Unifying approach for fluctuation theorems from joint probability distributions

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Any decomposition of the total trajectory entropy production for Markovian systems has a joint probability distribution satisfying a generalized detailed fluctuation theorem, when all the contributing terms are odd with respect to time reversal. The expression of the result does not bring into play dual probability distributions, hence easing potential applications. We show that several fluctuation theorems for perturbed nonequilibrium steady states are unified and arise as particular cases of this general result. In particular, we show that the joint probability distribution of the system and reservoir trajectory entropies satisfy a detailed fluctuation theorem valid for all times.

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The nonequilibrium stochastic thermodynamics of small systems has attracted a lot of attention. From the experimental side the development of techniques for microscopic manipulation has allowed one to study fluctuations in small systems [1,2]. From the theoretical side a group of exact relations known as fluctuation theorems (FTs) [3–8] has shed light into the principles governing dissipation and fluctuations in nonequilibrium phenomena, as in driven systems in contact with thermal bath. Formally, the generality of the FTs can be attributed to the way probability distribution functions of different observables behave under time-reversal symmetry-breaking perturbations (see [9,10] for reviews on FT).

Oono and Paniconi [11] proposed a phenomenological framework for a “nonequilibrium steady-state (NESS) thermodynamics” aimed at describing fluctuating systems subjected to an external protocol. In this approach, the total exchanged heat during a time interval \( \tau \) by a system initially prepared in a NESS is expressed as the sum of two contributions: \( Q^{\text{tot}}=Q^{\text{ex}}+Q^{\text{bk}} \). The “excess heat” \( Q^{\text{ex}} \) is, in average, associated with the energy exchange during transitions between steady states while the “housekeeping heat” \( Q^{\text{bk}} \) corresponds, in average, to the energy we need to supply to maintain the system in a NESS. Hatano and Sasa [12] introduced a formal framework for these phenomenological ideas and derived a FT which extends the second law of thermodynamics for transitions between NESSs controlled by external parameters \( \sigma(t) \). The Hatano and Sasa FT is applicable to trajectories \( x(t) \) evolved with a Langevin or more generally a Markovian dynamics starting from an initial condition sampled from a NESS compatible with the initial values \( \sigma(0) \) of the control parameters.

Under identical conditions different FTs were subsequently proposed for NESS, involving the above decomposition of the exchanged heat. We can distinguish between the so-called integral and detailed FTs for systems initially prepared as described above. The integral fluctuation theorems (IFTs) are exact relations for the average over histories of different stochastic trajectory functions \( W(x) \), such as \( \langle e^{-W} \rangle=1 \). Examples are the Jarzynski FT for the total work [7], the Hatano-Sasa FT [12], and the Speck-Seifert FT [13]. The so-called detailed FTs (DFTs) are, on the other hand, exact relations for the probability distribution functions (PDFs) of different observables \( W_x \), such as \( P(W)/P(-W)=e^Q \), where \( P(W) \) corresponds to the time-reversed protocol \( \sigma^{\text{R}}(t)=\sigma(-t) \), and a NESS initial condition compatible with \( \sigma(\tau) \). Examples are given by the Crooks relation [8] or Seifert fluctuation theorem [14]. While observables satisfying a DFT trivially satisfy an IFT, the opposite is not always true. In many recently formulated DFTs, a modified “dual” PDF \( P^{\text{R}}(W) \) enters into play [15,16], which corresponds to trajectories in a system with same stationary PDF but with reversed steady probability current [i.e., such that \( P^{\text{R}}(W)=P(W) \) when detailed balance holds]. In general the dual dynamics is different from the original dynamics of the system. Thus, the presence of dual distributions is a strong limitation to the experimental use of such a DFT. A central result of our work is that generalized DFTs can be established without relying on dual probabilities by considering joint probability distributions for different complementary observables, instead of single PDFs. The joint probability distributions arise naturally from the above mentioned separation of two contributions to the total heat exchanged in a NESS. From this joint DFT all the known DFTs and IFTs follow in a straightforward way.

