A fluctuation theorem for Floquet quantum master equations

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Abstract

We present a fluctuation theorem for Floquet quantum master equations. This is a detailed version of the famous Gallavotti–Cohen theorem. In contrast to the latter theorem, which involves the probability distribution of the total heat current, the former involves the joint probability distribution of positive and negative heat currents and can be used to derive the latter. A quantum two-level system driven by a periodic external field is used to verify this result.

Keywords: Floquet quantum master equations, Gallavotti–Cohen fluctuation theorem, large deviation principle, positive and negative heat currents

1. Introduction

The Gallavotti–Cohen (GC) fluctuation theorem states that the ratio of the probability distribution $p(\sigma)$ of having an average total entropy production rate $\sigma$ to that of having $-\sigma$ approaches $\exp(\sigma)$ as the time interval $t$ increases; that is,

$$\frac{p(\sigma)}{p(-\sigma)} \sim \exp(\sigma),$$

(1)

where the Boltzmann constant $k_B$ is set to 1 throughout this paper, and the symbol $\propto$ denotes asymptotic change as $t \to \infty$ [1]. The original GC fluctuation theorem was inspired by a relationship between the probabilities of fluctuations in the shear stress of fluids in nonequilibrium steady states [2] and was proved in modern dynamical system theory [3, 4]. Complicated techniques were used; see the latest review [5]. In contrast, its proof in stochastic systems, e.g. in classical Langevin systems or discrete jump systems, is simple [6–9]. Hence, stochastic dynamical systems are suitable to explore new fluctuation theorems.

The motivation of this paper is as follows. Let us imagine that a system contacts a heat bath having an inverse temperature $\beta$ and is in a nonequilibrium steady state due to some external force. The GC theorem can be reexpressed in terms of the probability distribution of the total heat current $j$, the total released heat averaged over the time interval $t$. Then, the exponent on the right-hand side of equation (1) is replaced by $t/\beta j$. We know that the total heat is composed of positive and negative parts. Accordingly, the total heat current $j$ can be divided into $j_+$ and $j_-$. Apparently, the individual current does not satisfy the GC fluctuation theorem. However, is the same true of the joined currents? Here, a positive answer is presented for the driven quantum systems described by Floquet quantum master equations [10–14].

The rest of this paper is organized as follows. In section 2, we review the Floquet quantum master equation and its stochastic thermodynamics. In section 3, we prove a fluctuation theorem. In section 4, a two-level quantum system is used to concretely verify this theorem. Section 5 concludes the paper.

2. Floquet quantum master equation and its stochastic thermodynamics

Given the Hamiltonian of a quantum system driven by periodic external forces, denoted as $H(t)$, we have

$$H(t + T) = H(t),$$

(2)

where $T = 2\pi/\Omega$ is the periodicity and $\Omega$ is the driving frequency. According to the Floquet theorem [15, 16], this periodic Hamiltonian satisfies an eigenvalue equation:

$$\langle H(t) - i\partial_t |u_n(t)\rangle = e_n|u_n(t)|,$$

(3)
where \( \epsilon_n \) and \(|u_n(t)|^2\) (\( n = 1, \cdots, N \)) are quasi-energies and Floquet bases, respectively, and we set \( h = 1 \). Note that the Floquet bases are orthonormal and periodic. In addition, we emphasize that these quasi-energies are restricted in a zone with a size of \( \Omega \). The heat bath that interacts with the quantum system has an inverse temperature \( \beta \). Under the weak system-bath coupling conditions and time scale separation assumptions, the evolution of the reduced density matrix of the quantum system \( \rho(t) \) can be described by the Floquet quantum master equation [10, 17, 18]:

\[
\partial_t \rho(t) = -i[H(t), \rho(t)] + D(t)[\rho(t)].
\]

(4)

The \( D \)-term represents the dissipation induced by the interaction between the system and the heat bath and is

\[
D(t)[\rho] = \sum_{\omega} r(\omega) \left[ A(\omega, t) \rho A^\dagger(\omega, t) - \frac{1}{2} \{ A(\omega, t) A(\omega, t), \rho \} \right].
\]

(5)

In the above equation, \( \omega \) are Bohr frequencies and are equal to \( \epsilon_n - \epsilon_m + q \Omega \), where \( q \) is a certain integer. The numbers may be positive or negative but always appear in pairs. Additionally, in the same equation, \( A(\omega, t) \) and \( A^\dagger(\omega, t) \) are called the Lindblad operators and are related by

\[
A(-\omega, t) = A^\dagger(\omega, t).
\]

