Comment on "Fluctuation theorem for hidden entropy production"

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Recently, Kawaguchi and Nakayama [Phys. Rev. E **88**, 022147 (2013)] claimed that the hidden entropy production associated with a coarse-graining procedure obeys the integral fluctuation theorem (IFT) only if the original process does not involve any odd-parity variable that changes its sign under time reversal. In this Comment, we show that this IFT holds in general, regardless of the presence of odd-parity variables. The discrepancy comes from their erroneous choice of the initial condition for the time-reverse process.

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Kawaguchi and Nakayama (KN) [1] recently claimed that the hidden entropy production, or the amount of entropy production ignored by coarse-graining, obeys the integral fluctuation theorem (IFT) when the original process involves only even-parity variables that are time-reversal invariant. This is consistent with the conventional wisdom that the average hidden entropy production should be non-negative. However, they also claimed that the IFT is not generally valid in the presence of odd-parity variables that are antisymmetric under time reversal. Specifically, the density function asymmetry for odd-parity variables is pointed out as the key source of the IFT violation. Their result implies that the total entropy may increase on average by the reduction of dynamics (coarse-graining), which is against the conventional wisdom. They cited the multibaker map [2] as an example of the IFT violation due to such odd-parity variables.

In this Comment, we show that (1) the hidden entropy production always obeys the IFT even in the presence of odd-parity variables and that (2) the multibaker map is no exception if the coarse-graining scheme adopted by KN is strictly applied.

Consider a Markov process of state variables x and y controlled by a time-dependent protocol $\lambda(t)$. Here, each of x and y may represent multiple variables. The process starts at $t = 0$ and ends at $t = \tau$. For convenience, we define a path variable $\mathbf{x}$ as $\mathbf{x}(t) \equiv \{x_t : t \in [0, \tau]\}$. The probability of a given path $\{\mathbf{x}, \mathbf{y}\}$ can be written as

$$P_\lambda(\mathbf{x}, \mathbf{y}) = P_0(x_0, y_0) W_\lambda(\mathbf{x}, \mathbf{y}|x_0, y_0), \tag{1}$$

where $P_0(x_0, y_0)$ is the probability distribution of the initial state (x_0, y_0) and $W_\lambda(\mathbf{x}, \mathbf{y}|x_0, y_0)$ is the conditional probability for the path $\{\mathbf{x}, \mathbf{y}\}$ starting from (x_0, y_0). In a Markov process, this conditional path probability can be factorized into an infinite product of infinitesimal conditional probabilities.

To characterize the irreversibility of the process, we define the corresponding time-reverse path $\{\mathbf{x}^\dagger, \mathbf{y}^\dagger\}$ as $\mathbf{x}^\dagger(t) = \bar{\mathbf{x}}(\tau - t)$ where $\bar{\mathbf{x}}$ represents the mirrored path with an extra minus sign for each odd-parity variable [3, 4]. The time-reverse path starts at the mirror state of the end point of the original path, $(x_0^\dagger, y_0^\dagger) = (\bar{x}_\tau, \bar{y}_\tau)$. Then, the probability for the time-reverse path is given as

$$P_{\lambda^\dagger}(\mathbf{x}^\dagger, \mathbf{y}^\dagger) = P_0^\dagger(x_0^\dagger, y_0^\dagger) W_{\lambda^\dagger}(\mathbf{x}^\dagger, \mathbf{y}^\dagger|x_0^\dagger, y_0^\dagger), \tag{2}$$

where $\lambda^\dagger(t) = \lambda(\tau - t)$ for the proper time-reverse process.

Each reverse path must be initiated by time-reversing the coordinates of the corresponding forward path at the end of the forward process [3, 4]. Thus, the initial state distribution of the reverse path must be related to the final state distribution of the forward path by

$$P_0^\dagger(x_0^\dagger, y_0^\dagger) = P_\tau(x_\tau, y_\tau). \tag{3}$$

We note that KN used a different condition, $P_0^\dagger(x_0^\dagger, y_0^\dagger) = P_\tau(\bar{x}_\tau, \bar{y}_\tau)$ [5], which is the source of various artifacts related to odd-parity variables.

