A Quantum Fluctuation Theorem

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Abstract

We consider a quantum system strongly driven by forces that are periodic in time. The theorem concerns the probability $P(e)$ of observing a given energy change $e$ after a number of cycles. If the system is thermostated by a (quantum) thermal bath, $e$ is the total amount of energy transferred to the bath, while for an isolated system $e$ is the increase in energy of the system itself. Then, we show that $P(e)/P(-e) = e^{\beta e}$, a parameter-free, model-independent relation.

In the past few years there has been a renewed interest in the study of quantum systems out of equilibrium, to a large extent stimulated by the design of new experimental settings and by the construction of new devices. If a system is well out of equilibrium, as for example when it is strongly driven by periodic forces, then linear response theory (understood as linear perturbations around the Gibbs measure) is insufficient.

Even in the context of classical mechanics not many generic results are available beyond linear response. An interesting new development consists of a number of relations for strongly out of equilibrium systems, mainly regarding the distribution of work and entropy production. The first of such fluctuation theorems was discovered by Evans et.al [1], who understood that the basic ingredient was time-reversal symmetry.

Two important further steps, made by Gallavotti and Cohen widened the scope and interest of the subject. On the one hand, it was realized [2] that the fluctuation theorems are indeed the far from equilibrium generalisations of the well-known equilibrium theorems (fluctuation-dissipation and Onsager reciprocity). Most intriguingly, a byproduct of their proof [3] was that, just as the validity of the fluctuation-dissipation relation is a strong indication of equilibration, the fact that a fluctuation formula holds in a driven stationary system strongly hints that the system can be considered ‘as ergodic as possible’ — with all the implications this entails.

These results concern deterministic systems. If instead a finite system is in contact with a stochastic thermal bath, then the ‘ergodicity’ questions become trivial, and all the fluctuation formulae are extremely simple to prove [4, 5, 6].
Particularly relevant for the present work are the simple and remarkable Jarzynski and other ‘work relations’ valid well out of equilibrium [7, 8, 9, 11], whose close relation to the fluctuation theorems was clarified by Crooks [10].

Except for Ref. [11], the developments described so far are restricted to classical mechanics. The purpose of this paper is to prove two versions of a fluctuation theorem for quantum systems under strong periodic drive, either isolated or in contact with a thermal bath. Very recently, these questions have become relevant in the context of detection of quantum ‘shot’ noise generated by currents flowing through devices, given the possibility it offers to observe different quasiparticle charges of the carriers [12].

We shall consider an evolution generated by a time-dependent Hamiltonian \( H(q, p, t) \) with real matrix elements, so that there is time-reversal symmetry in each infinitesimal time step. We shall assume the explicit time-dependence is periodic (with period \( t_0 \)) and that the cycles are symmetric [13]:

\[
H(q, p, t) = H(q, p, t) = H(q, p, -t)
\]

Splitting the evolution in infinitesimal steps \( t_1, \ldots, t_n \):

\[
|\phi(t_f)\rangle = U_n U_{n-1} \ldots U_2 U_1 |\phi(t_i)\rangle
\]

where \( n \) is large, \( U_r \equiv e^{i \tau r H} \) and \( \tau = (t_f - t_i)/n \to 0 \), the reality condition implies that: \( U_r^\dagger = U_r^\ast \) and, together with the symmetry of cycles Eq. (1) this implies that the evolution over a cycle satisfies time-reversibility: Consider the case in which the time \( t_f - t_i \) consists of an integer number of cycles, and hence \( U_r = U_{n-r+1} \) (cfr. [11]). Then:

\[
U^\dagger = U_1^\dagger U_2^\dagger \ldots U_{n-1}^\dagger U_n^\dagger = [U_1 U_2 \ldots U_{n-1} U_n]^\ast
\]

\[
= [U_n U_{n-1} \ldots U_2 U_1]^\ast = U^\ast
\]

a formula only valid for \((t_f - t_i)/t_0 = \text{integer}\), which we shall assume throughout this paper.

We denote the eigenvectors of the initial time Hamiltonian \( |\psi_\alpha\rangle \):

\[
H_1 |\psi_\alpha\rangle = \varepsilon_\alpha |\psi_\alpha\rangle
\]
and the corresponding partition function:

\[ Z = \text{Tr} e^{-\beta H_1} \]  

Consider the following protocol:

- With (canonical) probability \( p_\alpha = e^{-\beta \epsilon_\alpha}/Z \) we choose a wavefunction \( |\psi_\alpha\rangle \).
- We let it evolve through an integer number of cycles:
  \[ |\phi\rangle = U|\psi_\alpha\rangle = \sum_\gamma |\psi_\gamma\rangle \langle \psi_\gamma | \phi \rangle \]  
- We measure the final \( H_1 \) and record the energy difference \( e \) between initial and final times.

