

FAST TRACK COMMUNICATION

The Tasaki–Crooks quantum fluctuation theorem**Peter Talkner and Peter Hänggi**

Institut für Physik, Universität Augsburg, Universitätsstrasse 1, D-86135 Augsburg, Germany

E-mail: peter.talkner@physik.uni-augsburg.de

Received 24 April 2007

Published 12 June 2007

Online at stacks.iop.org/JPhysA/40/F569**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.

PACS numbers: 05.40.–a, 87.16.–b, 87.19.Nn

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

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

which is a mixed state for all finite β . Here, $Z(t_0) = \text{Tr} \exp\{-\beta H(t_0)\}$ 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.

$$G_{t_f, t_0}(u) = \int dw e^{i u w} p_{t_f, t_0}(w). \quad (2)$$

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 $\exp\{iuH(t_f)\}$ and $\exp\{-iuH(t_0)\}$. It explicitly reads

$$\begin{aligned} G_{t_f, t_0}(u) &= \langle e^{iuH(t_f)} e^{-iuH(t_0)} \rangle_{t_0} \\ &\equiv Z^{-1}(t_0) \text{Tr} U_{t_f, t_0}^+ e^{iuH(t_f)} U_{t_f, t_0} e^{-iuH(t_0)} e^{-\beta H(t_0)}, \end{aligned} \quad (3)$$

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 $S = \{u | 0 \leq \text{Im } u \leq \beta, -\infty < \text{Re } u < \infty\}$ ¹ where $\text{Re } u$ and $\text{Im } u$ denote the real and imaginary parts of u , respectively. Collecting the two exponential factors $e^{-iuH(t_0)}$ and $e^{-\beta H(t_0)}$ into one, and introducing the complex parameter $v = -u + i\beta \in S$, we find

$$\begin{aligned} Z(t_0)G_{t_f, t_0}(u) &= \text{Tr} U_{t_f, t_0}^+ e^{i(-v+i\beta)H(t_f)} U_{t_f, t_0} e^{ivH(t_0)} \\ &= \text{Tr} e^{-ivH(t_f)} e^{-\beta H(t_f)} U_{t_f, t_0} e^{ivH(t_0)} U_{t_f, t_0}^+ \\ &= \text{Tr} e^{-ivH(t_f)} e^{-\beta H(t_f)} U_{t_0, t_f}^+ e^{ivH(t_0)} U_{t_0, t_f} \\ &= \text{Tr} U_{t_0, t_f}^+ e^{ivH(t_0)} U_{t_0, t_f} e^{-ivH(t_f)} e^{-\beta H(t_f)} \\ &= Z(t_f)G_{t_0, t_f}(v), \end{aligned} \quad (4)$$

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

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

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:

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

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].

Acknowledgments

This work has been supported by the Deutsche Forschungs-gemeinschaft via the Collaborative Research Centre SFB-486, project A10. Financial support of the German Excellence Initiative via the *Nanosystems Initiative Munich* (NIM) is gratefully acknowledged as well.

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

References

- [1] Evans D J, Cohen E G D and Morriss G P 1993 *Phys. Rev. Lett.* **71** 2401
- [2] Gallavotti G and Cohen E G D 1995 *Phys. Rev. Lett.* **74** 2694
- [3] Jarzynski C 1997 *Phys. Rev. Lett.* **78** 2690
- [4] Crooks G E 1999 *Phys. Rev. E* **60** 2721
- [5] Kurchan J 1998 *J. Phys. A: Math. Gen.* **31** 3719
- [6] Tasaki H 1999 Jarzynski relations for quantum systems and some applications *Preprint cond-mat/0009244*
- [7] Mukamel S 2003 *Phys. Rev. Lett.* **90** 170604
- [8] Seifert U 2004 *J. Phys. A: Math. Gen.* **37** L517
- [9] Bustamante C, Liphardt J and Ritort F 2005 *Phys. Today* **58** (7) 43
- [10] Spohn H 1980 *Rev. Mod. Phys.* **52** 569
- [11] Talkner P, Lutz E and Hänggi P 2007 *Phys. Rev. E* **75** 050102 (*Preprint cond-mat/0703213*)
- [12] Haag R, Hugenholtz N M and Winnink M 1967 *Commun. Math. Phys.* **5** 215