For Markov processes, the path-dependent total entropy production for a given path $\{\mathbf{x}, \mathbf{y}\}$ can be defined as the ratio between the forward and reverse path probabilities [3, 4, 6, 7]

$$\Sigma(\mathbf{x}, \mathbf{y}) \equiv \ln \frac{P_\lambda(\mathbf{x}, \mathbf{y})}{P_{\lambda^\dagger}(\mathbf{x}^\dagger, \mathbf{y}^\dagger)}. \tag{4}$$

This definition, although not adopted by KN, has become standard because it is a natural way to relate the concept of entropy production to microscopic reversibility [7]. It also provides a convenient mathematical framework for understanding various detailed fluctuation theorems [6]. Once we accept Eq. (4), only Eq. (3) yields the correct formula for total entropy production [8], which is also used by KN. In contrast, the same formula cannot be derived from KN's initial condition for the time-reverse process. Thus, KN's choice of $P_0^\dagger(x_0^\dagger, y_0^\dagger)$ is inconsistent with the above standard definition for the total entropy production.

We define coarse-graining as integration over a subset of state variables, in accordance with [1]. Then, the coarse-grained path probabilities can be written as

$$\tilde{P}_\lambda(\mathbf{x}) \equiv \int \mathrm{d}\mathbf{y}\, P_\lambda(\mathbf{x},\mathbf{y}), \tag{5}$$

$$\tilde{P}_{\lambda^\dagger}(\mathbf{x}^\dagger) \equiv \int \mathrm{d}\mathbf{y}^\dagger\, P_{\lambda^\dagger}(\mathbf{x}^\dagger,\mathbf{y}^\dagger). \tag{6}$$

In the manner of Eq. (4), the total entropy production along a coarse-grained forward path is similarly defined as

$$\tilde{\Sigma}(\mathbf{x}) \equiv \ln \frac{\tilde{P}_\lambda(\mathbf{x})}{\tilde{P}_{\lambda^\dagger}(\mathbf{x}^\dagger)}. \tag{7}$$

As pointed out by KN, the coarse-grained process obtained from Eqs. (5) and (6) is generally non-Markovian, so the above definition may not represent the proper entropy production, i.e. the additivity of the entropy production over time may not be satisfied. Nevertheless, we proceed with this definition here as KN did with their own in [1].

The hidden entropy production is defined as

$$\Xi(\mathbf{x},\mathbf{y}) \equiv \Sigma(\mathbf{x},\mathbf{y}) - \tilde{\Sigma}(\mathbf{x}). \tag{8}$$

Then, it is trivial to prove the IFT for $\Xi(\mathbf{x},\mathbf{y})$ without making any further assumption about the state variables:

$$\begin{aligned}\langle e^{-\Xi(\mathbf{x},\mathbf{y})}\rangle &= \int \mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{y}\, P_\lambda(\mathbf{x},\mathbf{y}) \frac{P_{\lambda^\dagger}(\mathbf{x}^\dagger,\mathbf{y}^\dagger)}{P_\lambda(\mathbf{x},\mathbf{y})} \frac{\tilde{P}_\lambda(\mathbf{x})}{\tilde{P}_{\lambda^\dagger}(\mathbf{x}^\dagger)} \\ &= \int \mathrm{d}\mathbf{x}\, \frac{\tilde{P}_\lambda(\mathbf{x})}{\tilde{P}_{\lambda^\dagger}(\mathbf{x}^\dagger)} \int \mathrm{d}\mathbf{y}^\dagger\, P_{\lambda^\dagger}(\mathbf{x}^\dagger,\mathbf{y}^\dagger) \\ &= \int \mathrm{d}\mathbf{x}\, \tilde{P}_\lambda(\mathbf{x}) = 1. \end{aligned} \tag{9}$$

Hence, $\Xi(\mathbf{x},\mathbf{y})$ satisfies the IFT regardless of the parity of state variables. By Jensen's inequality, the IFT implies $\langle\Xi(\mathbf{x},\mathbf{y})\rangle \geq 0$, so the entropy production is reduced on average by coarse-graining, as expected.

In contradiction, KN presented a deterministic Hamiltonian-like model that is claimed to be coarse-grained into a probabilistic dynamics [1]. If this coarse-graining is possible, it is obvious that $\langle\Xi(\mathbf{x},\mathbf{y})\rangle$ can be negative, because $\langle\Sigma(\mathbf{x},\mathbf{y})\rangle = 0$ for a deterministic model with the time-reversal symmetry and $\langle\tilde{\Sigma}(\mathbf{x})\rangle > 0$ for a probabilistic model.

In the following, we show that this contradictory result originates from the Markovian truncation adopted by KN during the coarse-graining procedure, where the memory cutoff induces stochasticity and positive entropy production. Without any approximation in coarse-graining implemented by Eqs. (5) and (6), it is impossible to convert any deterministic process to a stochastic one and one can easily show that the coarse-grained system also does not produce entropy: $\langle\Xi(\mathbf{x},\mathbf{y})\rangle = 0$.