Let us calculate the probability distribution of \( e \). For a given value of \( \alpha \), this distribution reads:

\[ P_\alpha(e) = \sum_\gamma \delta[e - (\epsilon_\gamma - \epsilon_\alpha)] |\langle \psi_\gamma | U|\psi_\alpha\rangle|^2 e^{-\beta \epsilon_\alpha} \] (7)

The average distribution \( P(e) \) over initial conditions is:

\[ P(e) = \frac{1}{Z} \sum_{\gamma, \alpha} \delta[e - (\epsilon_\gamma - \epsilon_\alpha)] |\langle \psi_\gamma | U|\psi_\alpha\rangle|^2 e^{-\beta \epsilon_\alpha} \] (8)

Writing the delta function in integral form, we get:

\[ P(e) = \frac{1}{Z} \int_{-i\infty}^{i\infty} d\lambda e^{-\lambda e^{-(-\epsilon_\gamma - \epsilon_\alpha)}} \sum_{\gamma, \alpha} |\langle \psi_\gamma | U|\psi_\alpha\rangle|^2 e^{-\beta \epsilon_\alpha} \] (9)

where:

\[ Q(\lambda) = \sum_{\gamma, \alpha} e^{\lambda(\epsilon_\gamma - \epsilon_\alpha)} |\langle \psi_\gamma | U|\psi_\alpha\rangle|^2 e^{-\beta \epsilon_\alpha} \]
\[ = \sum_{\gamma, \alpha} e^{\lambda \epsilon_\gamma} \langle \psi_\alpha | U^\dagger | \psi_\gamma \rangle \langle \psi_\gamma | U|\psi_\alpha\rangle e^{-(\lambda + \beta) \epsilon_\alpha} \]
\[ = \text{Tr} \left[ U^\dagger e^{\lambda H_1} U e^{-(\lambda + \beta) H_1} \right] \] (10)

The fluctuation theorem can be proved very simply. Firstly, let us prove the following KMS-like relation. Let \( D \) be any real symmetric operator. Then:

\[ Q_D(\lambda) = \text{Tr} \left[ U^\dagger e^{\lambda D} U e^{-(\lambda + \beta) D} \right] = \text{Tr} \left[ U^\dagger e^{-(\lambda + \beta) D} U e^{\lambda D} \right] \]
\[ = Q_D(-\lambda^* - \beta)^* = Q_D(-\lambda - \beta) \] (11)
where we have used transposition, cyclic permutation and Eq. (3). Putting $D = H_1$, this is a form of the fluctuation theorem for $Q(\lambda) = Q_D(\lambda)$.

In order to see what the implications of (11) are for $P(e)$ we shall need to show that $Q(\lambda)$ is analytic on the stripe $-\beta \leq \text{Re}(\lambda) \leq 0$. To do this, we use the fact that:

$$|\text{Tr}AB|^2 \leq 2 (\text{Tr}AA^\dagger) (\text{Tr}BB^\dagger)$$

(12)

Putting $A = U^\dagger e^{\lambda H_1}$ and $B = U e^{-(\lambda + \beta) H_1}$:

$$|Q(\lambda)|^2 \leq 2 \left( \text{Tr} e^{2 \{\text{Re}(\lambda) + \beta\} H_1} \right) \left( \text{Tr} e^{2 \text{Re}(\lambda) H_1} \right)$$

(13)

Because the partition function (5) converges for positive temperatures, neither factor diverges if $-\beta < \text{Re}(\lambda) < 0$.

Inserting (11) with $D = H_1$ in (9), the analyticity result allows us to shift the integration from $\text{Re}(\lambda) = 0$ to $\text{Re}(\lambda) = -\beta$, and we get:

$$P(e) = P(-e)e^{\beta\epsilon}$$

(14)

This is the fluctuation theorem for the probability of energy changes in an isolated system. Note that we could have obtained this result directly, without writing the KMS equation, by using the (time-reversal) symmetry of $U$ (equation (3)) in (8).

Taking the expectation value of $e^{-\beta\epsilon}$ over an integer number of cycles, one obtains a quantum version of a Jarzynski work formula [11]:

$$\overline{e^{-\beta\epsilon}} = \int deP(e)e^{-\beta\epsilon} = \int deP(-e) = 1$$

(15)

where the overline denotes average over quantum amplitudes and initial conditions. This is a rather surprising model-independent result, which we can rewrite as:

$$0 = -\frac{1}{\beta} \ln \overline{e^{-\beta\epsilon}} \leq -\frac{1}{\beta} \ln \overline{e^{-\beta\epsilon}} = \overline{\epsilon}$$

(16)

We obtain the second principle, arising as the familiar inequality

$$\text{annealed average} \leq \text{quenched average}$$

(17)

with the initial conditions playing the role of disorder.
**Generalisation and Thermostated systems**

