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A generalized integral fluctuation theorem for general jump processes

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Abstract
Using the Feynman–Kac and Cameron–Martin–Girsanov formulae, we obtain a generalized integral fluctuation theorem (GIFT) for discrete jump processes by constructing a time-invariable inner product. The existing discrete IFTs can be derived as its specific cases. A connection between our approach and the conventional time-reversal method is also established. Unlike the latter approach that has been extensively employed in the existing literature, our approach can naturally bring out the definition of a time reversal of a Markovian stochastic system. Additionally, we find that the robust GIFT usually does not result in a detailed fluctuation theorem.

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1. Introduction

One of the most important developments in nonequilibrium statistic physics over the past two decades is the discovery of various fluctuation theorems. They are regarded as nonperturbative extensions of the fluctuation–dissipation theorems in the near equilibrium region to far from equilibrium region. According to their mathematical expressions, these theorems are roughly divided into two types: the integral fluctuation theorems (IFTs) [1–11] and the detailed fluctuation theorems (DFTs) [4, 12–15]. The former follows a unified expression

\[ \langle \exp[-A] \rangle = 1, \]  

where \(A\) is a functional of a stochastic trajectory of a concerned stochastic system and the angular brackets denote an average over the ensemble of the trajectories that start in a given
initial distribution. For instance, $A$ may be the dissipated work along a trajectory, and (1) is the celebrated Jarzynski equality (JE) [1, 2].

Due to the insightful work of Hummer and Szabo [16], we now know that these IFTs have an intimate connection with the famous Feynman–Kac formula (FK) [17, 18] in the stochastic theory of diffusion processes [19]. Recently, several works including ours have reinvestigated this issue from mathematical generalization and rigors [9, 20–23]. One of the findings is that the application of the FK formula in proving the IFTs is based on a construction of a time-reversed process of a diffusion process [22, 23]. Since the definition of a time reversal has some certain arbitrariness [22], we have obtained a generalized IFT (GIFT) by constructing a time-invariable integral and employing the FK and Cameron–Martin–Girsanov (CMG) formulae [24, 25] simultaneously, and the several IFTs [2, 5, 7, 9] were specific cases of the GIFT [23]. We should emphasize that all of the works focused on the continuous diffusion processes described by the Fokker–Planck (FK) equation.

In addition to the continuous case, there is still another kind of stochastic jump process described by Markovian discrete master equations. In many practical physical systems, the description of a discrete jump process is more satisfactory than the description of a continuous diffusion process, e.g., the systems only involving a few individual objects [26]. One may naturally think that there exists a GIFT in the discrete version, and the discrete IFTs in the literature [7, 11, 27, 28] are specific cases of it as well. At first sight, this effort seems trivial since a continuous diffusion process can always be discretized to a discrete jump process. However, in addition, one hardly ensures that the ‘discrete’ GIFT achieved in this way is really exact, we know that a jump process is not always equivalent to the discretization of a certain continuous process [26]. On the other hand, to our knowledge fewer works have formally studied the IFTs for general jump processes employing the FK and CMG formulae. Several authors have mentioned this possibility earlier [29, 30]. Therefore, in our opinion a rigorous derivation of an exact GIFT for discrete jump processes is essential and meaningful. In this communication, we present this effort. Because we focus on the general Markovian jump processes, little physics is mentioned here. The detailed discussions about the specific IFTs in the literature should suffice.

2. Generalized integral fluctuation theorem

We start with a Markovian jumping process described by a discrete master equation

\[ \frac{d p_n(t)}{dt} = [H(t)p(t)]_n, \]

where the $N$-dimensional column vector $p(t) = (p_1, \ldots, p_N)^T$ is the probability of the system at individual states at time $t$ (state index $n$ may be a vector), the matrix element of the time-dependent or time-independent rate $H_{mn} > 0 (m \neq n)$ and $H_{nn} = -\sum_{m \neq n} H_{mn}$. Given a normalized positive column vector $f(t) = (f_1, \ldots, f_N)^T$ and a $N \times N$ matrix $A$ that satisfies condition $f_n H_{mn} + A_{mn} > 0 (m \neq n)$ and $A_{nn} = -\sum_{m \neq n} A_{mn}$, we state that an inner product $f^T (t') v(t')$ is time invariable if the column vector $v(t') = (v_1, \ldots, v_N)^T$ satisfies