Among the fluctuation theorems formulated for Markovian dynamics, the total trajectory entropy production \( S[x;\sigma]=\ln[P_x^{\text{R}}/P_x] \) plays a fundamental role [5,6,14]. Here, \( P_x^{\text{R}}/P_x \) denotes the probability density of trajectory \( x \) (time-reversed trajectory \( x^R \)) in the forward (backward) protocol. We include in \( P \) the initial distribution of \( x \). We omit hereafter the final time \( \tau \) in all trajectory functionals and use calligraphic symbols to denote functionals and normal symbols to denote their values. The total trajectory entropy production is odd upon time reversal: \( S[x^R;\sigma^R]=-S[x;\sigma] \). We show that any decomposition of \( S \) in \( M \) distinct contributions, \( S[x;\sigma]=\sum M_A[x;\sigma] \), each of them being odd \( A[x^R;\sigma^R]=-A[x;\sigma] \), has a generating function satisfying the symmetry...
\( \langle \exp \left( - \sum_i^M \lambda_i A_i[x; \sigma] \right) \rangle = \left( \exp \left( - \sum_i^M (1 - \lambda_i) A_i[x; \sigma^2] \right) \right)_R, \)

(1)

where \( \lambda_i \) are arbitrary parameters and \( \langle \ldots \rangle_R \) denotes average over trajectories in the reversed protocol [17]. This symmetry is equivalent to the following generalized DFT for the joint probability of \( A_i[x; \sigma]'s \):

\[
P(A_1, A_2, \ldots, A_M) = \frac{P^R(-A_1, -A_2, \ldots, -A_M)}{P^R(-A_1, -A_2, \ldots, -A_M)} = e^S \text{ with } S = \sum_i^M A_i. \tag{2}
\]

Note that the result involves no use of dual PDFs. To prove Eq. (1) we start by noting that the average of any observable \( O[x] \) over trajectories satisfies the relation

\[
\langle O[x; \sigma] \rangle = \int DxP[x; \sigma^R]O[x; \sigma]e^{-S(x, \sigma^R)} = \langle O[x; \sigma^R]e^{-S(x, \sigma^R)} \rangle_R, \tag{3}
\]

where we have used \( S[x; \sigma]=S[x; \sigma^R] \) together with the change of variable \( x \rightarrow x^R \). Considering \( S[x; \sigma]=\sum_i^M A_i[x; \sigma] \) the proof comes around:

\[
\langle \exp(-\sum_i^M \lambda_i A_i[x; \sigma]) \rangle = \langle \exp(-\sum_i^M \lambda_i A_i[x; \sigma^R]) \rangle_R \tag{4}
\]

Equation (2) is proved in a similar way, or also follows from Eq. (1) since it is a symmetry for the generating function of the joint distribution \( P(A_1, \ldots, A_M) \). Before considering their particular application for explicit decompositions of \( S \) we note that symmetries (1) and (2) are valid for all times \( \tau \) for systems prepared in any initial distribution \( P(x(0)) \). In particular, we see that the total entropy production \( FTs (e^{-S}) \) is a time-translation invariant and in particular, we see that the total entropy production \( FTS (e^{-S}) \) is equal to the average of any observable \( O \) with initial distribution \( P^R(-x, -\sigma^R) \) over trajectories in the reversed protocol.

We will consider two generic frameworks where our result applies: systems described (i) by Langevin dynamics and (ii) by a Markovian dynamics on discrete configurations, exemplifying their parallel features. First we consider a particle driven by a constant force \( f \) in a potential \( U \),

\[
x = -\partial_x U(x; \alpha(t)) + f + \xi, \tag{5}
\]

where \( \alpha(t) \) represents a set of control parameters and \( \xi(t) \) is the Gaussian white noise, with \( \langle \xi(t) \xi(0) \rangle = 0 \) and \( \langle \xi(t) \xi(t') \rangle = 2T \delta(t-t') \) due to a thermal bath at temperature \( T \). For example, this system can be out of equilibrium when \( U \) has periodic boundary conditions. We consider for simplicity a single degree of freedom \( x \), but our results are easily generalized, e.g., in larger dimensions and/or with more particles. For a stochastic trajectory generated by Eq. (4) we define the total exchanged heat as

\[
\beta Q^\text{tot}[x; \sigma] = -\beta \int_0^\tau d\xi_t [\partial_x U(x; \alpha) - f]. \tag{6}
\]

