

Generalized entropy production fluctuation theorems for quantum systems

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MS received 5 June 2012; accepted 24 July 2012

Abstract. Based on trajectory-dependent path probability formalism in state space, we derive generalized entropy production fluctuation relations for a quantum system in the presence of measurement and feedback. We have obtained these results for three different cases: (i) the system is evolving in isolation from its surroundings; (ii) the system being weakly coupled to a heat bath; and (iii) system in contact with reservoir using quantum Crooks fluctuation theorem. In Case (iii), we build on the treatment carried out by H T Quan and H Dong [[arXiv/cond-mat:0812.4955](https://arxiv.org/abs/0812.4955)], where a quantum trajectory has been defined as a sequence of alternating work and heat steps. The obtained entropy production fluctuation theorems (FTs) retain the same form as in the classical case. The inequality of second law of thermodynamics gets modified in the presence of information. These FTs are robust against intermediate measurements of any observable performed with respect to von Neumann projective measurements as well as weak or positive operator-valued measurements.

Keywords. Fluctuation theorems; entropy production; measurement and feedback; mutual information.

PACS Nos 05.40.–a; 05.70.Ln; 03.65.Ta

1. Introduction

Nonequilibrium processes are common in nature, but a general framework to understand them is lacking as compared to equilibrium systems. However, recent development in the field of nonequilibrium statistical mechanics, had led to the discovery of FTs [1–7], which are exact equalities that are valid even when the system of interest is driven far away from equilibrium. For such a nonequilibrium system, the statistical distribution of thermodynamic quantities such as work, heat, entropy, etc. exhibit universal relations. These thermodynamic quantities have now been generalized to a single trajectory of system evolving in phase space. They are random variables depending on the phase space trajectory (stochastic thermodynamics [8]). The physical origin of FTs rely on the time-reversal symmetry of the dynamics [4,5] and they are expected to have important applications in

nanoscience and biophysics. The second law of thermodynamics emerges in the form of inequalities from these theorems [3,6]. It can be shown that the second law is valid on an average. Here averaging is done over different trajectories, thus not ruling out the possibility of transient violations of second law for individual realization [9]. These theorems have helped us in understanding how thermodynamic irreversibility arises from the underlying time-reversible dynamics [10].

One of the FTs was initially put forward by Jarzynski [3] in the form of the nonequilibrium work theorem, by means of which one can extract information about equilibrium changes in free energy ΔF by measuring the nonequilibrium work W performed on a system by the external drive. The system is initially prepared in equilibrium, and then driven away from equilibrium using some predetermined protocol $\lambda(t)$, which runs from $t = 0$ to $t = \tau$. The Jarzynski equality is given by

$$\langle e^{-\beta W} \rangle = e^{-\beta \Delta F}. \quad (1.1)$$

The work W depends on trajectory of the system, whose initial state is sampled from equilibrium distribution. The angular brackets denote averaging over an ensemble of such trajectories and the free energy differences $\Delta F = F(\lambda(\tau)) - F(\lambda(0))$. A stronger fluctuation theorem was provided by Crooks [4,5] in the form

$$\frac{P_f(W)}{P_r(-W)} = e^{\beta(W - \Delta F)}, \quad (1.2)$$

$P_f(W)$ and $P_r(W)$ being the work probability densities generated under the forward protocol $\lambda(t)$ and the reverse protocol $\lambda(\tau - t)$, respectively.

A more general FT was put forward by Seifert [7] which contains the Jarzynski and the Crooks theorems as special cases. A system which is in contact with a heat bath, is initially prepared in some arbitrary distribution $p_0(x_0)$ of phase-space points and is perturbed by varying an external parameter $\lambda(t)$ up to time $t = \tau$. In the reverse process, the system evolves from some other initial distribution $p_1(x_\tau)$ under the time-reversed protocol $\lambda(\tau - t)$. The Seifert's fluctuation theorem states that, the probability of a phase space trajectory along the forward process, $P[x(t)]$, is related to that along the reverse process, $\tilde{P}[\tilde{x}(t)]$, as

$$\frac{P[x(t)]}{\tilde{P}[\tilde{x}(t)]} = \frac{P[x(t)|x_0]p_0(x_0)}{\tilde{P}[\tilde{x}(t)|x_\tau]p_1(x_\tau)} = \frac{p_0(x_0)}{p_1(x_\tau)} \exp[\Delta S_B], \quad (1.3)$$

where ΔS_B is the change in entropy of the bath ($\Delta S_B = (Q/T)$, where Q is the heat absorbed by the bath). $P[x(t)|x_0]$ is a short notation for functional of a path starting at x_0 and $x(t)$ is the phase-space trajectory ending at x_τ . If, in particular, the distribution $p_1(x_\tau)$ in the final distribution at time τ is as dictated by dynamics, then the above relation gives the integral fluctuation theorem (IFT) for total entropy production [7]:

$$\langle e^{-\Delta S_{\text{tot}}} \rangle = 1, \quad (1.4)$$

where

$$\Delta S_{\text{tot}} = \Delta S + \Delta S_B = \ln \frac{p_0(x_0)}{p_1(x_\tau)} + \frac{Q}{T}. \quad (1.5)$$

Here, $\ln(p_0(x_0)/p_1(x_\tau))$ is the change of system entropy along a given trajectory. For details, we refer to Seifert's article [7]. If the system is in steady state, one can also obtain detailed entropy production fluctuation theorem (DFT), namely

$$\frac{p(\Delta S_{\text{tot}})}{p(-\Delta S_{\text{tot}})} = e^{\Delta S_{\text{tot}}}. \quad (1.6)$$

The IFT follows directly from the DFT. Using Jensen's inequality in eq. (1.4) we get

$$\langle \Delta S_{\text{tot}} \rangle \geq 0. \quad (1.7)$$

This is a statement of second law of thermodynamics, expressed in the form of inequality for the average change in total entropy.

