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Meng Zeng and Ee Hou Yong

Division of Physics and Applied Physics, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore 637371, Singapore

E-mail: eehou@ntu.edu.sg

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Abstract

Following the recent work by Deffner and Saxena (2015 *Phys. Rev. Lett.* **114** 150601), where the Jarzynski equality is generalised to non-Hermitian quantum mechanics, we prove in this work a stronger form of Jarzynski equality, the Crooks fluctuation theorem, also in the non-Hermitian formalism when the system is in the unbroken $\mathcal{PT}$ -symmetric phase.

1. Introduction

Near-equilibrium systems are relatively well understood [1–4], but systems far from equilibrium are much less so and are still under intensive study. The first breakthrough in quantitatively characterising systems arbitrarily far away from equilibrium came with the works of Evans *et al* [5, 6] and Gallavotti *et al* [7], where the entropy production fluctuation theorems for such systems were firstly formulated. In a seminal paper [8] and a paper following [9] in 1997, Jarzynski derived an equality relating the work fluctuations with the free energy difference when a classical thermodynamic system is driven from an equilibrium state to another state. The equality reads

$$\langle e^{-\beta W} \rangle = e^{-\beta \Delta F}, \quad (1)$$

where W is the work done to the system by the external driving force, ΔF is the change in the system's free energy during the driving process, and the left hand side of the equality is averaged over all the phase space trajectories of the system. Two years later in 1999, Crooks proved a stronger form of the Jarzynski equality, the entropy production fluctuation theorem [10]. The Crooks fluctuation theorem relates the forward entropy production distribution along phase space trajectories with the backward entropy production distribution along the time-reversed trajectories. The fluctuation theorem reads

$$\frac{P_F(+\omega)}{P_R(-\omega)} = e^{+\omega}, \quad (2)$$

where $+\omega$ ($-\omega$) is the entropy production (decrease) during the non-equilibrium process, $P_F(\omega)$ is the forward entropy production distribution for all the phase space trajectories and $P_R(-\omega)$ is the entropy decrease distribution for all the time-reversed phase space trajectories. Equation (2) has another equivalent form that replaces the entropy by the non-equilibrium work and equilibrium free energy difference and thus is closer in form with the Jarzynski equality given by equation (1). This version of the fluctuation theorem is given by

$$\frac{P_F(+\beta W)}{P_R(-\beta W)} = e^{\beta(W - \Delta F)}, \quad (3)$$

where the W and ΔF have the same physical meaning as in equation (1). Equation (3) reduces to equation (1) if $P_R(-\beta W)$ is moved over to the right hand side followed by an integration on both sides with respect to W . Soon after the discovery of the classical fluctuation theorems, efforts had been made to generalise the fluctuation theorems to quantum regime [11–14]. Especially in [15], the authors pointed out that quantum work is not an observable. Instead, quantum work should be represented using correlation functions, which will be an important ingredient of this paper.

Almost at around the same time of the discovery of the Jarzynski equality, Bender *et al* discovered new classes of complex Hamiltonians that are non-Hermitian, but come with real spectra [16]. These Hamiltonians, not necessarily Hermitian, are supposed to satisfy a weaker condition: the so-called $\mathcal{PT}$ -symmetry. More precisely, $[H, \mathcal{PT}] = 0$, where $\mathcal{P}$ is the parity operator and $\mathcal{T}$ is the time-reversal operator. For $\mathcal{PT}$ -symmetric Hamiltonian systems, there are two phases: broken $\mathcal{PT}$ -symmetry, where the energy eigenvalues appear as complex conjugate pairs, and the unbroken $\mathcal{PT}$ -symmetry, where all the energy eigenvalues are real [17].

In the recent work [18, 19], the authors proved that the quantum Jarzynski equality can be readily generalised to non-Hermitian quantum systems with unbroken $\mathcal{PT}$ -symmetry, by adopting a modified unitary time-evolution operator suitable for the formalism of non-Hermitian quantum mechanics. However, to the best of our knowledge, the more general Crooks fluctuation theorem has not been proved in the $\mathcal{PT}$ -symmetric quantum mechanical framework, and this is the purpose of our present work. We are going to show that the Crooks fluctuation theorem still holds in non-Hermitian quantum systems with unbroken $\mathcal{PT}$ -symmetry.