\[ \frac{d v_n(t')}{dt'} = -(H^T v)_n - f_n^{-1} [\partial_t f - HF]_n v_n + f_n^{-1} [(A1)_n v_n - (A^T v)_n], \]

where the final condition of $v_n(t)$ is $g_n (t' < t)$, and the column vector is $1 = (1, \ldots, 1)^T$. This is easily proved by noticing a time differential $d_t [f^T (t') v(t')] = d_t (f^T) v + f^T d_t (v)$ and the transpose property of a matrix. Employing the FK and CMG formulae for jump processes
(for a simple derivation about the latter see appendix A), (3) has a stochastic representation given by

\[ v_n(t') = E^{n,t'} \left[ e^{-\mathcal{J}[x,f,A]} q_{x(t)} \right] \]  

(4)

and

\[ \mathcal{J}[x,f,A] = \int_{t'}^t f_{x,1}^{-1} \left[ -\partial_x f + H f + A \right] d\tau - \int_{t'}^t f_{x,1}^{-1} A_{x,1}^{x,1} d\tau \]

\[ - \sum_{i=1}^k \ln \left[ 1 + \frac{A_{x,i}^{x,i} f_{x,i}^{x,i} q_{x(t)}}{f_{x,i}^{x,i} q_{x(t)}} \right] \]

(5)

the expectation \( E^{n,t'} \) is over all trajectories \( x \) generated from (2) with fixed initial state \( n \) at time \( t' \), \( x(t') \) is the discrete state at time \( t' \), \( x(t_i') \) and \( x(t_i') \) represent the states just before and after a jump occurring at time \( t_i \), respectively, and we assumed that the jumps occur \( k \) times for a trajectory. The readers are reminded that the first and last two terms of the functional are the consequences of the FK and GCM formulae, respectively. We see that the last term is significantly different from that in the continuous processes ((11) in [23]). Combining the stochastic representation and the time-invariant quantity and choosing \( t' = 0 \), we obtain the exact discrete GIFT for a jump process,

\[ N \sum_{m=1}^N f_m(0) E^{m,0} \left[ e^{-\mathcal{J}[x,f,A]} q_{x(t)} \right] = f_T(t) q. \]

(6)

Particularly, the right-hand side of the equation becomes 1 if \( q = 1 \).

3. Relationship between GIFT and existing IFTs

The abstract (6) includes several discrete IFTs in the literature. First, we investigate the case in which the discrete system has a transient steady-state solution \( H(t) p_{ss}(t) = 0 \). Choosing matrix \( A = 0 \) and vector \( f(t) = p_{ss}(t) \), (5) is immediately simplified into

\[ \mathcal{J} = - \int_0^t \partial_t p_{ss}^{x,s}(\tau) d\tau. \]

(7)

If one further regards \( p_{ss} \) as satisfying a time-dependent detailed balance condition \( H_{mn}(t) p_{ss}^{x,m}(t) = H_{nm}(t) p_{ss}^{x,n}(t) \), the above functional may be analogous to the dissipated work and (6) is the discrete version of the JE [1, 2]. On the other hand, if \( p_{ss} \) is a transient nonequilibrium steady-state without detailed balance, (7) could be rewritten as

\[ \mathcal{J} = \ln \frac{p_{ss}^{x,s}(0)}{p_{ss}^{x,s}(t)} + \sum_{i=1}^k \ln \frac{p_{ss}^{x,i}(t_i)}{p_{ss}^{x,i}(t_i)}. \]

(8)

where we used the following relationship:

\[ -d t \ln p_{ss}^{x,i}(t) = \delta(t - t_i) \ln \left[ p_{ss}^{x,i}(t_i) / p_{ss}^{x,i}(t_i) \right]. \]

Then we may interpret the first term in (8) as the entropy change of the system and the second term as the ‘excess’ heat of the driven jump process. Under this circumstance, (6) is the discrete version of the Hatano–Sasa equality [5].