If the systems are driven by the feedback-controlled protocols, which in turn depend on the measurement outcomes of the state of the system at intermediate times (information gain), then IFT gets modified to the form [11]

$$\langle e^{-\Delta S_{\text{tot}} - I} \rangle = 1, \quad (1.8)$$

where I is the mutual information which quantifies the change in uncertainty of the state of the system upon making measurements. Application of Jensen's inequality generalizes second law for total entropy production:

$$\langle \Delta S_{\text{tot}} \rangle \geq -\langle I \rangle. \quad (1.9)$$

The average mutual information $\langle I \rangle$ is always non-negative [12]. Thus, the average entropy change can be made negative by feedback control, and the lower bound is given by $-\langle I \rangle$. There are few attempts to extend the IFT (eq. (1.4)) to the quantum domain [13–15]. In our present work, we extend the IFT for ΔS_{tot} to quantum systems, in the presence of multiple measurements and feedback. We assume that the measurement procedure involves errors that are classical in nature. We show the robustness of FTs against intermediate measurements of any system observable (both von Neumann projective measurements or generalized positive operator-valued measurements (POVM)).

We obtain these theorems for three different cases: (i) the system evolves in isolation from its surroundings; (ii) it is weakly coupled to a heat bath; and (iii) evolution of system coupled to heat bath is modelled in terms of work steps and heat steps following closely the treatment given in ref. [16] and is described in §4. Our treatment is based on path probability in state space. The measurement is assumed to be von Neumann type, i.e., projective measurement which results in the collapse of system state to one of the eigenstates of the corresponding observable. Case (i), namely, isolated quantum system is discussed in detail. DFT is obtained for various situations, i.e., (a) system evolving unitarily, (b) in the presence of measurement and feedback, and finally (c) in the presence of intermediate measurements, of any observables of the system. The IFT follows from DFT. For Cases (ii) and (iii), we have derived generalized IFT. In the Appendix, we have given a proof of IFT in the presence of weak measurements. In passing, we note that all the extended quantum FTs retain the same form as their classical counterparts.

2. Isolated quantum system

2.1 Unitary evolution

In this section, we consider an isolated quantum system given by Hamiltonian $H(\lambda(t))$, where $\lambda(t)$ is some external time-dependent protocol. To clarify our notation and for completeness, we rederive DFT for this system following the treatment of ref. [14]. Initially at time $t = 0$, energy measurement is performed and system is found to be in eigenstate $|i_0\rangle$, with energy eigenvalue E_0 . It then evolves unitarily from time 0 to τ under the protocol $\lambda(t)$. The energy measurement at final time τ is performed and system is found to be at state $|i_\tau\rangle$ with energy eigenvalue E_τ . If the initial probability density of the state $|i_0\rangle$ is $p(i_0)$, then the joint probability of $|i_0\rangle$ and $|i_\tau\rangle$ (forward state trajectory) is given by

$$\begin{aligned} P_F(i_\tau, i_0) &= p(i_\tau|i_0)p(i_0) \\ &= |\langle i_\tau|U_\lambda(\tau, 0)|i_0\rangle|^2 p(i_0), \end{aligned} \quad (2.1)$$

where $U_\lambda(t_2, t_1)$ denotes the unitary evolution operator for a given $\lambda(t)$ from time t_1 to time t_2 . It is defined as

$$U_\lambda(t_2, t_1) = T \exp\left(-\frac{i}{\hbar} \int_{t_1}^{t_2} H(\lambda(t))dt\right). \quad (2.2)$$

Here, T denotes time ordering.

The system entropy is defined as $S(t) = -\ln p(i_t)$. As the system is isolated, there is no generation of heat, i.e, $Q = 0$. Using eq. (1.5), the total change in entropy production ΔS_{tot} during the evolution from time 0 to τ is equal to the change in system entropy alone.

$$\Delta S_{\text{tot}} = -\ln \frac{p(i_\tau)}{p(i_0)}, \quad (2.3)$$

where $p(i_\tau)$ is the final probability of state $|i_\tau\rangle$ at time τ . The probability density $P_F(\Delta S_{\text{tot}})$ for the forward path is by definition

$$\begin{aligned} P_F(\Delta S_{\text{tot}}) &= \sum_{i_\tau, i_0} \delta\left(\Delta S_{\text{tot}} + \ln \frac{p(i_\tau)}{p(i_0)}\right) P_F(i_\tau, i_0) \\ &= \sum_{i_\tau, i_0} \delta\left(\Delta S_{\text{tot}} + \ln \frac{p(i_\tau)}{p(i_0)}\right) p(i_\tau|i_0)p(i_0). \end{aligned} \quad (2.4)$$

We now introduce time-reversal operator Θ . The time-reversed state of $|i\rangle$ is defined as $|\tilde{i}\rangle = \Theta|i\rangle$. It can be readily shown that [11]

$$p(i_2|i_1) = |\langle i_2|U_\lambda(t_2, t_1)|i_1\rangle|^2 = |\langle \tilde{i}_1|U_{\lambda^\dagger}(\tilde{t}_1, \tilde{t}_2)|\tilde{i}_2\rangle|^2 = p(\tilde{i}_1|\tilde{i}_2), \quad (2.5)$$

where $\tilde{t} = \tau - t$ and $\lambda^\dagger(\tilde{t}) = \lambda(\tau - t)$ is the time-reversed protocol of $\lambda(t)$. The evolution of the system from the given time-reversed state $\Theta|i_2\rangle$ to the time-reversed state $\Theta|i_1\rangle$, under the time-reversed protocol $\lambda^\dagger(t)$, is given by the conditional probability $p(\tilde{i}_1|\tilde{i}_2)$.