The total exchanged heat in a trajectory can be split as \( Q^\text{tot} = Q^\text{kin} + Q^\text{ct} \) [11]. Defining \( \phi(x; \sigma) = -\ln p_{SS}(x; \sigma) \) from the steady-state probability density \( p_{SS}(x; \sigma) \) at fixed values of \( \sigma=(\alpha, f) \) Hatano and Sasa [12] proposed

\[
\beta Q^\text{tot}[x; \sigma] = \int_0^\tau d\xi_t [\partial_x \phi(x; \sigma) - \beta \partial_x U(x; \alpha) - f], \tag{7}
\]

for the housekeeping heat, and

\[
\beta Q^\text{ex}[x; \sigma] = -\int_0^\tau d\xi_t \partial_x \phi(x; \sigma), \tag{8}
\]

for the excess heat. The Hatano-Sasa functional [12] \( \mathcal{Y}[x; \sigma] \) is then defined as

\[
\mathcal{Y}[x; \sigma] = \int_0^\tau d\tau [\partial_x \phi(x; \sigma) + \beta \partial_x U(x; \alpha)] \tag{9}
\]

Similar decompositions also exist for Markovian dynamics: we consider now discrete configurations \( \{C\} \) with transition rates \( W(C \rightarrow C'); \sigma \) between configurations. They depend on \( \sigma \), an external control parameter which may vary in time. The probability density at time \( t \) obeys the Markovian dynamics

\[
\partial_t P(C, t) = \sum_{C'} W(C' \rightarrow C; \sigma(t)) P(C', t) - r(C; \sigma(t)) P(C, t), \tag{10}
\]

meaning that the mean value of an history-dependent observable \( O \) is given by \( \langle O \rangle = \sum_{C'=0}^K \sum_{\sigma} \int d\sigma \int d\tau \partial_x \phi(x; \sigma)[P(C; \sigma)] \tag{11} \]

where \( \phi(x; \sigma) = \exp[-\int_0^\tau [\partial_x U(C(t); \sigma(t)) - \beta \partial_x U(x; \alpha)] dt] \) and

\[
\beta Q^\text{tot}[x; \sigma] = \sum_{C'=0}^K \sum_{\sigma} \int d\sigma \int d\tau \partial_x \phi(x; \sigma) W(C; \sigma) = -\int_0^\tau d\tau \partial_x \phi(x; \sigma) \tag{12}
\]

Although there is no natural definition of \( \beta \) we write \( \beta Q^\text{tot} \) to exemplify the parallel with Langevin dynamics.

Turning to the first decomposition, let us assume that the initial distribution is steady state: \( P_{\sigma} = p_{SS}(\alpha, \sigma) \). One directly checks that the Hatano-Sasa functional \( \mathcal{Y}[C; \sigma] \) can be written as

\[
\int_0^\tau d\tau [\partial_x U(C(t); \sigma(t)) - \beta \partial_x U(x; \alpha)]. \tag{13}
\]

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The corresponding IFTs can be written as

$$\mathcal{Y} = \left[ \phi(C, \sigma) \right]_R - \sum_{k=1}^K \left[ \phi(C_k, \sigma_k) - \phi(C_{k-1}, \sigma_{k-1}) \right].$$

Besides, defining the housekeeping work as

$$\beta Q^{hk}[C, \sigma] = \sum_{k=1}^K \log \frac{W(C_{k-1} \rightarrow C_k, \sigma_k)}{W(C_k \rightarrow C_{k-1}, \sigma_k)} + \sum_{k=1}^K \phi(C_k, \sigma_k) - \phi(C_{k-1}, \sigma_{k-1}),$$

we check that the decomposition $S = \mathcal{Y} + \beta Q^{hk}$ holds [19]. The parallel between Markovian and Langevin frameworks also appears by specializing to rates $W(k \rightarrow k \pm 1) = e^{-\beta[2f(V_k \cdot \sigma + V_{k+1} \cdot \sigma)]}$ of jumping on a one-dimensional lattice from site $k$ to $k \pm 1$ in a tilted potential $V_k = U_k - kf$: in the continuum limit, one recovers the Langevin observables [19].

In the first decomposition, $\mathcal{Y}$ can be identified with the so-called nonadiabatic contribution (since it vanishes for quasistatic protocols) to the trajectory entropy $S_{\text{na}} = \mathcal{Y}$, while $\beta Q^{hk}$ (which is continuously produced in the steady state) can be identified with the so-called adiabatic part $S_{\text{a}} = \beta Q^{hk}$ [16]. On the other hand, in the second decomposition of $S$, $\Delta \phi$ can be identified with the system contribution $S_s = \Delta \phi$ while $\beta Q^{tot}$ can be identified with the reservoir contribution $S_r = \beta Q^{tot}$ to the total trajectory entropy production.

