Generalized detailed fluctuation theorem under nonequilibrium feedback control

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It has been shown recently that the Jarzynski equality is generalized under nonequilibrium feedback control [T. Sagawa and M. Ueda, Phys. Rev. Lett. **104**, 090602 (2010)]. The presence of feedback control in physical systems should modify both the Jarzynski equality and the detailed fluctuation theorem [K. H. Kim and H. Qian, Phys. Rev. E **75**, 022102 (2007)]. However, the generalized Jarzynski equality under forward feedback control has been proved by considering that the physical systems under feedback control should locally satisfy the detailed fluctuation theorem. We use the same formalism and derive the generalized detailed fluctuation theorem for nonequilibrium driven systems under feedback control. We find that the feedback control in a physical system should preserve the detailed fluctuation theorem if the system has the same feedback information measure in forward and reverse directions.

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I. INTRODUCTION

There are very few relations in statistical dynamics which are used to calculate the equilibrium thermodynamic properties for the systems driven arbitrarily far from equilibrium [1–3]. In particular, the Jarzynski's equality [1] and the Crooks detailed fluctuation theorem [2] can be used to calculate equilibrium free-energy differences from nonequilibrium work measurements. Consider a system initially in equilibrium at temperature (inverse) $\beta=1/k_BT$ (k_B is the Boltzmann constant) which is externally driven from its initial state to final state by nonequilibrium process. The work W performed on the system satisfies the detailed fluctuation theorem $P(W)/P(-W)=\exp[\beta(W-\Delta F)]$, where $P(\pm W)$ is the work probability distribution in forward (+) and reverse (−) directions and ΔF is the free-energy difference between its final and initial equilibrium states. The Jarzynski equality, $\langle\exp(-\beta W)\rangle=\exp(-\beta\Delta F)$, is the integrated version of the detailed fluctuation theorem. The average $\langle\cdots\rangle$ is over a statistical ensemble of realizations of a given thermodynamic process. These two nonequilibrium work relations have been verified in experiments [4,5] as well as in simulations [6,7] and widely used in many branches of science (see, e.g., [8,9]).

The evolution of the physical systems can be modified or controlled by the repeated operation of an external agent called controller [10,11]. The action of the controller is to regulate the system dynamics and increase its performance. The controller can operate on the system blindly or it can use information about the state of the system. The former is known as the open loop controller and the latter one is called the feedback or closed loop controller. The feedback controller measures the partial performance of the system, and its action on the system depends on the measurement outcome [12]. For example, in a single molecule atomic force microscopy experiment, the external agent is an electric feedback circuit which detects the motion of the cantilever and manipulates the control force proportional to its velocity [13]. The proper utilization of the information about the state of the system in feedback control effectively improves the system performance [10–14]. If the experiments or simulations have been performed under feedback control, both the Jarzynski equality and the fluctuation theorem should be extended into more general forms [13]. Since the work that performed on a thermodynamic system can be lowered by feedback control [12–14], this feedback mechanism can be helpful in simulations for sampling rare trajectories and in calculating precise free-energy differences [15].

Recently, the Jarzynski equality is generalized to an experimental condition in which the system is driven between two equilibrium states via a nonequilibrium process under forward feedback control [16]. The equilibrium free-energy difference for the driven system (which locally satisfies the detailed fluctuation theorem) under nonequilibrium feedback control can be calculated from the generalized Jarzynski equality [16]

$$\langle e^{-\sigma-I}\rangle=1, \tag{1}$$

where $\sigma=\beta(W-\Delta F)$ and I is the mutual information measure obtained by the feedback controller [16]. The average is taken from the work distribution in the forward direction with feedback control.

The presence of feedback control in physical system modifies both the Jarzynski equality and the fluctuation theorem [13]. However, the generalized Jarzynski equality [Eq. (1)] under forward feedback control has been proved by considering that the physical systems under feedback control should locally satisfy the detailed fluctuation theorem [16]. In this paper, we use the same formalism and derive the generalized detailed fluctuation theorem for nonequilibrium driven systems under feedback control. In order to calculate the free-energy differences precisely in simulations, one requires information of work distribution in both forward and reverse directions [17–19]. In this aspect, one needs the generalized detailed fluctuation theorem under nonequilibrium feedback control.