We consider the initial distribution of reverse trajectory to be equal to the final distribution of forward trajectory

$$p(\tilde{i}_\tau) = p(i_\tau). \quad (2.6)$$

The states $|i\rangle$ and $|\tilde{i}\rangle$ have one-to-one correspondence. Multiplying and dividing by $p(i_\tau)$ in the summand in eq. (2.4) and using eqs (2.5) and (2.6), we get

$$\begin{aligned} P_F(\Delta S_{\text{tot}}) &= \sum_{i_\tau, i_0} \delta\left(\Delta S_{\text{tot}} + \ln \frac{p(i_\tau)}{p(i_0)}\right) p(\tilde{i}_0|i_\tau) p(\tilde{i}_\tau) \frac{p(i_0)}{p(i_\tau)} \\ &= \sum_{i_\tau, i_0} \delta\left(\Delta S_{\text{tot}} + \ln \frac{p(i_\tau)}{p(i_0)}\right) p(\tilde{i}_0|i_\tau) p(\tilde{i}_\tau) e^{\Delta S_{\text{tot}}} \\ &= e^{\Delta S_{\text{tot}}} \sum_{i_\tau, i_0} \delta\left(\Delta S_{\text{tot}} + \ln \frac{p(\tilde{i}_\tau)}{p(\tilde{i}_0)}\right) p(\tilde{i}_0|\tilde{i}_\tau) p(\tilde{i}_\tau) \\ &= e^{\Delta S_{\text{tot}}} \sum_{i_\tau, i_0} \delta\left(\Delta S_{\text{tot}} - \ln \frac{p(\tilde{i}_0)}{p(\tilde{i}_\tau)}\right) P_R(\tilde{i}_\tau, \tilde{i}_0) \\ &= e^{\Delta S_{\text{tot}}} P_R(-\Delta S_{\text{tot}}). \end{aligned} \quad (2.7)$$

To arrive at this result, we have used eq. (2.3) in the second step and eq. (2.6) in the third step. $P_R(\tilde{i}_\tau, \tilde{i}_0)$ is the joint probability of the corresponding states in the reverse direction. If ΔS_{tot} is the total entropy change for forward path, then the total entropy change in the corresponding reverse path is $-\Delta S_{\text{tot}}$. It follows from the fact that $p(i_\tau)$ and $p(\tilde{i}_0)$ are the initial and final probability distribution of states in the time-reversed process because of unitary evolution. Equation (2.7) can be written in the form

$$\frac{P_F(\Delta S_{\text{tot}})}{P_R(-\Delta S_{\text{tot}})} = e^{\Delta S_{\text{tot}}}. \quad (2.8)$$

This is the detailed FT for change in total entropy, extended to the quantum regime. Simple cross-multiplication followed by integration over ΔS_{tot} leads to the integral form of the above theorem:

$$\langle e^{-\Delta S_{\text{tot}}} \rangle = 1. \quad (2.9)$$

2.2 Isolated quantum system with feedback

So far we have been dealing with a predetermined protocol, also known as open-loop feedback. Often to increase the efficiency of a physical process (e.g., engines at nanoscale, molecular motor, etc.), we need to perform intermediate measurements and change the protocol as per the outcomes of these measurements [17–24]. Such a process is known as closed-loop feedback. Let the system evolve under some external protocol $\lambda_0(t)$, from its initial energy eigenstate $|i_0\rangle$ measured at time t_0 . At time t_1 , we perform a measurement of some arbitrary observable and system collapses to state $|i_1\rangle$. We assume that

measurement process leading to information gain involves classical errors. Here y_1 is the measured outcome with a probability $p(y_1|i_1)$, while the system's actual state is $|i_1\rangle$. Depending on the value of y_1 the protocol is changed to $\lambda_{y_1}(t)$. Under this new protocol, the system evolves unitarily up to time t_2 , where another measurement is performed and so on. This process terminates at time τ when the system collapses to its final energy eigenvalue $|i_\tau\rangle$. We should note that initial and final measurements are energy measurements. The joint probability of the corresponding state trajectory for n number of intermediate measurements y_1, y_2, \dots, y_n at times t_1, t_2, \dots, t_n , respectively is [11]

$$\begin{aligned}
 P_F(i_\tau, \dots, i_1, i_0, y_n, \dots, y_1) &= p(i_\tau|i_n) \cdots p(y_2|i_2)p(i_2|i_1)p(y_1|i_1)p(i_1|i_0)p(i_0) \\
 &= |\langle i_\tau|U_{\lambda_{y_n}}(\tau, t_1)|i_n\rangle|^2 \cdots p(y_2|i_2)|\langle i_2|U_{\lambda_{y_1}}(t_2, t_1)|i_1\rangle|^2 p(y_1|i_1) \\
 &\quad \times |\langle i_1|U_{\lambda_0}(t_1, 0)|i_0\rangle|^2 p(i_0). \tag{2.10}
 \end{aligned}$$

It may be noted that the joint probability of the path is expressed using classical probability rules. This is because we perform projective measurement on the system which collapses to one of the eigenvalues of the measured observables [11,25]. As a consequence, it wipes out the previous memory of evolution and the post-measurement evolution becomes uncorrelated to the pre-measurement evolution. Thus, if one performs intermediate measurements along two paths, the interference effects between the two paths disappear and the quantum effects are suppressed. Hence, in the presence of measurement, path probability in state-space obeys classical probability rules, and is given by product of transition probability of paths between consecutive measurements. However, it may be noted that quantum mechanics enters through the explicit calculation of transition probability between two consecutive states.

To generate the reverse trajectory of a path in state-space given in eq. (2.10), we first choose one of the forward protocols with probability $p(y_n, \dots, y_2, y_1)$, and then blindly time-reverse the protocol. We perform measurements at the appropriate times along the reverse path to allow the state to collapse to the corresponding time-reversed eigenstates. We do not use these measurements to perform any feedback to respect causality [24]. Then, the expression for the joint probability of reverse trajectory is given by

$$\begin{aligned}
 P_R(\tilde{i}_\tau, \dots, \tilde{i}_0, y_n, \dots, y_1) &= p(\tilde{i}_N|\tilde{i}_\tau) \cdots p(\tilde{i}_0|\tilde{i}_1)p(i_\tau)p(y_n, \dots, y_1). \tag{2.11}
 \end{aligned}$$

The mutual information gain due to measurements between the measured values and the actual value is defined as [11,24]

$$I = \ln \frac{p(y_n|i_n) \cdots p(y_2|i_2)p(y_1|i_1)}{p(y_n, \dots, y_2, y_1)}. \tag{2.12}$$