(6)

The interaction operator of the quantum system and the heat bath is given as \( A \otimes B \), where \( A \) and \( B \) are the system and heat bath components, respectively. These Lindblad operators are obtained by performing a Fourier-like expansion of the interaction-picture operator of \( A \) [17]:

\[
A(\omega, t) = \sum_{m,n,q} \delta_{\omega, \epsilon_m - \epsilon_n + q \Omega} \langle \langle u_m | A | u_n \rangle \rangle_q |u_m(t)\rangle \langle u_n(t)| e^{-i \lambda t},
\]

(7)

where \( \delta \) is the Kronecker symbol, and the time-independent coefficient \( \langle \langle u_m | A | u_n \rangle \rangle_q \) is the \( q \)th harmonic of the transition amplitude \( \langle u_m(t) | A | u_n(t) \rangle \); that is,

\[
\langle \langle u_m | A | u_n \rangle \rangle_q = \frac{1}{T} \int_0^T \langle u_m(t) | A | u_n(t) \rangle e^{i \omega t} dt.
\]

(8)

The last ingredient of the Floquet quantum master equation is the assumption that the heat bath is always in a thermal state. Then, \( r(\omega) \), the Fourier transformation of the correlation function of the operator \( B \), satisfies the important Kubo–Martin–Schwinger condition [19, 20]:

\[
r(-\omega) = r(\omega) e^{-\beta \omega}.
\]

(9)

Stochastic thermodynamics can be established for the Floquet quantum master equation [14, 21, 22]. Roughly, equation (4) is unraveled into the dynamics of individual quantum systems [23–26]. The evolution of each system is composed of a continuous process alternating with discrete random jumps. Assume that these jumps occur at time points \( t_i \) (\( i = 1, \cdots \)). Each jump indicates that a quantum \( \omega_i \) is released to the heat bath [21, 22, 27–31]. The subscript \( i \) represents the time points of these energy exchanges. When the evolution of a quantum system ends at time \( t \), a quantum jump trajectory is generated and marked as \( \bar{\omega} = \{ \omega_1, \cdots \} \). If the density matrices of these individual quantum systems are \( \tilde{\rho}(\omega, t) \), their average weighted by the probabilities of all possible quantum jump trajectories is just the reduced density matrix \( \rho(t) \) of equation (4). From a thermodynamic point of view, the quanta are the heat released to the heat bath. Hence, given a quantum jump trajectory \( \bar{\omega} \), we define the total heat along it as

\[
Q(\bar{\omega}) = \sum_{i=1}^{\infty} \omega_i = Q_+(\bar{\omega}) + Q_-(\bar{\omega}).
\]

(10)

In the second equation, we specifically define the positive and negative heat, \( Q_+(\bar{\omega}) \) and \( Q_-(\bar{\omega}) \), respectively; clearly, they are simply equal to the sums of positive and negative Bohr frequencies.

3. A fluctuation theorem

Because the occurrences of quantum jump trajectories and time points of quantum jumps are random events, all three types of heat are stochastic quantities. Let the joint probability distribution of the positive and negative heat, \( Q_+ \) and \( Q_- \), respectively, be \( p(Q_+, Q_-) \). We can construct its histogram by directly simulating quantum jump trajectories [21, 22]. Because we are interested in the statistics over long time limits, a more practical approach is to compute its moment generation function,

\[
\Phi(\chi_+, \chi_-) = \int dQ_+ dQ_- p(Q_+, Q_-) e^{\chi_+ Q_+ + \chi_- Q_-} = \text{Tr}[\hat{\rho}(t)].
\]

(11)

We introduce a characteristic operator \( \hat{\rho}(t) \) in the second equation above and find that it satisfies an evolution equation:

\[
\partial_t \hat{\rho}(t) = -i[H(t), \hat{\rho}] + D(t, \chi_+, \chi_-)[\hat{\rho}(t)],
\]