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II. DETAILED FLUCTUATION THEOREM UNDER FEEDBACK CONTROL

The feedback control enhances our controllability of small thermodynamic systems [10–14]. At any given time, the controller measures the partial state of the system. The result of the measurement determines the action of the controller. The additional information on the system provided by the measurement further determines the state of the system. Suppose that the controller performs a measurement on a stochastic thermodynamic system at time t_m. Let Γ_m be the phase-space point of the system at that time, $P[\Gamma_m]$ its probability, and y the measurement. Depending on the controller measurements, the outcome y can occur with a probability $P[y]$ [16]. The information obtained by the controller can be characterized by the mutual (feedback) information measure [16,20],

$$I[y,\Gamma_m] = \ln\left[\frac{P[y|\Gamma_m]}{P[y]}\right], \tag{2}$$

where $P[y|\Gamma_m]$ is the conditional probability of obtaining the outcome y on the condition that the state of the system is Γ_m. The above equation can be rewritten as

$$e^{I[y,\Gamma_m]} = \frac{P[y|\Gamma_m]}{P[y]}. \tag{3}$$

In experiments and simulations, the free-energy difference between two equilibrium states can be calculated in general by pulling the system from one equilibrium state to another state along a switching path. The path connecting the two states in the time period τ will be parametrized using the variable λ, with $0 \le \lambda \le 1$. The switching rate describes the nature of the switching process to be an equilibrium (infinitely slow) or nonequilibrium (fast). If the experiments are performed under feedback control, the switching control parameter λ depends on the outcome y after t_m [16]. That is, whenever the controller makes measurements, there is a corresponding change in the switching parameter for the next time step, which is denoted as $\lambda_{(t;y)}$. Between every stage of the controller measurements, the value of the outcome y is to be fixed and the corresponding switching parameter $\lambda_{(t;y)}$ does not change. In this time interval for each stage of $\lambda_{(t;y)}$, we consider that the system should locally satisfy the detailed fluctuation theorem [16],

$$\frac{P_{\lambda_{(t;y)}}[\Gamma(t)]}{P_{\lambda^\dagger_{(t;y)}}[\Gamma^\dagger(t)]} = e^{\sigma[\Gamma(t)]}, \tag{4}$$

where $P_{\lambda_{(t;y)}}[\Gamma(t)]$ is the probability of obtaining the outcome y in the forward direction with a switching protocol $\lambda_{(t;y)}$, and $P_{\lambda^\dagger_{(t;y)}}[\Gamma^\dagger(t)]$ is the probability of obtaining the same outcome y [16] in the reverse direction of phase point, $\Gamma^\dagger(t)$, with the corresponding switching protocol $\lambda^\dagger_{(t;y)}$. Here, $\sigma[\Gamma(t)]$ is the work value obtained in the forward direction and its time reversal work value

$$\sigma[\Gamma^\dagger(t)] = -\sigma[\Gamma(t)]. \tag{5}$$

Let $P_F[\tilde{X}] \equiv P_F[\sigma[\tilde{\Gamma}], I[\tilde{y},\tilde{\Gamma}]]$ be the joint probability of obtaining the work value $\sigma[\tilde{\Gamma}]$ for a given feedback information $I[\tilde{y},\tilde{\Gamma}]$ of the measurement outcome $\tilde{y}$ in the forward direction. The particular outcome $\tilde{y}$ may often occur in different realizations of the repeated experiment. Analogous to previous studies [21,22], this (joint) probability can be obtained from the nonequilibrium ensemble of variable (forward) switching trajectories as

$$P_F[\tilde{X}] = \int P[y'|\Gamma'_m]P_{\lambda_{(t;y')}}[\Gamma(t)]\,\delta(I[y',\Gamma'_m] - I[\tilde{y},\tilde{\Gamma}])\,\delta(\sigma[\Gamma(t)] - \sigma[\tilde{\Gamma}])dy'D[\Gamma(t)], \tag{6}$$

where $\delta(x)$ is the Dirac delta function which has a property $\delta(-x)=\delta(x)$. It should be noted that y' and Γ'_m in the above equation are dummy variables, and they have appropriate values for each outcome of the controller measurements [see Eq. (3)].