We now calculate the joint probability density $P_F(\Delta S_{\text{tot}}, \mathcal{I})$ of the entropy production and \mathcal{I} along the forward path, which is

$$\begin{aligned}
 & P_F(\Delta S_{\text{tot}}, \mathcal{I}) \\
 &= \int dy_n \cdots dy_1 \sum_{i_\tau, \dots, i_1, i_0} \delta\left(\Delta S_{\text{tot}} + \ln \frac{p(i_\tau)}{p(i_0)}\right) \delta(\mathcal{I} - I(i_n, \dots, i_1, y_n, \dots, y_1)) \\
 &\quad \times P_F(i_\tau, \dots, i_1, i_0, y_n, \dots, y_1) \\
 &= \int dy_n \cdots dy_1 \sum_{i_\tau, \dots, i_1, i_0} \delta\left(\Delta S_{\text{tot}} + \ln \frac{p(i_\tau)}{p(i_0)}\right) \delta(\mathcal{I} - I(i_n, \dots, i_1, y_n, \dots, y_1)) \\
 &\quad \times p(i_\tau|i_n) \cdots p(y_2|i_2) p(i_2|i_1) p(y_1|i_1) p(i_1|i_0) p(i_0) \\
 &= \int dy_n \cdots dy_1 \sum_{i_\tau, \dots, i_1, i_0} \delta\left(\Delta S_{\text{tot}} + \ln \frac{p(i_\tau)}{p(i_0)}\right) \delta(\mathcal{I} - I(i_n, \dots, i_1, y_n, \dots, y_1)) \\
 &\quad \times p(\tilde{i}_N|\tilde{i}_\tau) \cdots p(\tilde{i}_0|\tilde{i}_1) p(i_\tau) p(y_n, \dots, y_1) e^{\Delta S_{\text{tot}} + \mathcal{I}} \\
 &= \int dy_n \cdots dy_1 \sum_{i_\tau, \dots, i_1, i_0} \delta\left(\Delta S_{\text{tot}} + \ln \frac{p(i_\tau)}{p(i_0)}\right) \delta(\mathcal{I} - I(i_n, \dots, i_1, y_n, \dots, y_1)) \\
 &\quad \times P_R(\tilde{i}_\tau, \dots, \tilde{i}_0, y_n, \dots, y_1) e^{\Delta S_{\text{tot}} + \mathcal{I}} \\
 &= e^{\Delta S_{\text{tot}} + \mathcal{I}} \int dy_n \cdots dy_1 \sum_{i_\tau, \dots, i_1, i_0} \delta\left(\Delta S_{\text{tot}} + \ln \frac{p(i_\tau)}{p(i_0)}\right) \\
 &\quad \times \delta(\mathcal{I} - I(i_n, \dots, i_1, y_n, \dots, y_1)) \times P_R(\tilde{i}_\tau, \dots, \tilde{i}_0, y_n, \dots, y_1) \\
 &= e^{\Delta S_{\text{tot}} + \mathcal{I}} P_R(-\Delta S_{\text{tot}}, \mathcal{I}). \tag{2.13}
 \end{aligned}$$

In deriving the above result, we have made use of eqs (2.10), (2.11), (2.12). The path variable $I(i_n, \dots, i_1, y_n, \dots, y_1)$ is given by eq. (2.12), and \mathcal{I} denotes its value. It is important to note that the probability density function $P_R(-\Delta S_{\text{tot}}, \mathcal{I})$ gives the probability of reverse trajectories along which the entropy change is $-\Delta S_{\text{tot}}$ and whose corresponding forward trajectory has the mutual information \mathcal{I} between its measured outcomes and actual states. Once again, the initial and final distributions of states along forward trajectory get interchanged in the reverse trajectory because of unitary evolution between measurements. Along the reverse trajectory, the change in total entropy is $-\Delta S_{\text{tot}}$. Thus, we obtain the DFT

$$\frac{P_F(\Delta S_{\text{tot}}, \mathcal{I})}{P_R(-\Delta S_{\text{tot}}, \mathcal{I})} = e^{\Delta S_{\text{tot}} + \mathcal{I}}. \tag{2.14}$$

From the above equation, the extended version of IFT and second law, eqs (1.8) and (1.9) can be readily obtained as discussed in the earlier subsection.

2.3 Isolated system under multiple measurements

In this subsection, we restrict ourselves on the influence of intermediate measurements of arbitrary observables on the statistics of ΔS_{tot} . To this end, we do not involve any

feedback. Following closely the discussions in §2.2, of path probability in state-space is given by

$$\begin{aligned}
 P(i_\tau, \dots, i_1, i_0) &= p(i_\tau|i_n) \cdots p(i_2|i_1)p(i_1|i_0)p(i_0) \\
 &= |\langle i_\tau|U_{\lambda_{y_n}}(\tau, t_1)|i_n\rangle|^2 \cdots \\
 &\quad |\langle i_2|U_{\lambda_{y_1}}(t_2, t_1)|i_1\rangle|^2 |\langle i_1|U_{\lambda_0}(t_1, 0)|i_0\rangle|^2 p(i_0). \quad (2.15)
 \end{aligned}$$

From the preceding section, we now calculate the probability density $P_F(\Delta S_{\text{tot}})$ of the total entropy change along the forward path

$$\begin{aligned}
 P_F(\Delta S_{\text{tot}}) &= \sum_{i_\tau, \dots, i_1, i_0} \delta\left(\Delta S_{\text{tot}} + \ln \frac{p(i_\tau)}{p(i_0)}\right) P(i_\tau, \dots, i_1, i_0) \\
 &= \sum_{i_\tau, \dots, i_1, i_0} \delta\left(\Delta S_{\text{tot}} + \ln \frac{p(i_\tau)}{p(i_0)}\right) p(i_\tau|i_n) \cdots p(i_2|i_1)p(i_1|i_0)p(i_0) \\
 &= \sum_{i_\tau, \dots, i_1, i_0} \delta\left(\Delta S_{\text{tot}} + \ln \frac{p(i_\tau)}{p(i_0)}\right) p(\tilde{i}_N|\tilde{i}_\tau) \cdots p(\tilde{i}_0|\tilde{i}_1)p(i_\tau) e^{\Delta S_{\text{tot}}} \\
 &= \sum_{i_\tau, \dots, i_1, i_0} \delta\left(\Delta S_{\text{tot}} + \ln \frac{p(i_\tau)}{p(i_0)}\right) P_R(\tilde{i}_\tau, \dots, \tilde{i}_0) e^{\Delta S_{\text{tot}}} \\
 &= e^{\Delta S_{\text{tot}}} \sum_{i_\tau, \dots, i_1, i_0} \delta\left(\Delta S_{\text{tot}} + \ln \frac{p(i_\tau)}{p(i_0)}\right) P_R(\tilde{i}_\tau, \dots, \tilde{i}_0), \quad (2.16)
 \end{aligned}$$