In the most physical setting, we have a system in contact with a bath. The bath can be modeled for example with an infinite set of harmonic oscillators coupled to each variable in the system. Consider for simplicity the case of one system variable:

\[ H(x, p_x, y_1, p_1, ..., y_M, p_M) = H_{\text{system}} + H_{\text{int}} + H_{\text{bath}} \]  

with:

\[ H_{\text{bath}} = \sum_i \left( \frac{p_i^2}{2m} + m\omega_i^2 y_i^2 \right) \]  

\[ H_{\text{int}} = \sum_i C_i y_i x \]  

and, say:

\[ H_{\text{system}} = \frac{p_x^2}{2m_x} + V(x, t) \]  

(The interested reader will find an extensive literature on this implementation of heat baths in [15] and references therein.)

We can define the following bases of eigenvalues:

\[ H_{\text{bath}} |\chi_\alpha\rangle = \varepsilon_\alpha |\chi_\alpha\rangle \]

\[ O_{\text{system}} |\psi_{\alpha'}\rangle = o_{\alpha'} |\psi_{\alpha'}\rangle \]  

\( O \) is any real symmetric operator corresponding to an observable depending *exclusively* on the system variables, with a spectrum bounded from below (e.g. \( H_{\text{system}}(t_i) \)). The wavefunctions \( |\chi_\alpha\rangle \) and \( |\psi_{\alpha'}\rangle \) depend only on bath and system variables, respectively.

We consider an initial condition with no correlations between bath and system constructed as follows:

- We choose a bath wavefunction \( |\chi_\alpha\rangle \) with canonical probability \( \propto e^{-\beta \varepsilon_\alpha} \).
- We choose a system wavefunction \( |\psi_{\alpha'}\rangle \) with probability \( p_{\alpha'} \propto e^{-\beta o_{\alpha'}} \). This distribution is quite general, given the freedom of choice of \( O \). It could be for example a canonical distribution at higher temperature (\( O = \frac{\beta'}{\beta} H_1 \)), as resulting from a temperature quench.
• We start with the initial state $|\chi_{\alpha}\rangle \otimes |\psi_{\alpha'}\rangle$ and let it evolve.

• We measure

$$D \equiv H_{\text{bath}} + O$$

at the beginning and at the end, and record the difference. Note that at this stage the operator $O$ which we are measuring is forced by the initial condition we are choosing.

It is now easy to prove that the fluctuation formula (14) holds, with $e$ measuring the difference in value of bath energy plus observed value of $O$. To do this one uses (11) with $D$ as in (23). In order to guarantee the analyticity of $Q_{D}$, one must assure that (see argument leading to (13))

$$\text{Tr} \left[ e^{-2\{\text{Re}(\lambda)+\beta\}D} \right] = \text{Tr} \left[ e^{-2\{\text{Re}(\lambda)+\beta\}H_{\text{bath}}} \right] \times \text{Tr} \left[ e^{-2\{\text{Re}(\lambda)+\beta\}O} \right] < \infty$$

(24)

and

$$\text{Tr} \left[ e^{2\text{Re}(\lambda)D} \right] = \text{Tr} \left[ e^{2\text{Re}(\lambda)H_{\text{bath}}} \right] \text{Tr} \left[ e^{2\text{Re}(\lambda)O} \right] < \infty$$

(25)

for $-\beta < \text{Re}(\lambda) < 0$. The traces over the bath variables are bounded, since they correspond to the bath partition function. For the initial probabilities of the system, these conditions require that:

$$\text{Tr} \left[ e^{-2\beta\mu O} \right] \propto \sum_{\alpha} p_{\alpha}^{2\mu}$$

(26)

is finite for $0 < \mu < 1$, a condition we assume.

We are now in a position of discussing a general system in contact with a an infinite heat bath after many cycles have elapsed ($t_f - t_i \rightarrow \infty$). If we have that, under these circumstances:

i) The expected value of $O$ — a property of the system — stays finite as $t_f$ grows.

ii) The bath receives by virtue of the time-dependent forces an energy proportional to the number of cycles $e = (t_f - t_i)e_o + e_1$, with $e_1$ finite and and $e_o$ independent of the initial configuration.

Then, the derivation above of the fluctuation theorem carries over for long times to any initial distribution and to leading order in $t_f - t_i$, equation (14) will be a statement about the probability distribution of the energy $e_o$ the bath received, i.e. its entropy increase (17). Measuring the
fluctuation formula in a concrete situation becomes then a test for a property of the ‘stationary’ (i.e. periodical) asymptotic quantum state.

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[17] Note that whenever we invoke the limit of large time-differences, we understand it as taken after the limit of large heat bath size $M$. 