Combining Eqs. (3) and (4), Eq. (6) is modified as

$$P_F[\tilde{X}] = \int e^{\sigma[\Gamma(t)]+I[y',\Gamma'_m]}P[y']P_{\lambda^\dagger_{(t;y')}}[\Gamma^\dagger(t)]\,\delta(I[y',\Gamma'_m] - I[\tilde{y},\tilde{\Gamma}])\,\delta(\sigma[\Gamma(t)] - \sigma[\tilde{\Gamma}])dy'D[\Gamma(t)],$$

$$P_F[\tilde{X}] = e^{\sigma[\tilde{\Gamma}]+I[\tilde{y},\tilde{\Gamma}]}\int P[y']P_{\lambda^\dagger_{(t;y')}}[\Gamma^\dagger(t)]\,\delta(I[y',\Gamma'_m] - I[\tilde{y},\tilde{\Gamma}])\,\delta(\sigma[\Gamma(t)] - \sigma[\tilde{\Gamma}])dy'D[\Gamma(t)]. \tag{7}$$

Let $P_R[\tilde{X}^\dagger] \equiv P_R[-\sigma[\tilde{\Gamma}], I[\tilde{y}^\dagger,\tilde{\Gamma}]]$ be the joint probability of obtaining the work value $-\sigma[\tilde{\Gamma}]$ for a given feedback information $I[\tilde{y}^\dagger,\tilde{\Gamma}]$ of the measurement outcome $\tilde{y}^\dagger$ in the reverse direction. This (joint) probability can be obtained from the nonequilibrium ensemble of variable (reverse) switching trajectories as

$$P_R[\tilde{X}^\dagger] = \int P[y'|\Gamma'_m]P_{\lambda^\dagger_{(t;y')}}[\Gamma^\dagger(t)]\,\delta(I[y',\Gamma'_m] - I[\tilde{y}^\dagger,\tilde{\Gamma}])\,\delta(\sigma[\Gamma^\dagger(t)] + \sigma[\tilde{\Gamma}])dy'D[\Gamma^\dagger(t)]. \tag{8}$$

In what follows, we will use above equations and derive the generalized detailed fluctuation theorem under feedback control either in the forward direction [16] or in both directions.

A. Feedback control in forward and reverse directions

If the system has the same feedback control in both directions, then under the controller measurement condition, $I[\tilde{y}^\dagger,\tilde{\Gamma}]=I[\tilde{y},\tilde{\Gamma}]$, and using Eq. (3), we can rewrite Eq. (8) as

$$P_R[\tilde{X}^\dagger] = e^{I[\tilde{y},\tilde{\Gamma}]}\int P[y']P_{\lambda^\dagger_{(t;y')}}[\Gamma^\dagger(t)]\,\delta(I[y',\Gamma'_m] - I[\tilde{y},\tilde{\Gamma}])\,\delta(\sigma[\Gamma^\dagger(t)] + \sigma[\tilde{\Gamma}])dy'D[\Gamma^\dagger(t)]. \tag{9}$$

Since $\delta(-x)=\delta(x)$ and $D[\Gamma^\dagger(t)]=D[\Gamma(t)]$ [16], combining Eqs. (5) and (9) in Eq. (7) we can obtain the generalized detailed fluctuation theorem under feedback control in both directions as

$$P_F[\tilde{X}] = e^{\sigma[\tilde{\Gamma}]+I[\tilde{y},\tilde{\Gamma}]}P_R[\tilde{X}^\dagger]e^{-I[\tilde{y},\tilde{\Gamma}]},$$

$$\frac{P_F[\tilde{X}]}{P_R[\tilde{X}^\dagger]} = e^{\sigma[\tilde{\Gamma}]}. \tag{10}$$

The above equation can be written simply as

$$\frac{P_F[\sigma,I]}{P_R[-\sigma,I]} = e^{\sigma}. \tag{11}$$

Although the feedback control in classical systems in general modifies the detailed fluctuation theorem, our result shows that for a given feedback information measure I in both directions, the physical system under repeated measurements of the feedback controller does not modify the detailed fluctuation theorem. Since the feedback control enhances our controllability of small thermodynamic systems, the proper choice of feedback mechanism in free-energy simulations can be useful for precise free-energy estimates [15].