The entropy expressions of Eq. (9) satisfy the conditions for the application of identity (1) or (2) since each term is odd with respect to time reversal in both decompositions. We can thus write DFTs (valid for all times $\tau$) for the joint probabilities as

$$P(Y, \beta Q^{hk}) = e^{\mathcal{Y} + \beta Q^{hk}},$$

$$P(\Delta \phi, \beta Q^{tot}) = e^{\Delta \phi + \beta Q^{tot}}.$$

The corresponding IFTs can be written as

$$\langle e^{-\lambda \mathcal{Y}} \rangle = \langle e^{-(1-\lambda)\mathcal{Y}} \rangle R,$$

$$\langle e^{-\lambda \Delta \phi} \rangle = \langle e^{-(1-\lambda)\Delta \phi} \rangle R.$$
From the analysis of $\langle e^{-\beta H(t)} \rangle_R$ for specific cases of experimental errors, one can estimate the dispersion of the experimentally obtained $\langle e^{-\beta H(t)} \rangle_R$ around $\langle e^{-\beta H} \rangle = 1$ [19].

As a second example let us consider a system initially prepared in a NESS with a variation of its parameters $\sigma(t) = \sigma^0 + \delta \sigma(t)$ in such a way that $|\delta \sigma(t)/\sigma^0| < 1$, with $\sigma^0 = \sigma(0)$ and $\delta \sigma(0) = 0$. In this case a modified fluctuation-dissipation theorem has been derived in [22], which relates dissipation under small perturbations around a NESS with fluctuations in the corresponding steady state. Expanding the exponentials in Eq. (15) up to second order in $\delta \sigma$ and then to second order in $\lambda$ and order zero in $\kappa$, we arrive at (see [19] for details)

$$\langle B_j(0, \tau) \rangle_0 = \left\langle B_j(\tau, 0) \exp \left[ - \beta \int_0^\tau dt \dot{x}(t) v_j(x(t); \sigma^0) \right] \right\rangle_0,$$  \hspace{1cm} (22)

where $B_j(0, \tau) = [\delta \dot{x}(x(t); \sigma^0)/\partial \sigma^0][\dot{x}(x(t); \sigma^0)/\partial \sigma^0]$ and $v_j = B_j^T \partial \partial \sigma^0 - B_j^T \partial \sigma^0$ corresponds to the average velocity in the NESS associated with $\sigma$. For a Boltzmann-Gibbs steady state, this result reduces to the symmetry $C_j(\tau) = C_j(-\tau)$, with $C_j(\tau) = \langle B_j(0, \tau) \rangle_0$. Equation (22) can also be derived from Eq. (19) in Ref. [15]. With the use of the joint PDF we can obtain further new results. Let us introduce a weighted correlation function as

$$C_j^{0}(\tau, 0) = \left\langle \exp \left[ - \frac{\beta}{2} \int_0^\tau dt \dot{x}(t) v_j(x(t); \sigma^0) \right] \right\rangle_0.$$  \hspace{1cm} (23)

This correlation function carries explicit information about the lack of detailed balance and reduces to the usual one when the system is able to equilibrate. Using Eq. (15) with $\kappa = \frac{1}{2}$ and repeating the same procedure used to obtain Eq. (22) we arrive at the symmetry $C_j^{0}(\tau, 0) = C_j^{0}(0, \tau)$, which reduces to the known result for equilibrium dynamics when detailed balance holds.

In conclusion, identities (1) and (2) and their immediate consequences for Markovian systems are the main results of this work. Equation (1) or Eq. (2) indeed contains, as particular cases, several known FTs such as the ones previously derived by Hatano and Sasa [12], Speck and Seifert [13], Seifert [14], Chernyak et al. [15], and Esposito and Van den Broeck [16]. In addition, an exact DFT, valid for all times $\tau$, holds for the joint distribution of the reservoir and system entropy contributions to the total trajectory entropy production, although each contribution does not do it separately, as given by Eq. (14). Also a similar DFT holds for the joint distribution of the adiabatic and nonadiabatic entropy contributions to the total trajectory entropy, as given by Eq. (13). For the type of NESS discussed here, two-variable joint PDFs are all that is needed for the corresponding DFTs since there are $M = 2$ decompositions of the total trajectory entropy production, like Eq. (9), for this case. We have shown an example with $M = 3$ for handling experimental errors in the Hatano-Sasa FT. In any case, in the light of Eqs. (1) and (2), obtaining an adequate minimal $M$ decomposition of the total trajectory entropy production constitutes the cornerstone toward the derivation of generalized FTs for nonequilibrium systems.

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