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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.

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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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