where $P_R(\tilde{i}_\tau, \dots, \tilde{i}_0)$ is the probability of the reverse path. The DFT for ΔS_{tot} follows from the above equation:

$$\frac{P_F(\Delta S_{\text{tot}})}{P_R(-\Delta S_{\text{tot}})} = e^{\Delta S_{\text{tot}}}. \quad (2.17)$$

We observe from eq. (2.17), the robustness of this FT against intermediate measurements [26,27]. It retains the same form as in the classical case. The path probability, however, gets modified in the presence of measurements and statistics of ΔS_{tot} is strongly influenced by the intermediate measurements. In the next section, we derive IFT in the presence of feedback for a quantum system coupled weakly to a bath. In the Appendix, we have shown that the IFT for ΔS_{tot} is also robust against weak or generalized intermediate measurements.

3. Weakly coupled quantum system

Consider a driven system which is weakly coupled to a bath. The total Hamiltonian will be

$$H(\lambda(t)) = H_S(\lambda(t)) + H_B + H_{SB}. \quad (3.1)$$

The external time-dependent drive $\lambda(t)$ only affects the system Hamiltonian $H_S(\lambda(t))$, while the bath Hamiltonian H_B and interaction Hamiltonian H_{SB} are time-independent.

As the system is weakly coupled, it is assumed that H_{SB} is negligibly small compared to $H_{\text{S}}(\lambda(t))$ and H_{B} . Initially, the super-system (system+bath) is coupled to a large reservoir of inverse temperature β [27,28]. At time $t = 0$, the large reservoir is decoupled from the super-system. Hence, initially the super-system will be in a canonical distribution,

$$\rho(\lambda_0) = \frac{e^{-\beta H(\lambda(0))}}{Y(\lambda(0))}, \quad (3.2)$$

where $Y(\lambda(0)) = \text{Tr} e^{-\beta H(\lambda(0))}$. The system and the bath Hamiltonians commute with each other, hence we can measure simultaneously the energy eigenstates for the system as well as the bath. At $t = 0$, the measured energy eigenvalues of the system and the bath are denoted by E_0^{S} and E_0^{B} , respectively. We perform N number of intermediate measurements of some arbitrary observables at time t_1, t_2, \dots, t_N between time 0 to τ . Initially, the protocol was $\lambda_0(t)$. At t_1 , the measured output is y_1 , while its actual state is i_1 , with probability $p(y_1|i_1)$. Now, the protocol is changed to $\lambda_{y_1}(t)$ and system evolves up to time t_2 . Again, measurement is performed and protocol is changed according to the output at intermediate times and so on. Finally at $t = \tau$, joint measurement is performed on the system and the bath Hamiltonians, and the measured eigenvalues are E_{τ}^{S} and E_{τ}^{B} , respectively. The system–reservoir interaction energy can be neglected in the presence of weak coupling. Hence, during the evolution process from time $t = 0$ to $t = \tau$ for a single realization, the change in the internal energy of the system is given by [28]

$$\Delta U = E_{\tau}^{\text{S}} - E_0^{\text{S}} \quad (3.3)$$

and the heat dissipated to the bath is

$$Q = E_{\tau}^{\text{B}} - E_0^{\text{B}}. \quad (3.4)$$

If i_0 and i_{τ} denote initial and final system energy eigenstates, then system entropy change is

$$\Delta S_{\text{sys}} = -\ln \frac{p(i_{\tau})}{p(i_0)}, \quad (3.5)$$

and the total entropy change is

$$\Delta S_{\text{tot}} = \Delta S_{\text{sys}} + \Delta S_{\text{B}} = -\ln \frac{p(i_{\tau})}{p(i_0)} + \frac{Q}{T}, \quad (3.6)$$

where T is the temperature of the bath. The mutual information between the state trajectory $\{i_1, i_2, \dots, i_N\}$ and the measurement trajectory $\{y_1, y_2, \dots, y_N\}$ is

$$I \equiv \ln \left[\frac{p(y_1|i_1) \cdots p(y_N|i_N)}{P(y_1, \dots, y_N)} \right]. \quad (3.7)$$

Denoting initial and final states of the bath by α_0 and α_{τ} , it can be written from microscopic reversibility [21,24]

$$p(i_{\tau}, \alpha_{\tau}|i_0, \alpha_0) = p(\tilde{i}_0, \tilde{\alpha}_0|\tilde{i}_{\tau}, \tilde{\alpha}_{\tau}), \quad (3.8)$$

where $p(i_\tau, \alpha_\tau | i_0, \alpha_0)$ is the total transition probability for the system and the reservoir to evolve from state $|i_0, \alpha_0\rangle$ to $|i_\tau, \alpha_\tau\rangle$ under the full Hamiltonian. Here, $|\tilde{i}, \tilde{\alpha}\rangle \equiv \Theta|i, \alpha\rangle$ is the time-reversed state of $|i, \alpha\rangle$. To generate the reverse trajectory, proper causal protocol has to be used which has been discussed in §2.2. Thus, the forward and the reverse path probabilities of trajectories are respectively given by

$$P_F(A \rightarrow B) = p(i_\tau, \alpha_\tau | i_N, \alpha_N) \cdots p(y_1 | i_1) p(i_1, \alpha_1 | i_0, \alpha_0) p(i_0, \alpha_0), \quad (3.9)$$

$$P_R(A \leftarrow B) = p(\tilde{i}_0, \tilde{\alpha}_0 | \tilde{i}_1, \tilde{\alpha}_1) \cdots p(\tilde{i}_N, \tilde{\alpha}_N | \tilde{i}_\tau, \tilde{\alpha}_\tau) p(\tilde{i}_\tau, \tilde{\alpha}_\tau) p(y_1, y_2, \dots, y_N). \quad (3.10)$$