The last case is about nonvanishing \( A(t) \). We choose matrix element

\[ A_{mn}(t') = H_{mn}(t') f_m(t') - H_{mn}(t') f_n(t') \quad (m \neq n), \]

(10)
or flux $J_{mn}(t')$ between states $m$ and $n$ for a distribution $\mathbf{f}(t)$. Obviously, the condition of $f_n\mathbf{H}_{mn} + A_{mn} > 0$ is satisfied. Substituting this matrix into (5), we obtain

$$J = - \int_0^t \partial_\tau \ln f_{s(t)}(\tau) \, d\tau + \sum_{i=1}^k \ln \frac{H_{x_i'(t)}x_i(t)}{H_{x_i'(\tau)}x_i(\tau)} f_{s(t)}(t_i),$$

(11)

The physical meaning of the above equation becomes clear when we again employ (9) and have

$$J = \ln \frac{f_{s(0)}(0)}{f_{s(t)}(t)} + \sum_{i=1}^k \ln \frac{H_{x_i'(t)}x_i(t)}{H_{x_i'(\tau)}x_i(\tau)} f_{s(t)}(t_i).$$

(12)

Hence, if $\mathbf{f}(t)$ is the distribution of the system itself satisfying the evolution (2), the first term in the equation is just the entropy change of the system and the second term is interpreted as the entropy change of the environment [7, 11]. In other words, the GIF with (12) is about the total entropy change of a stochastic jump process.

4. GIFT and time reversal for jump processes

Similar to the case of continuous diffusion processes [23], in the following we establish a connection between the time-invariable inner product and a jump process that is a time reversal of the original process. Multiplying $f_n(t')$ and rearranging on both sides of (3), we have

$$\frac{d}{dt'}[f_n(t')v_n(t')] = - \sum_{m=1}^N f_{m}^{-1}(t') [\mathbf{H}_{mn} f_n + A_{mn}] f_m v_m + f_n v_n \sum_{m=1}^N f_{m}^{-1}(t') [\mathbf{H}_{mn} f_m + A_{mn}].$$

(13)

Then we define a new function $q_{\bar{n}}(s) = f_n(t')v_n(t')$, where $s = t - t'$ and $\bar{n}$ represents an index whose components are the same or the minus of the components of index $n$ depending on whether they are even or odd under time reversal ($t \rightarrow -t$). We also define a new rate matrix $\mathbf{H}(s)$ whose elements are

$$\mathbf{H}_{\bar{n}n}(s) = f_m^{-1}(t')[\mathbf{H}_{mn}(t') f_n(t') + A_{mn}(t')] \quad (m \neq n),$$

(14)

and $\mathbf{H}_{n\bar{n}}(s) = - \sum_{\bar{n} \neq n} \mathbf{H}_{n\bar{n}}(s)$. Hence, (13) can be rewritten as

$$\frac{dq_{\bar{n}}(s)}{ds} = (\mathbf{H}(s)q(s))_{\bar{n}}.$$

(15)

Because of variable $s = t - t'$, we interpret $\mathbf{H}(t)$ as a time reversal of the original $\mathbf{H}(t)$. Equation (15) directly presents the reason of the time-invariable inner product $\mathbf{f}(t')\mathbf{v}(t')$ that equals $\mathbf{f}(t)\mathbf{v}(t)$; the latter is a constant due to probability conservation.

The generalized time reversal (14) includes several types of time reversals in the literature [5, 11, 31]. For convenience, we only consider even components only in the state index $n$. First, if the matrix $\mathbf{A} = 0$ and $\mathbf{f}(t') = \mathbf{p}(t')$ satisfy the time-dependent detailed balance condition, the time-reversed rate matrix $\mathbf{H}(t') = \mathbf{H}(s)$ simply. The process governed by this rate matrix was termed a backward process [11] (or a reversed protocol in [31]). In contrast, if $\mathbf{p}(t')$ is the transient nonequilibrium steady state, a process determined by $\mathbf{H}(t') = f_n(s)\mathbf{H}_{mn}(s)/f_m(s)$ was termed an adjoint process [11] (or the current reversal in [22]). Intriguingly, if we choose $A_{mn}(s)$ to be flux $J_{mn}$ (10) between states $m$ and $n$ for a distribution $\mathbf{f}(s)$, we reobtain $\mathbf{H}(t') = \mathbf{H}(s)$ that is the same as in the first case. Considering that these choices of $\mathbf{f}$ and $\mathbf{A}$ here are corresponding to those in section 3, respectively, we conclude that the JE and the IFT of the total entropy have the same physical origin. It is expected in physics that the realization
of a reversed protocol is usually possible and does not depend on whether the system satisfies a time-dependent detailed balance condition. We should point out that one may construct infinite time reversals since $f$ and $A$ are almost completely arbitrary, e.g., $A_{mn}(s) = \alpha J_{mn}(s)$ and $0 \leq \alpha \leq 1$. Before ending this section, we give two comments about relationship $q_{\bar{n}}(s) = f_n(t') v_n(t')$. First, for a time-independent $H$, if $f_n$ is the equilibrium solution of the rate matrix, (3) with zero $A$ is just the backward master equation [26]. Second, employing the relationship repeatedly, we may obtain the detailed DFTs for the specific vectors $f(t')$ and matrixes $A(t')$ in section 3. In general, the GIFT is not equivalent to the detailed DFT (for more details see appendix B).