2. Non-Hermitian quantum thermodynamics

For non-Hermitian Hamiltonian with $\mathcal{PT}$ -symmetry, the Hamiltonian is still diagonalisable, but not unitarily diagonalisable. The left eigenstate and right eigenstate do not have the usual bra-ket correspondence as in Hermitian quantum mechanics, simply because the Hamiltonian is non-Hermitian and we no longer have the formal left-right symmetry [20, 21]. Based on the non-Hermitian formalism, we have the modified ket-bra correspondence $|\phi\rangle \leftrightarrow \langle g\phi| = \langle\phi|g^\dagger = \langle\phi|g$, where g is a Hermitian operator, i.e. $g^\dagger = g$. As a result, the normalisation condition will be given by $\langle\phi|g|\phi\rangle = 1$ and the completeness relation will be given by $\sum_m |\phi_m\rangle \langle\phi_m|g = 1$.

For a quantum system coupled to a thermal bath and thus in equilibrium at time t_0 , with Hamiltonian $H(t_0)$, an external driving force is applied and the system starts to evolve with a time-dependent Hamiltonian $H(t)$, till some final time t_f . The system is decoupled from the heat bath starting at time t_0 such that the system remains isolated except there is a driving force during the process.

It has been shown that the time evolution in non-Hermitian quantum mechanics has to be modified to preserve unitarity [22]. In this framework, the modified Schrodinger equation is given by

$$i\frac{\partial}{\partial t}|\psi\rangle = (H(t) + A(t))|\psi\rangle, \quad (4)$$

where $H(t)$ is the time-dependent Hamiltonian of the system and $A(t) = -\frac{i\hbar}{2}g_t^{-1}\partial_t g_t$ is a time-dependent gauge field term that has been added in to ensure unitarity of the non-Hermitian quantum dynamics when all the energy eigenvalues are real. The corresponding time evolution operator then is given by

$$U_{t_0, t_f} = \mathcal{T}e^{\int_{t_0}^{t_f} H(t) + A(t) dt}, \quad (5)$$

where U_{t_0, t_f} is the time evolution operator from initial time t_0 to some final time t_f and $\mathcal{T}$ is the time-ordering operator. When the system is in the unbroken $\mathcal{PT}$ -symmetric phase, it has real spectrum and thus the dynamics generated by the above time evolution operator is unitary in the sense that probability is preserved. This does not mean that the evolution operator U_{t_0, t_f} is unitary. Instead, the conventional unitarity condition of the time evolution operator $U_{t_0, t_f}^\dagger U_{t_0, t_f} = 1$ should be replaced by

$$U_{t_0, t_f}^\dagger g_{t_f} U_{t_0, t_f} = g_{t_0}. \quad (6)$$

The latter reduces to the former when g is set to be the identity. We can see from this formalism that the non-Hermitian quantum mechanics serves to generalise the conventional Hermitian quantum mechanics.

Since we are using the non-Hermitian formalism to solve problems in quantum thermodynamics, some of the basic mathematical manipulations have to be modified to be consistent with the theory of statistical mechanics and experimental observations. One essential change is the form of inner product. In the non-Hermitian formalism the inner product has to be modified to $\langle g\phi|\psi\rangle = \langle\phi|g|\psi\rangle$. Correspondingly, the definition of the trace operation, which is a crucial part of the definition of density operator and calculation of thermodynamic observables, will also have to be modified as the following:

$$\text{Tr}_g\{O\} = \sum_m \langle\phi_m|gO|\phi_m\rangle, \quad (7)$$

where O is some arbitrary operator, and $\{|\phi_m\rangle\}$ form a complete basis of the Hilbert space and we have assumed that the spectrum is discrete and non-degenerate for simplicity. There are two simple facts regarding the modified trace operation that will be useful in our later discussions. The first fact is that the usual cyclic property still holds in the modified version, i.e.

$$\text{Tr}_g\{AB\} = \text{Tr}_g\{BA\}. \quad (8)$$

The second fact is that trace is preserved under the unitary dynamics generated by equation (5):

$$\text{Tr}_g\{O\}_{t_0} = \text{Tr}_g\{O\}_{t_f}. \quad (9)$$

The proofs of the the above two facts are provided in the [appendix](#).