The notations A and B respectively denote initial and final values of the forward protocol. For reverse trajectory, we have chosen the outcome of the forward trajectory with probability $p(y_1, y_2, \dots, y_N)$ and have blindly reversed the protocol, but performing measurements (without any feedback) at appropriate time instants. From eqs (3.9) and (3.10) we get

$$\begin{aligned} & \frac{P_F(A \rightarrow B)}{P_R(A \leftarrow B)} \\ &= \frac{p(i_\tau, \alpha_\tau | i_N, \alpha_N) \cdots p(y_1 | i_1) p(i_1, \alpha_1 | i_0, \alpha_0) p(i_0, \alpha_0)}{p(\tilde{i}_0, \tilde{\alpha}_0 | \tilde{i}_1, \tilde{\alpha}_1) \cdots p(\tilde{i}_N, \tilde{\alpha}_N | \tilde{i}_\tau, \tilde{\alpha}_\tau) p(\tilde{i}_\tau, \tilde{\alpha}_\tau) p(y_1, y_2, \dots, y_N)} \\ &= \frac{p(y_N | i_N) \cdots p(y_1 | i_1) p(i_0, \alpha_0)}{P(y_1, \dots, y_N) p(\tilde{i}_\tau, \tilde{\alpha}_\tau)} \\ &= e^I \frac{p(i_0) p(\alpha_0)}{p(\tilde{i}_\tau) p(\tilde{\alpha}_\tau)}. \end{aligned} \quad (3.11)$$

In arriving at eq. (3.11), we have used microreversibility eq. (3.8) and have assumed that the system and the bath are weakly coupled. The joint probability of the system and the bath states is approximated as a product of individual state probabilities. Correction to this factorized initial state is at least of second order in system–bath interaction, and therefore they can be neglected in the limit of weak coupling. The bath probability can be considered canonical with inverse temperature β . This leads to

$$\frac{P_F(A \rightarrow B)}{P_R(A \leftarrow B)} = e^I e^{\Delta S_{\text{sys}}} \frac{e^{-\beta E_0^B} / Z_B}{e^{-\beta E_\tau^B} / Z_B} = e^I e^{\Delta S_{\text{sys}}} e^{Q/T} = e^{\Delta S_{\text{tot}} + I}. \quad (3.12)$$

A simple cross-multiplication and integration over paths gives the extended IFT. It may be noted that in our framework, we can also obtain the DFT, provided the system either begins and ends in equilibrium or in the same nonequilibrium steady state [5]. In the next section, we prove the same IFT for ΔS_{tot} by means of the method developed in ref. [16] by using the quantum mechanical generalization of the Crook’s FT.

4. IFT using quantum Crooks FT

We consider the system to be coupled to a bath, but there is no assumption made with regard to the strength of the coupling. Each time step in the entire evolution is divided into

two substeps. In the first substep, the protocol is changed while in the second, the protocol is kept fixed and the system relaxes by dissipation of heat. The total evolution is divided into N steps. Each step starts at t_n and ends at t_{n+1} , where $n = 0, 1, 2, \dots, N - 1$. We closely follow the treatment in ref. [16].

For a quantum adiabatic process, the protocol changes slowly and the system remains in the same eigenstate in the work step. However, in the present case, the work step is almost instantaneous and the process is non-adiabatic. As a consequence, the eigenstates before and after work step may be different. The system starts to evolve under a predetermined protocol λ_0 . For simplicity, let us consider the observable measured at intermediate times to be the Hamiltonian itself. It can be readily generalized to the case of other observables. We consider that the feedback is applied at the beginning of each work step and we change the protocol subsequently according to the result obtained from the measurement, as discussed earlier. The conditional probability $p(y_{n-1}|i_{n-1})$ denotes that the measured outcome is y_{n-1} , while the actual collapsed state is $|i_{n-1}, \lambda_{n-1}\rangle$, at the beginning of the n th work step. Within the ket notation, i_{n-1} represents the state of the system and λ_{n-1} is the value of the control parameter. After the measurement of t_{n-1} , the protocol is changed to $\lambda_n(y_{n-1})$ from $\lambda_{n-1}(y_{n-2})$. During the work step, the system evolves unitarily from t_{n-1} to t'_{n-1} , where it is measured to be in state $|i'_{n-1}, \lambda_n\rangle$. The time taken in the work substep is considered to be too small for the system to relax. In the n th heat step, the system relaxes from state $|i'_{n-1}, \lambda_n\rangle$ to $|i_n, \lambda_n\rangle$. Therefore, the path followed by the system in state-space of the measured eigenstates from state $|i_0, \lambda_0 = A\rangle$ to $|i_\tau, \lambda_\tau = B\rangle$ is represented as $|i_0, \lambda_0\rangle \rightarrow |i'_0, \lambda_1\rangle \rightarrow |i_1, \lambda_1\rangle \rightarrow |i'_1, \lambda_2\rangle \rightarrow \dots \rightarrow |i_{N-1}, \lambda_{N-1}\rangle \rightarrow |i'_{N-1}, \lambda_N\rangle \rightarrow |i_N, \lambda_N\rangle$. Let $E(i_n, \lambda_n)$ be the energy eigenvalue of state $|i_n, \lambda_n\rangle$. By adding the contributions from all the work steps, the total work done on the system is given by

$$W = \sum_{n=0}^{N-1} [E(i'_n, \lambda_{n+1}) - E(i_n, \lambda_n)], \quad (4.1)$$

while heat dissipated into the bath is

$$Q = - \sum_{n=0}^{N-1} [E(i_{n+1}, \lambda_{n+1}) - E(i'_n, \lambda_{n+1})]. \quad (4.2)$$

The change in internal energy of the system along the trajectory is

$$\Delta E = Q + W = E(i_N, \lambda_N) - E(i_0, \lambda_0). \quad (4.3)$$

As before, the mutual information is

$$I = \ln \frac{p(y_n|i_n) \cdots p(y_2|i_2)p(y_1|i_1)}{p(y_n, \dots, y_2, y_1)}. \quad (4.4)$$

