The Tasaki–Crooks quantum fluctuation theorem

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Abstract
Starting out from the recently established quantum correlation function expression of the characteristic function for the work performed by a force protocol on the system in Talkner *et al* (2007 *Phys. Rev.* E **75** 050102 (*Preprint* cond-mat/0703213)) the quantum version of the Crooks fluctuation theorem is shown to emerge almost immediately by the mere application of an inverse Fourier transformation.

Work and fluctuation theorems have ignited much excitement during the recent decade [1–4]. These theorems have prompted further theoretical investigations [5–8] as well as experimental research [9]. We here consider a quantum system staying in *weak thermal contact* with a heat bath at the inverse temperature β until a time t_0. At time t_0 the contact to the heat bath is then either kept at this weak level, or may even be switched off altogether. A classical time-dependent force solely acts on the system according to a prescribed protocol until time t_f. A *protocol* defines a family of Hamiltonians $\{H(t)\}_{t_f,t_0}$ which govern the time evolution of the system during the indicated interval of time $[t_0, t_f]$ in the presence of the external force. The weak action of the heat bath on the system can be neglected for any protocol of finite duration $t_f - t_0$ [10]. The work performed by the force on the system is a random quantity because of the quantum nature of the considered system and because the system is prepared in the thermal equilibrium state

$$\rho(t_0) = Z^{-1}(t_0) \exp\{-\beta H(t_0)\} \tag{1}$$

which is a mixed state for all finite β. Here, $Z(t_0) = \mathrm{Tr} \exp\{-\beta H(t_0)\}$ denotes the partition function. As a random quantity, the work is characterized by a probability density $p_{t_f,t_0}(w)$ or equivalently by the corresponding characteristic function $G_{t_f,t_0}(u)$, which is defined as the Fourier transform of the probability density, i.e.

$$G_{t_f,t_0}(u) = \int \mathrm{d}w \, \mathrm{e}^{\mathrm{i}uw} p_{t_f,t_0}(w). \tag{2}$$

In a recent work, [11] we have demonstrated that the characteristic function $G_{t_f,t_0}(u)$ of the work can be expressed as a quantum correlation function of the two exponential operators $\exp\{\mathrm{i}uH(t_f)\}$ and $\exp\{-\mathrm{i}uH(t_0)\}$. It explicitly reads

$$\begin{aligned} G_{t_f,t_0}(u) &= \langle \mathrm{e}^{\mathrm{i}uH(t_f)}\,\mathrm{e}^{-\mathrm{i}uH(t_0)}\rangle_{t_0} \\ &\equiv Z^{-1}(t_0)\,\mathrm{Tr}\,U^+_{t_f,t_0}\,\mathrm{e}^{\mathrm{i}uH(t_f)}U_{t_f,t_0}\,\mathrm{e}^{-\mathrm{i}uH(t_0)}\,\mathrm{e}^{-\beta H(t_0)}, \end{aligned} \tag{3}$$

where the index at the bracket signifies the fact that the average is taken over the initial density matrix $\rho(t_0)$.

For a protocol consisting of Hamiltonians $H(t)$, each of which is bounded from below and has a purely discrete spectrum, the characteristic function $G_{t_f,t_0}(u)$ is an analytic function of u in the strip $S = \{u|0 \leqslant \mathrm{Im}\,u \leqslant \beta, -\infty < \mathrm{Re}\,u < \infty\}$ [1] where $\mathrm{Re}\,u$ and $\mathrm{Im}\,u$ denote the real and imaginary parts of u, respectively. Collecting the two exponential factors $\mathrm{e}^{-\mathrm{i}uH(t_0)}$ and $\mathrm{e}^{-\beta H(t_0)}$ into one, and introducing the complex parameter $v = -u + \mathrm{i}\beta \in S$, we find

$$\begin{aligned} Z(t_0)G_{t_f,t_0}(u) &= \mathrm{Tr}\,U^+_{t_f,t_0}\,\mathrm{e}^{\mathrm{i}(-v+\mathrm{i}\beta)H(t_f)}\,U_{t_f,t_0}\,\mathrm{e}^{\mathrm{i}vH(t_0)} \\ &= \mathrm{Tr}\,\mathrm{e}^{-\mathrm{i}vH(t_f)}\,\mathrm{e}^{-\beta H(t_f)}\,U_{t_f,t_0}\,\mathrm{e}^{\mathrm{i}vH(t_0)}\,U^+_{t_f,t_0} \\ &= \mathrm{Tr}\,\mathrm{e}^{-\mathrm{i}vH(t_f)}\,\mathrm{e}^{-\beta H(t_f)}\,U^+_{t_0,t_f}\,\mathrm{e}^{\mathrm{i}vH(t_0)}\,U_{t_0,t_f} \\ &= \mathrm{Tr}\,U^+_{t_0,t_f}\,\mathrm{e}^{\mathrm{i}vH(t_0)}\,U_{t_0,t_f}\,\mathrm{e}^{-\mathrm{i}vH(t_f)}\,\mathrm{e}^{-\beta H(t_f)} \\ &= Z(t_f)G_{t_0,t_f}(v), \end{aligned} \tag{4}$$

where we used the unitarity of the time evolution operator, i.e. $U^+_{t_f,t_0} = U^{-1}_{t_f,t_0} = U_{t_0,t_f}$. We hence obtain

$$G_{t_f,t_0}(u) = \frac{Z(t_f)}{Z(t_0)}G_{t_0,t_f}(-u + \mathrm{i}\beta). \tag{5}$$

The ratio of the canonical partition functions can be expressed in terms of the difference of free energies ΔF between the two thermal equilibrium systems as $Z(t_f)/Z(t_0) = \exp\{-\beta\Delta F\}$. The quantity $G_{t_0,t_f}(v)$ coincides with the characteristic function of the work performed on a system that is initially prepared in the thermal equilibrium state $Z^{-1}(t_f)\exp\{-\beta H(t_f)$ under the influence of the *time-reversed* protocol $\{H(t)\}_{t_0,t_f}$. Applying the inverse Fourier transform on both sides of equation (5) we obtain the following fluctuation theorem:

$$\frac{p_{t_f,t_0}(w)}{p_{t_0,t_f}(-w)} = \frac{Z(t_f)}{Z(t_0)}\,\mathrm{e}^{\beta w} = \mathrm{e}^{-\beta(\Delta F - w)}. \tag{6}$$

It relates the probability density of performed work for a given protocol to that of the work for the time-reversed process. This process can in principle be realized by preparing the Gibbs state $Z^{-1}(t_f)\exp\{-\beta H(t_f)\}$ as the *initial* density matrix and letting run the time-reversed protocol $\{H(t)\}_{t_0,t_f}$.

In the classical context this fluctuation theorem was proved by Gavin Crooks [4], while its quantum version goes back to Hal Tasaki [6].

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[1] This can be proved in the same way as the analyticity properties of equilibrium correlation functions that underly the KMS condition, cf [12].

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