To address this problem explicitly, we consider an area-preserving deterministic (Hamiltonian) process with the time-reversal symmetry, of which the extended multibaker map is one example. Since the process is deterministic, the path is uniquely determined by its initial state, which is denoted by $\{\hat{\mathbf{x}}(x_0,y_0), \hat{\mathbf{y}}(x_0,y_0)\}$. Then, the conditional path probability is given as

$$W_\lambda(\mathbf{x},\mathbf{y}|x_0,y_0) = \delta[\mathbf{x}-\hat{\mathbf{x}}(x_0,y_0)]\cdot\delta[\mathbf{y}-\hat{\mathbf{y}}(x_0,y_0)], \tag{10}$$

where δ represents an infinite product of delta functions over the path $\{\mathbf{x},\mathbf{y}\}$. Using Eqs. (1) and (5), the probability of a coarse-grained path is given by

$$\tilde{P}_\lambda(\mathbf{x}) = \int \mathrm{d}y_0\, P_0(x_0,y_0)\ \delta[\mathbf{x}-\hat{\mathbf{x}}(x_0,y_0)] \tag{11}$$

Note that the area preservation condition guarantees $P_\tau(x_\tau,y_\tau) = P_0(x_0,y_0)$ with (x_τ,y_τ) uniquely determined by (x_0,y_0).

Similarly for the time-reverse path, we get

$$W_{\lambda^\dagger}(\mathbf{x}^\dagger,\mathbf{y}^\dagger|x_0^\dagger,y_0^\dagger) = \delta[\mathbf{x}^\dagger-\hat{\mathbf{x}}^\dagger(x_0^\dagger,y_0^\dagger)]\cdot\delta[\mathbf{y}^\dagger-\hat{\mathbf{y}}^\dagger(x_0^\dagger,y_0^\dagger)]. \tag{12}$$

Due to the time-reversal symmetry of the deterministic process, the time-reverse path should trace exactly back along the forward path with the initial condition $(x_0^\dagger,y_0^\dagger) = (\bar{x}_\tau,\bar{y}_\tau)$. Hence, $W_{\lambda^\dagger}(\mathbf{x}^\dagger,\mathbf{y}^\dagger|x_0^\dagger,y_0^\dagger)$ is identical to $W_\lambda(\mathbf{x},\mathbf{y}|x_0,y_0)$. Then, the probability of the coarse-grained reverse path is obtained as

$$\begin{aligned}\tilde{P}_{\lambda^\dagger}(\mathbf{x}^\dagger) &= \int \mathrm{d}y_0^\dagger\, P_0^\dagger(x_0^\dagger,y_0^\dagger)\delta[\mathbf{x}^\dagger-\hat{\mathbf{x}}^\dagger(x_0^\dagger,y_0^\dagger)] \\ &= \int \mathrm{d}y_\tau\, P_\tau(x_\tau,y_\tau)\delta[\mathbf{x}-\hat{\mathbf{x}}(x_0,y_0)] \\ &= \tilde{P}_\lambda(\mathbf{x}), \end{aligned} \tag{13}$$

where Eq. (3) and the area-preserving property are used. Hence, in contrast to the claim by KN [1], the entropy production is zero even after the coarse-graining, which means $\Xi(\mathbf{x},\mathbf{y}) = 0$ for every path. This implies that the coarse-graining does not invoke any irreversibility from a time-reversal symmetric deterministic process.

Why does the coarse-grained process fail to produce any entropy? It is simply because it is still deterministic except for the uncertainty associated with the initial state variable y_0, as indicated by Eq. (11). Once the initial uncertainty is resolved by fixing y_0, the everlasting memory of the initial state ensures that the rest of the coarse-grained process has no random elements. Thus, there is no chance left for the entropy production. In order to give rise to stochasticity and positive entropy production, the memory cutoff at a Markovian time scale must be built into the coarse-graining scheme. This additional requirement was implicitly assumed when KN claimed that the multibaker map could be coarse-grained to the one-dimensional random walk [1]. In that case, the violation of the IFT should be attributed not to the presence of odd-parity variables, but to the memory cutoff.

In conclusion, the hidden entropy production due to the coarse-graining by integration over a subset of state variables always satisfies the IFT, irrespective of the presence of odd-parity variables. The IFT can be violated only if an additional memory cutoff (Markovian truncation) is built into the coarse-graining scheme.

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