(12)

where the super-operator

\[
D(t, \chi_+, \chi_-)[\hat{\rho}]
\]

is

\[
\begin{align*}
\sum_{\omega > 0} r(\omega) &\left[ e^{i \chi_+ \omega} A(\omega, t) \hat{\rho} A^\dagger(\omega, t) - \frac{1}{2} \{ A(\omega, t) A(\omega, t), \hat{\rho} \} \right] \\
\sum_{\omega < 0} r(\omega) &\left[ e^{i \chi_- \omega} A(\omega, t) \hat{\rho} A^\dagger(\omega, t) - \frac{1}{2} \{ A(\omega, t) A(\omega, t), \hat{\rho} \} \right]
\end{align*}
\]

(13)

If \( \chi_+ = 0 \), equation (13) reduces to equation (4). This result comes from a simple extension of the previous equation (equation (19) in [21]), which concerned the moment-generating function of the total heat, and we can reobtain it by letting \( \chi_+ = \chi_- \) in equation (13). Because the derivation is the same, we do not repeat it here.

The abstract equation (12) is not the most convenient to use in analyses. According to equation (11), \( \Phi(\chi_+, \chi_-) \) is equal to a sum of diagonal elements of \( \hat{\rho}(t) \). Hence, we write
the evolution equations for $P_n(t) = \langle u_n(t)|\hat{\rho}(t)|u_n(t)\rangle$ in the Floquet bases:

$$\frac{d}{dt} P(t) = R(\chi_+, \chi_-)P(t),$$

(14)

where the vectors $P(t) = (P_1(t), \cdots, P_n(t))^T$ and $R$ represents the transpose, the nondiagonal elements of the $R$-matrix are

$$[R(\chi_+, \chi_-)]_{mn} = \sum_{\omega > 0} e^{\gamma_+ r(\omega)} \langle u_n(t)|A(\omega, t)|u_m(t)\rangle^2$$

$$+ \sum_{\omega < 0} e^{\gamma_- r(\omega)} \langle u_n(t)|A(\omega, t)|u_m(t)\rangle^2,$$

(15)

$$m\neq n), and the diagonal elements are

$$[R(\chi_+, \chi_-)]_{nn} = \sum_{\omega > 0} e^{\gamma_+ r(\omega)} \langle u_n(t)|A(\omega, t)|u_n(t)\rangle^2$$

$$+ \sum_{\omega < 0} e^{\gamma_- r(\omega)} \langle u_n(t)|A(\omega, t)|u_n(t)\rangle^2$$

$$- \sum_{\omega} r(\omega) \sum_m \langle u_m(t)|A(\omega, t)|u_n(t)\rangle^2.$$ (16)

Note that equation (7) reminds us that $R(\lambda_+ , \lambda_-)$ is in fact a constant matrix. We can easily prove that this matrix possesses symmetry:

$$[R(\chi_+, \chi_-)]^T = R(-\beta - \chi_+, -\beta - \chi_+).$$

(17)

Using this property, we obtain a fluctuation theorem by simply following a standard procedure, e.g. that presented by Lebowitz and Spohn [7]. First, because the transpose matrix has the same eigenvalues as the original matrix, equation (17) implies that the scaled cumulant generating function $[1]$, $\phi(\chi_+, \chi_-)$, or the maximal eigenvalue of the $R$-matrix has the same symmetry:

$$\phi(\chi_+, \chi_-) = \phi(-\beta - \chi_+, -\beta - \chi_+).$$

(18)

Given the large deviation function $I(j_+, j_-)$ of the distribution $p(j_+, j_-)$ for the positive heat current $j_+ = Q_+/t$ and the negative heat current $j_- = Q_-/t$, and because the function is a Legendre transform of the scaled cumulant generating function, equation (18) immediately leads to

$$I(j_+, j_-) = I(-j_-, -j_+) - \beta(j_+ + j_-).$$

(19)

Then, the probability distribution for these two heat currents satisfies the fluctuation theorem

$$p(j_+, j_-) = e^{\beta(j_+ + j_-)}.$$ (20)

The conventional GC fluctuation theorem (1) can be easily derived from equation (20).