B. Feedback control in the forward direction

If the system has feedback control only in the forward direction, the generalized detailed fluctuation theorem under forward feedback control can be obtained from the following reverse experimental condition. Based on the information about forward switching protocols, without feedback control, we can perform the same variable switching protocol experiment in the reverse direction [16]. This is equivalent to operation of the open loop controller in the reverse direction on the system. In such a case, $P[y'|\Gamma'_m]=P[y']$ in the reverse direction, and the open loop controller implicitly has information about the forward feedback information measure $I[\tilde{y},\tilde{\Gamma}]$ for the corresponding switching parameter $\lambda^\dagger_{(t;y')}$ in the reverse direction [see Eqs. (3) and (4)]. Then, we can write Eq. (8) as

$$P_R[\tilde{X}^\dagger] = \int P[y']P_{\lambda^\dagger_{(t;y')}}[\Gamma^\dagger(t)]\delta(I[y',\Gamma'_m] - I[\tilde{y},\tilde{\Gamma}])\delta(\sigma[\Gamma^\dagger(t)] + \sigma[\tilde{\Gamma}])dy'D[\Gamma^\dagger(t)]. \tag{12}$$

Similar to the earlier derivation, using Eqs. (5) and (12) in Eq. (7) we can obtain the generalized detailed fluctuation theorem under forward feedback control as

$$P_F[\tilde{X}] = e^{\sigma[\tilde{\Gamma}]+I[\tilde{y},\tilde{\Gamma}]}P_R[\tilde{X}^\dagger],$$

$$\frac{P_F[\tilde{X}]}{P_R[\tilde{X}^\dagger]} = e^{\sigma[\tilde{\Gamma}]+I[\tilde{y},\tilde{\Gamma}]}. \tag{13}$$

In order to prove the generalized Jarzynski equality under forward feedback control, we measure the quantity

$$\langle e^{-\sigma-I}\rangle = \int P_F[\tilde{X}]e^{-\sigma[\tilde{\Gamma}]-I[\tilde{y},\tilde{\Gamma}]}d\tilde{y}d\tilde{\Gamma}.$$

From Eq. (13),

$$\langle e^{-\sigma-I}\rangle = \int P_R[\tilde{X}^\dagger]d\tilde{y}d\tilde{\Gamma} = 1, \tag{14}$$

we obtained the generalized Jarzynski equality under forward feedback control [16]. In order to get more insight into the forward mutual information measure, we calculate the quantity

$$\langle e^{-\sigma}\rangle = \int P_F[\tilde{X}]e^{-\sigma[\tilde{\Gamma}]}d\tilde{y}d\tilde{\Gamma}.$$

Using Eq. (13), the average of above equation can be written as

$$\langle e^{-\sigma}\rangle = \int P_R[\tilde{X}^\dagger]e^{I[\tilde{y},\tilde{\Gamma}]}d\tilde{y}d\tilde{\Gamma} = \int P_R[\widetilde{X^{\star\dagger}}]d\tilde{y}d\tilde{\Gamma} = \gamma, \tag{15}$$

where $\gamma=\int P_R[\widetilde{X^{\star\dagger}}]d\tilde{y}d\tilde{\Gamma}$ is the feedback control characteristic, which is a measure of the correlation between the dissipation and the information [16]. $P_R[\widetilde{X^{\star\dagger}}]=P_R[\tilde{X}^\dagger]e^{I[\tilde{y},\tilde{\Gamma}]}$ is the special case [16] of the joint probability distribution in the reverse direction.

Even though there is no feedback control in the reverse direction, due to the implementation of variable (reverse) switching protocols in accordance with forward feedback control experiment, we can also obtain the forward mutual information measure from the reverse direction as

$$I[\tilde{y},\tilde{\Gamma}] = \ln\left[\frac{P_R[\widetilde{X^{\star\dagger}}]}{P_R[\tilde{X}^\dagger]}\right]. \tag{16}$$

III. CONCLUSION

We have derived the generalized detailed fluctuation theorem under nonequilibrium feedback control. The central finding of our result [Eq. (11)] shows that for the same feedback information measure, the repeated measurements of the feedback controller in both directions do not modify the detailed fluctuation theorem. It is well known that the exponential average in one direction limits the accurate calculation of free-energy differences in simulations. The knowledge of measurements from both directions usually gives improved results. Thus, the generalized detailed fluctuation theorem can be very useful in free-energy simulations for systems driven under nonequilibrium feedback control.

In a recent investigation of quantum fluctuation theorem, it was shown that the action of intermediate projective quantum measurements does not affect the fluctuation theorem [23]. It would be interesting to carry out an investigation of how the repeated controller measurements in quantum systems with feedback control can affect the quantum fluctuation theorem.

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