5. Conclusion

In this work, we derive a GIFT for general jump processes. The existing IFTs for discrete master equations are its special cases. We see that the form of the GIFT for the jump cases is significantly distinct from that for the continuous diffusions that we obtained earlier [23]. Additionally, we also find that this robust GIFT usually does not result into a detailed fluctuation theorem. Compared to other approaches, the major advantage of our two works is that the time reversal comes out automatically during the constructions of the time-invariable integral or the inner product, which is direct and obvious. Of course, the limit of these works is that we did not show any applications of the two GIFTs in physical systems. We hope that this weakness will be remedied in the near future.

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Appendix A. The Cameron–Martin–Girsanov formula for jump processes

Compared to the CMG formula for continuous diffusion processes, not much of the literature has discussed the CMG formula for discrete jump processes. For the convenience of the readers, we give a simple derivation of the formula here. Given a master equation with rate matrix $H$. The probability of observing a trajectory $x$ which starts state $n_1$ at time $t_0 = 0$, jumps at time $t_1$ to state $n_2$, . . . , finally jumps at time $t_k$ to $n_{k+1}$ and stays till time $t_{k+1} = t$ is

$$\text{prob}[x] = \prod_{i=1}^{k} \exp \left[ \int_{t_{i-1}}^{t_i} H_{x(t_i)} x(t_i) (\tau) d\tau \right] H_{x(t_k)} x(t_k) \times \exp \left[ \int_{t_k}^{t} H_{x(t_k)} x(t_k) (\tau) d\tau \right].$$  \hspace{1cm} (A.1)

where $x(t_i^-) = n_i$ and $x(t_i^+) = n_{i+1}$ ($i = 1, \ldots, k$). We assume that there is another master equation with a different rate matrix $H' = H + A$, where the matrix elements of $A$ may be negative. Then the ration of the probabilities of observing the same trajectory in these two equations is simply

$$\text{prob}'[x] = \text{prob}[x] e^{-Q[x]},$$  \hspace{1cm} (A.2)

where

$$Q[x] = -\int_{0}^{t} A_{x(t) x(t)} (\tau) d\tau - \sum_{i=1}^{k} \ln \left( 1 + \frac{A_{x(t_i^-) x(t_i^+)} H_{x(t_k)} x(t_k)}{H_{x(t_i^-) x(t_i^+)} H_{x(t_k)} x(t_k)} \right).$$  \hspace{1cm} (A.3)
Obviously, (A.2) results in an IFT
\[ \langle e^{-Q(x)} \rangle = 1, \] (A.4)
where the average is over an ensemble of trajectories generated from the stochastic system with rate matrix \( \mathbf{H} \) and with any initial distribution. Choosing a specific
\[ A_{mn}(t) = p_{mn}^\alpha(t)^{-1} \left[ H_{mn}(t)p_{m\alpha}^\alpha(t) - H_{mm}(t)p_{m\alpha}^\alpha(t) \right] \quad (m \neq n) \quad (A.5) \]
and \( A_{nn} = - \sum_{m \neq n} A_{mn}(t) = 0 \), we obtain the IFT of the house-keeping heat [8, 11] in the discrete version, where
\[ Q_{hk}[x] = \sum_{i=1}^k H_{x|s_{i-1}^\alpha}(t_i)p_{x|s_{i-1}^\alpha}(t_i) \quad (A.6) \]