The forward and the reverse path probabilities are respectively given by

$$P_F(A \rightarrow B) = p(i_0, \lambda_0) \prod_{n=0}^{N-1} p(y_n | i_n) p_F(|i_n, \lambda_n\rangle \rightarrow |i'_n, \lambda_{n+1}\rangle) \times p_F(|i'_n, \lambda_{n+1}\rangle \rightarrow |i_{n+1}, \lambda_{n+1}\rangle) \quad (4.5)$$

and

$$P_R(A \leftarrow B) = p(i_N, \lambda_N) p(y_N, \dots, y_1) \prod_{n=0}^{N-1} p_R(|\tilde{i}_n, \lambda_n\rangle \leftarrow |\tilde{i}'_n, \lambda_{n+1}\rangle) \times p_R(|\tilde{i}'_n, \lambda_{n+1}\rangle \leftarrow |\tilde{i}_{n+1}, \lambda_{n+1}\rangle). \quad (4.6)$$

As mentioned earlier, during the work step, the system can be regarded as an isolated quantum system and evolution is completely determined by the time-dependent Hamiltonian $H_S(\lambda(t))$. Thus, the evolution is unitary. Microscopic reversibility for the work step gives [16]

$$p_F(|i_n, \lambda_n\rangle \rightarrow |i'_n, \lambda_{n+1}\rangle) = p_R(|\tilde{i}_n, \lambda_n\rangle \leftarrow |\tilde{i}'_n, \lambda_{n+1}\rangle). \quad (4.7)$$

The heat steps or relaxation steps are assumed to be microscopically reversible and obey the local detailed balance for all the fixed values of the external parameter λ . The detailed balance condition in relaxation substep implies

$$\frac{P_F(|i'_n, \lambda_{n+1}\rangle \rightarrow |i_{n+1}, \lambda_{n+1}\rangle)}{P_R(|\tilde{i}'_n, \lambda_{n+1}\rangle \leftarrow |\tilde{i}_{n+1}, \lambda_{n+1}\rangle)} = \exp[-\beta(E_{n+1}, \lambda_{n+1} - E(i'_n, \lambda_{n+1}))]. \quad (4.8)$$

Using the above two equations, we get

$$\frac{P_F(A \rightarrow B)}{P_R(A \leftarrow B)} = \frac{p(y_N | i_N) \cdots p(y_2 | i_2) p(y_1 | i_1)}{p(y_N, \dots, y_2, y_1)} \frac{p(i_0, \lambda_0)}{p(i_N, \lambda_N)} \times \prod_0^{N-1} \exp[-\beta(E_{n+1}, \lambda_{n+1} - E(i'_n, \lambda_{n+1}))]. \quad (4.9)$$

The total entropy change along the trajectory, $\Delta S_{\text{tot}} = \Delta S + \Delta S_B$, which is a trajectory-dependent random variable, where $\Delta S \equiv -\ln(P(i_N, \lambda_N)/P(i_0, \lambda_0))$ is the change in system entropy, and $\Delta S_B \equiv Q/T$ is the entropy change of the bath, along a single trajectory. Using eqs (4.2) and (4.4), eq. (4.9) simplifies to

$$\frac{P_F(A \rightarrow B)}{P_R(A \leftarrow B)} = e^I e^{\Delta S_{\text{sys}}} e^{Q/T} = e^{\Delta S_{\text{tot}} + I}. \quad (4.10)$$

This immediately leads to the generalized integral fluctuation theorem for total entropy change, in the presence of measurement and feedback. In the above derivation, we have taken measurements for feedback at the beginning of the work steps for simplicity. These

measurements can be performed at any time in between the work steps. The result will not be affected. It would only make the notations more complicated and would not provide any new physical insight. Feedback cannot be performed within the heat step which by definition requires protocol to be held constant.

As in Case (ii), the DFT for ΔS_{tot} can be obtained if the initial and final distributions are in the equilibrium or in the same nonequilibrium steady state [5].

5. Conclusions

Based on the path probability formulation in state-space, we have derived the generalized total entropy production FTs for quantum systems in the presence of measurement and feedback, for three different cases. They retain the same form as in classical case. The second law of thermodynamics gets modified in the presence of information and feedback (eq. (1.9)). For isolated quantum system with feedback, we have derived the generalized DFT for the total entropy. For this case, DFT retains the same form in the presence of multiple measurements of any system observable, thus showing the robustness of these FTs against measurements (von Neumann-type or generalized measurements). For Case (ii) of a weakly coupled quantum system under feedback, we have derived the extended IFT for total entropy. In Case (iii), we have derived the extended IFT for ΔS_{tot} , using the quantum Crooks FT, where quantum trajectory is characterized by a sequence of alternating work and heat steps. IFT is valid for any initial arbitrary state of a system. DFT in Cases (ii) and (iii) can be obtained only when the system either begins or ends in equilibrium or remains in the same nonequilibrium steady state. By using our approach, the generalized DFT can be proved, but we have not provided the details. The derivation of the robustness of the FT against intermediate measurements is given only for Case (i), namely, for the isolated quantum system. Following the same treatment, the robustness of FT can be readily demonstrated for Cases (ii) and (iii) as well.

In conclusion, we have generalized total entropy production fluctuation theorem in the presence of feedback to the quantum domain using three different approaches.

Acknowledgement

One of the authors (AMJ) thanks DST, India for financial support.