3. Proof of Crooks fluctuation theorem in unbroken $\mathcal{PT}$ -symmetric phase

The calculation of the work done on the system is based on the two-time energy measurement [15, 23]. An energy projection measurement is performed on the system at the initial time t_0 , resulting in $E(t_0)$, after which the system is allowed to evolve by the Hamiltonian $H(t)$ till some final time t_f when a second energy measurement is performed, resulting in $E(t_f)$. Then the work done for this particular quantum process is given by $W = E(t_f) - E(t_0)$. Average is done over all the possible realisations of the two-time energy measurement and the probability measure is given by the Gibbs distribution

$$\rho = \frac{e^{-\beta H}}{Z} = \frac{e^{-\beta H}}{\text{Tr}_g e^{-\beta H}}. \quad (10)$$

In order to prove the Crooks fluctuation theorem, we first calculate the work distribution for the non-equilibrium process. Based on the two-time energy measurement, the work distribution is given by [15]

$$P_{t_0, t_f}(W) = \sum_{m, n} \delta(W - (E_n(t_f) - E_m(t_0))) P(|\phi_m(t_0)\rangle) P(|\phi_m(t_0)\rangle \rightarrow |\phi_n(t_f)\rangle), \quad (11)$$

where $P(|\phi_m(t_0)\rangle)$ denotes the probability for the system to be found in the eigenstate $|\phi_m(t_0)\rangle$ for the first measurement at t_0 and $P(|\phi_m(t_0)\rangle \rightarrow |\phi_n(t_f)\rangle)$ denotes the transition probability from $|\phi_m(t_0)\rangle$ to $|\phi_n(t_f)\rangle$ under time evolution. Assuming the system is initially thermalised and follows the Boltzmann–Gibbs distribution equation (10), then we have

$$P(|\phi_m(t_0)\rangle) = \text{Tr}_g\{\rho(t_0)\Pi_m(t_0)\} = \frac{e^{-\beta E_m(t_0)}}{Z(t_0)}, \quad (12)$$

where $\Pi_m(t_0) = |\phi_m(t_0)\rangle\langle\phi_m(t_0)|g_{t_0}$ is the projection operator for energy measurement at t_0 . The transition probability is given by

$$P(|\phi_m(t_0)\rangle \rightarrow |\phi_n(t_f)\rangle) = |\langle\phi_n(t_f)|g_{t_f} U_{t_0, t_f} |\phi_m(t_0)\rangle|^2. \quad (13)$$

Following the same method used in [14] to prove the Hermitian quantum Crooks fluctuation theorem, we calculate the Fourier transform of the work distribution function

$$\begin{aligned} \tilde{P}_{t_0, t_f}(u) &= \int dW e^{iuW} P_{t_0, t_f}(W) \\ &= \sum_{m, n} e^{iu(E_n(t_f) - E_m(t_0))} e^{-\beta E_m(t_0)} \frac{1}{Z(t_0)} |\langle\phi_n(t_f)|g_{t_f} U_{t_0, t_f} |\phi_m(t_0)\rangle|^2 \\ &= 1/Z(t_0) \text{Tr}_g\{U_{t_0, t_f}^{-1} e^{iuH(t_f)} U_{t_0, t_f} e^{-iuH(t_0)} e^{-\beta H(t_0)}\}_{t_0} \\ &= \langle U_{t_0, t_f}^{-1} e^{iuH(t_f)} U_{t_0, t_f} e^{-iuH(t_0)} \rangle_{t_0}, \end{aligned} \quad (14)$$

where the completeness relation $\sum_m |\phi_m(t_0)\rangle\langle\phi_m(t_0)|g_{t_0} = 1$ and the cyclic property of the trace have been used. We also have for the time-reversed distribution, following [14] and setting $v = -u + i\beta$,

$$\begin{aligned} \tilde{P}_{t_f, t_0}(v) &= \int dW e^{ivW} P_{t_f, t_0}(W) = \langle U_{t_f, t_0}^{-1} e^{ivH(t_0)} U_{t_f, t_0} e^{-ivH(t_f)} \rangle_{t_f} \\ &= 1/Z(t_f) \text{Tr}_g\{U_{t_f, t_0}^{-1} e^{ivH(t_0)} U_{t_f, t_0} e^{-ivH(t_f)} e^{-\beta H(t_f)}\}_{t_0} \\ &= 1/Z(t_f) \text{Tr}_g\{U_{t_f, t_0} e^{iuH(t_f)} U_{t_f, t_0}^{-1} e^{-iuH(t_0)} e^{-\beta H(t_0)}\}_{t_0}, \end{aligned} \quad (15)$$

where we have used both of the two aforementioned facts for the trace operation defined in the non-Hermitian formalism. We can see from the above derivations that in the non-Hermitian case, the characteristic function (the Fourier transform of the work distribution) of the work performed during the non-equilibrium process can again be identified as a correlation function, which is in a slightly different form with the one given in [15] due to the modified unitarity condition. Comparing equation (14) with (15), it immediately follows that

$$Z(t_0) \tilde{P}_{t_0, t_f}(u) = Z(t_f) \tilde{P}_{t_f, t_0}(v) = Z(t_f) \tilde{P}_{t_f, t_0}(-u + i\beta). \quad (16)$$