Fluctuation theorem (20) has a time-reversal explanation. Analogous to that of classical stochastic processes [7], the ratio of the probability distribution $P[\tilde{\omega}]$ of observing a quantum jump trajectory $\tilde{\omega} = \{\omega_1, \cdots, \omega_m\}$ to $P[\omega]$ of observing its reversed trajectory $\omega = \{-\omega_m, \cdots, -\omega_1\}$ approaches $\exp(\beta Q[\omega])$ as the time interval $t$ increases [22]. Note that not only is the time order of the quantum jumps reversed in the reversed trajectory, but the signs of these Bohr frequencies are reversed, we obtain $Q_\omega[\tilde{\omega}] = -Q_\omega[\omega]$ and

$$p(j_+, j_-) = \int D\tilde{\omega} \delta(Q_\omega[\tilde{\omega}] - Q_\omega) \times \delta(Q_\omega[\omega] - Q_\omega) \times \delta(Q_\omega[\omega] + Q_\omega)$$

$$= e^{\beta(j_+ + j_-)}.$$ (21)

Some unimportant constants are ignored here. This rough proof explains why the positions of $j_+$ and $j_-$ in the probability distribution on the right-hand side are exchanged and minus signs are added simultaneously; they are just the consequences of the time-reversal. Equations (19) and (20) are the central results of this paper. In the next section, we use a two-level quantum system to concretely show these results.

4. Two-level quantum system

Consider the Hamiltonian of a two-level quantum system [12–15, 17, 32]

$$H(t) = \frac{1}{2} \omega_0 \sigma_z + \frac{1}{2} \Omega_\theta (\sigma_z e^{-i\theta t} + \sigma_x e^{i\theta t}),$$

(22)

where $\omega_0$ is the transition frequency of the bare system, $\Omega_\theta$ is the Rabi frequency, and $\Omega$ is the frequency of the periodic external field. The Floquet bases and the quasi-energies of this system are

$$|u_\pm(t)\rangle = \frac{1}{\sqrt{2\Omega'}} \left( \pm \sqrt{\Omega' \pm \frac{\delta}{2\Omega'}} \right).$$

(23)

and $\epsilon_\pm = (\Omega \pm \Omega')/2$, respectively, where $\Omega' = \sqrt{\Omega^2 + \Omega_\theta^2}$ and the detuning parameter $\delta = \omega_0 - \Omega$. Here, we additionally set $\Omega > \Omega'$. Assume that the coupling between the two-level system and the heat bath is $\sigma_z$-coupling. There are six Lindblad operators, and the Bohr frequencies are $\pm \Omega$, $\pm (\Omega - \Omega')$, and $\pm (\Omega + \Omega')$. By performing some simple derivations, the $R$-matrix is obtained:

$$R_{11} = (e^{i\chi_0} - 1) \Gamma_0 + (e^{i\chi_0} - 1) \Gamma_0$$

$$= \Gamma_0(\Gamma_0 - \Omega + \gamma),$$

$$R_{12} = e^{i\chi_0} (\Omega - \Omega') \Gamma_0(\Omega - \Omega') + e^{i\chi_0} (\Omega + \Omega') \Gamma_0(\Omega + \Omega'),$$

$$R_{13} = e^{-i\chi_0} (\Omega - \Omega') \Gamma_0(\Omega - \Omega') + e^{-i\chi_0} (\Omega + \Omega') \Gamma_0(\Omega + \Omega'),$$

$$R_{14} = (e^{i\chi_0} - 1) \Gamma_0 + (e^{i\chi_0} - 1) \Gamma_0$$

$$= \Gamma_0(\Gamma_0 - \Omega + \gamma).$$

(24)
This observation reminds us that simply simulating quantum jump trajectories is not enough to solve the full large deviation function.

5. Conclusion

In this paper, we present a detailed GC fluctuation theorem for the quantum systems described by the Floquet quantum master equations. Although this theorem is proved for systems that interact with one heat bath, its generalization to the case of multiple heat baths is straightforward. For instance, for the case of two heat baths, we have [33]

$$\frac{p(j_1^+, j_2^+, j_1^-, j_2^-)}{p(-j_1^-, -j_2^-, j_1^+, j_2^+)} \propto e^{\delta \Omega (j_1^+ + j_1^-) + \delta \Omega (j_2^+ + j_2^-)},$$

where $j_1^+$ and $j_1^-$ are the positive and negative heat currents of the quantum system released to the heat bath with the inverse temperature $\beta_k$ ($k = 1, 2$). Finally, if a quantum system contacts two heat baths at two different temperatures and can be described by a Lindblad quantum master equation, the system is able to evolve into a nonequilibrium steady state without external driving fields. In such a situation, by carrying out the same argument presented here, we can prove that the fluctuation theorem (28) is still true.

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