A. Appendix

A.1 Isolated system under weak measurements

In this Appendix, we derive IFT for ΔS_{tot} under weak measurement (POVM), as opposed to projective von Neumann-type measurements considered in §2.1. We follow the mathematical treatment given in ref. [29]. For simplicity, we consider that only one weak measurement is performed at intermediate time. The generalization to multiple weak measurements is straightforward. Consider that an isolated quantum system is controlled externally through time-dependent protocol $\lambda(t)$. Initially at $t = 0$, energy measurement

is performed and the system is found to be in state $|n, 0\rangle$ with probability density p_n . The density matrix becomes

$$\rho_n(0^+) = \frac{\Pi_n^0 \rho_0 \Pi_n^0}{p_n}, \quad (\text{A.1})$$

where ρ_0 is the density matrix of the system before measurement, Π_n^0 denotes von Neumann projective measurement operator and $p_n = \text{Tr} \Pi_n^0 \rho_0$. The system then evolves unitarily up to time t_1 and a weak measurement is performed and we get the density matrix

$$\rho_n(t_1^+) = \sum_r M_r U_\lambda(t_1, 0) \rho_n(0^+) U_\lambda^\dagger(t_1, 0) M_r^\dagger. \quad (\text{A.2})$$

M_r is the weak measurement operator with property $\sum_r M_r M_r^\dagger = 1$. The system undergoes further evolution unitarily and finally the projective measurement is performed and the system is found to be in state $|m, \tau\rangle$ at time τ . The conditional probability $P_\lambda(m, \tau|n, 0)$ for a system initially in state $|n, 0\rangle$ and finally in state $|m, \tau\rangle$ is given by

$$P_\lambda(m, \tau|n, 0) = \text{Tr} \Pi_m^f U_\lambda(\tau, t_1) \rho_n(t_1^+) U_\lambda^\dagger(\tau, t_1). \quad (\text{A.3})$$

Thus, the probability of the change in total entropy,

$$\Delta S_{\text{tot}} = -\ln p_m + \ln p_n, \quad (\text{A.4})$$

for a given pre-determined protocol $\lambda(t)$ is

$$P_\lambda(\Delta S_{\text{tot}}) = \sum_{m,n} \delta(\Delta S_{\text{tot}} + \ln p_m - \ln p_n) P_\lambda(m, \tau|n, 0) p_n, \quad (\text{A.5})$$

where p_m is the probability of the system to stay at the end of protocol at final time τ . The Fourier transform of this probability is

$$G_\lambda(u) = \int d\Delta S_{\text{tot}} P_\lambda(\Delta S_{\text{tot}}) e^{iu\Delta S_{\text{tot}}}. \quad (\text{A.6})$$

Substituting the expression for $P_\lambda(\Delta S_{\text{tot}})$ from eq. (A.5) and using eqs (A.3), (A.2), (A.1) we get

$$\begin{aligned} G_\lambda(u) &= \sum_{m,n,r} e^{iu(-\ln p_m + \ln p_n)} \text{Tr} \Pi_m^f U_\lambda(\tau, t_1) M_r U_\lambda(t_1, 0) \\ &\quad \times \Pi_n^0 \rho_0 \Pi_n^0 U_\lambda^\dagger(t_1, 0) M_r^\dagger U_\lambda^\dagger(\tau, t_1) \\ &= \sum_{m,n,r} \text{Tr} \Pi_m^f e^{-iu \ln \rho_\tau} U_\lambda(\tau, t_1) M_r U_\lambda(t_1, 0) \\ &\quad \times \Pi_n^0 e^{iu \ln \rho_0} \rho_0 U_\lambda^\dagger(t_1, 0) M_r^\dagger U_\lambda^\dagger(\tau, t_1) \\ &= \sum_r \text{Tr} e^{-iu \ln \rho_\tau} U_\lambda(\tau, t_1) M_r U_\lambda(t_1, 0) e^{iu \ln \rho_0} \rho_0 U_\lambda^\dagger(t_1, 0) M_r^\dagger U_\lambda^\dagger(\tau, t_1) \\ &= \sum_r \text{Tr} U_\lambda^\dagger(t_1, 0) M_r^\dagger U_\lambda^\dagger(\tau, t_1) e^{-iu \ln \rho_\tau} U_\lambda(\tau, t_1) M_r U_\lambda(t_1, 0) e^{iu \ln \rho_0} \rho_0. \end{aligned} \quad (\text{A.7})$$

ρ_f is the final density matrix which is diagonal in the energy basis. In the second step, we have used the completeness relation $\sum_m \Pi_m^f = 1$ and $\sum_n \Pi_n^0 = 1$ for the projective operator. Substituting $u = i$, for the Fourier transform variable, we get from eq. (A.6) $G_\lambda(i) = \langle e^{-\Delta S_{\text{tot}}} \rangle$ and hence

$$\begin{aligned}
 \langle e^{-\Delta S_{\text{tot}}} \rangle &= \sum_r \text{Tr} U_\lambda^\dagger(t_1, 0) M_r^\dagger U_\lambda^\dagger(\tau, t_1) e^{\ln \rho_f} U_\lambda(\tau, t_1) M_r U_\lambda(t_1, 0) e^{-\ln \rho_0} \rho_0 \\
 &= \sum_r \text{Tr} U_\lambda^\dagger(t_1, 0) M_r^\dagger U_\lambda^\dagger(\tau, t_1) e^{\ln \rho_f} U_\lambda(\tau, t_1) M_r U_\lambda(t_1, 0) \\
 &= \sum_r \text{Tr} U_\lambda(\tau, t_1) M_r U_\lambda(t_1, 0) U_\lambda^\dagger(t_1, 0) M_r^\dagger U_\lambda^\dagger(\tau, t_1) e^{\ln \rho_f} \\
 &= \sum_r \text{Tr} U_\lambda(\tau, t_1) M_r M_r^\dagger U_\lambda^\dagger(\tau, t_1) e^{\ln \rho_f} \\
 &= \text{Tr} U_\lambda(\tau, t_1) U_\lambda^\dagger(\tau, t_1) e^{\ln \rho_f} \\
 &= \text{Tr} e^{\ln \rho_f} = \text{Tr} \rho_f = 1.
 \end{aligned} \tag{A.8}$$

In the second line, we make use of $e^{-\ln \rho_0} \rho_0 = 1$, while the cyclic property of trace is used in the third line. Operator identity $\sum_r M_r M_r^\dagger = 1$ is used in the fourth step.

We have proved that the IFT holds in the same form as in eq. (1.4) under intermediate weak measurements. This can be readily generalized to the multiple intermediate weak measurements, which corroborates the robustness of FT under weak or generalized measurements.

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