After inverse Fourier transforming both sides of equation (16), we readily obtain

$$P_{t_0, t_f}(W) = P_{t_f, t_0}(-W) \frac{Z(t_f)}{Z(t_0)} e^{\beta W} = P_{t_f, t_0}(-W) e^{\beta(W - \Delta F)}, \quad (17)$$

which is equivalent to equation (3), and hence the Crooks fluctuation theorem is proved in the non-Hermitian quantum mechanical setting. It has to be noted that the above derivations have assumed that the non-Hermitian system is in its unbroken $\mathcal{PT}$ -symmetric phase, and thus the dynamics is unitary, which is crucial for the proof. It has been pointed out in [18] that the Jarzynski equality no longer holds if the dynamics is non-unitary. Following the same argument, we can conclude that the Crooks fluctuation theorem also breaks down when the $\mathcal{PT}$ -symmetry is broken.

4. Conclusion and outlook

By deriving a similar expression [15] regarding the characteristic function of quantum work using non-Hermitian formalism, we have generalised the quantum Crooks fluctuation theorem to the non-Hermitian case with unbroken $\mathcal{PT}$ -symmetry. It has to be emphasised that what we have done assumes the system-bath coupling is switched off during the driving process. For non-zero system-bath coupling, i.e. open quantum systems, the effects of quantum decoherence and dissipation will have to be considered. There has been recent theoretical work on quantum fluctuation theorems when decoherence is explicitly considered [24] and their experimental confirmations [25]. Therefore, an interesting and natural extension of the present work would be to investigate the validity of non-Hermitian fluctuation theorems in the presence of quantum decoherence, which would involve generalising the open quantum dynamics to one with non-Hermitian Hamiltonian.

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Appendix

The cyclic property of Tr_g is shown as the following:

$$\begin{aligned} \text{Tr}_g\{AB\} &= \sum_m \langle \phi_m | gAB | \phi_m \rangle \\ &= \sum_{m,n} \langle \phi_m | gA | \phi_n \rangle \langle \phi_n | gB | \phi_m \rangle \\ &= \sum_{m,n} \langle \phi_n | gB | \phi_m \rangle \langle \phi_m | gA | \phi_n \rangle \\ &= \sum_n \langle \phi_n | gBA | \phi_n \rangle \\ &= \text{Tr}_g\{BA\}. \end{aligned} \quad (18)$$

The invariance of Tr_g under the unitary dynamics generated by equation (5) is proved below:

$$\begin{aligned} \text{Tr}_g\{O\}_{t_0} &= \sum_m \langle \phi_m(t_0) | g_{t_0} O | \phi_m(t_0) \rangle \\ &= \sum_m \langle \phi_m(t_0) | U_{t_0, t_f}^\dagger (U_{t_0, t_f}^\dagger)^{-1} g_{t_0} O U_{t_0, t_f}^{-1} U_{t_0, t_f} | \phi_m(t_0) \rangle \\ &= \sum_m \langle \tilde{\phi}_m(t_f) | (U_{t_0, t_f}^\dagger)^{-1} g_{t_0} O U_{t_0, t_f}^{-1} | \tilde{\phi}_m(t_f) \rangle \\ &= \sum_m \langle \tilde{\phi}_m(t_f) | g_{t_f} U_{t_0, t_f} O U_{t_0, t_f}^{-1} | \tilde{\phi}_m(t_f) \rangle \\ &= \sum_m \langle \tilde{\phi}_m(t_f) | g_{t_f} O | \tilde{\phi}_m(t_f) \rangle \\ &= \text{Tr}_g\{O\}_{t_f}, \end{aligned} \quad (19)$$

where use has been made of the unitarity condition equation (6) and the cyclic property equation (8). Here we have defined that $|\tilde{\phi}_m(t_f)\rangle = U_{t_0, t_f} |\phi_m(t_0)\rangle$. It has to be noted that even if $|\phi_m(t_0)\rangle$ is an energy eigenstate of the initial Hamiltonian $H(t_0)$, the time-evolved final state $|\tilde{\phi}_m(t_f)\rangle$ may not necessarily be the eigenstate of the final

Hamiltonian $H(t_f)$. That is why $|\tilde{\phi}_m(t_f)\rangle$ is used to distinguish it from the true energy eigenstate $|\phi_m(t_f)\rangle$. This, however, does not prevent $\{|\tilde{\phi}_m(t_f)\rangle\}$ to form a valid basis for the Hilbert space at t_f .

ORCID iDs

Ee Hou Yong  <https://orcid.org/0000-0002-4583-4071>

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