Intuitively, replacing \( p_{mn}^\alpha \) above by the real probability distribution \( p_m(t) \) of the system \( \mathbf{H} \), one obtains a new IFT with
\[ Q[x] = \int_0^t \partial_x \ln \left[ \Phi(t, t') \right] dt + \sum_{i=1}^k \frac{H_{x|s_{i-1}^\alpha}(t_i)p_{x|s_{i-1}^\alpha}(t_i)}{H_{x|s_{i-1}^\alpha}(t_i)p_{x|s_{i-1}^\alpha}(t_i)} \quad (A.7) \]

We note that this functional is almost the same as that of the IFT of the total entropy (11) except that the symbol of the first term is plus here. In addition, the average of (A.7) is the same as the average of the total entropy (11) since the first terms of them vanish. We are not very clear whether (A.7) has new physical interpretation.

Appendix B. The detailed fluctuation theorem

Given the transition probability of (15) to be \( q_h(s'|m, s), (0 < s < s' < t) \), the previous relationship implies
\[ q_h(s'|m, s) f_{\alpha}(t - s) = f_{\alpha}(t - s') e^{-\int_0^{s'} J(t - s', t - t') dt} \delta_{0,m} \] (B.8)

if one notes the initial condition \( q_h(s|m, s) = \delta_{0,m} \), where we use \( J(t - s', t - s) \) to denote the functional (5) with the lower and upper limits \( t - s' \) and \( t - s \), respectively, and \( \delta \) is the Kronecker’s. Now we consider a mean of a \((k + 1)\)-point function over the time-reversed system (15),
\[ \langle F[x(t_0), \ldots, x(t_k)] \rangle_{TR} = \sum_{n_0, \ldots, n_k} q_{n_k}(s_k | n_{k-1}, s_{k-1}) \cdots q_{n_1}(s_1 | n_0, s_0) q_{n_0}(s_0) F(n_k, \ldots, n_0), \quad (B.9) \]

where \( 0 = s_0 < s_1 < \cdots < s_k = t \) and \( q(s_0) \) is the initial distribution. If we choose a specific \( q_{n_k}(s_0) = f_{n_k}(t - s_0) \) and employ (B.8) repeatedly, the right-hand side of the above equation becomes
\[ \langle e^{-J[x,f,a]} F[x(t_0), \ldots, x(t_k)] \rangle = \sum_{n_k} f_{n_k}(t - s_k) e^{\int_0^{s_k} J(t - s_k, t - t_k) dt} \left[ e^{-\int_0^{s_k} J(t - s_k, t - t_k) dt} F[x(t - s_k), \ldots, x(t - s_0)] \right]. \quad (B.10) \]

Here we define \( t_k = t - s_{k-1} \) and \( 0 = t_0 < t_1 < \cdots < t_k = t \). On the basis of the above discussion, if \( k \to \infty \), function \( F \) becomes a functional \( \mathcal{F} \) over the space of all trajectories \( x \), and we get an identity
\[ \langle \mathcal{F}[x] \rangle_{TR} = \langle e^{-\int J[x,f,a]} \mathcal{F} \rangle, \quad (B.11) \]

where \( \mathcal{F}(x) = \mathcal{F}(\bar{x}) \) and \( \bar{x} \) is simply the time-reversed trajectory of \( x \). This is a generalization of Crooks’ relation [4]. Obviously, choosing the \( \mathcal{F} \) constant, one obtains the GIFT (6). An
important following question is whether the GIFT results in a DFT. For the specific matrixes $A(t)$ and vectors $f(t)$ in section 3, we indeed obtain several DFTs

$$P_{TR}(-J) = P(J)e^{-J},$$

by choosing $\mathcal{F}(x) = \delta(\mathcal{J}[x, f, A] - J)$, where $P(J)$ is the probability distribution for quantity $\mathcal{J}$ achieved from the jump process (2) and $P_{TR}(J)$ is the corresponding distribution from the time-revered system (15). According to the expression of (5), for any pair of $A$ and $f$, (B.13) usually does not hold. Of course, one may obtain an alternative identity

$$\bar{P}_{TR}(J) = P(J)e^{-J},$$

by formally introducing a probability distribution $\bar{P}_{TR}(J)$ for quantity $\bar{J}[\bar{x}, f, A] = \mathcal{J}[\bar{x}, f, A]$ from the time-reversed system.

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