \ln(1/2). \end{aligned} \tag{27}$$

By Jensen's inequality [19], Eq. (20) implies

$$\langle \sigma \rangle_{x_\tau, y_\tau} \geq I_\tau(x_\tau, y_\tau). \tag{28}$$

Thus coupling $x_\tau = 0, y_\tau = 0$ accompanies on average entropy production at least $\ln(3/2)$ which is greater than 0. Coupling $x_\tau = 0, y_\tau = 1$ does not produce entropy on average. Coupling $x_\tau = 0, y_\tau = 2$ on average may produce negative entropy by $\ln(1/2) = -\ln 2$.

5. Conclusions

We have proved the fluctuation theorem of information exchange conditioned at a coupled-microstates, Eq. (20), and its corollary, Eq. (26). Those theorems make it clear that local mutual information encodes as a state function of coupled-states entropy production within an ensemble of paths that reach the coupled-states. Eq. (20) also reproduces lower bound of entropy production, Eq. (28), within a subset of path-ensembles, which provides more detailed information than the fluctuation theorem involved in the ensemble of all paths. Eq. (26) enables us to know the exact relationship between work, non-equilibrium free energy, and mutual information. This end-point conditioned version of the theorem also provides more detailed information on the energetics for coupling than current approaches in the literature. This robust framework may be useful to analyze thermodynamics of dynamic molecular information processes [31–33] and to analyze dynamic allosteric transitions [34,35].

Funding: L.J. was supported by the National Research Foundation of Korea Grant funded by the Korean Government (NRF-2010-0006733, NRF-2012R1A1A2042932, NRF-2016R1D1A1B02011106), and in part by Kwangwoon University Research Grant in 2017.

Conflicts of Interest: The authors declare no conflict of interest.

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