Quantum fluctuation theorem: Can we go from micro to meso?

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Abstract
Quantum extensions of the Gallavotti-Cohen fluctuation theorem (FT) for the entropy production have been discussed by several authors. There is a practical gap between microscopic forms of FT and mesoscopic (i.e. not purely Hamiltonian) forms for open systems. In a microscopic setup, it is easy to state and to prove FT. In a mesoscopic setup, it is difficult to identify fluctuations of the entropy production. (This difficulty is absent in the classical case.) We discuss a particular mesoscopic model: a Lindblad master equation, in which we state FT and, more importantly, connect it rigorously with the underlying microscopic FT. We also remark that FT is satisfied by the Lesovik-Levitov formula for statistics of charge transport.

1. Introduction

A goal of nonequilibrium statistical mechanics is to make good, yet simple, models of complicated phenomena out of equilibrium and to analyze them. Such models should answer correctly questions like: “What is the structure of an object’s state that is kept between two heat reservoirs at different temperatures? How does it look like locally and how does it fluctuate?” or “When and how does a liquid flow become turbulent?”. In equilibrium, we have a good and simple guiding rule for making dynamical models: detailed balance. Surely, any nonequilibrium dynamics should break detailed balance, but can one formulate a general rule as to how to fix this detailed balance breaking?

It is here that the celebrated Gallavotti-Cohen fluctuation theorem (FT) (see [18,19,20]) for the entropy production comes into the picture. It turns out that there is such a general rule and it reads (for every path $\sigma$ of the dynamics, with corresponding probability $\text{Prob}[\sigma]$)

$$\log \frac{\text{Prob}[\sigma]}{\text{Prob}[\theta \sigma]} = \text{Entropy production along } \sigma + o(t)$$

(1)

where $\theta \sigma$ is the time reversed path $\sigma$. The FT itself

$$\log \frac{\text{Prob}[\text{Entropy production up to time } t \text{ equals } st]}{\text{Prob}[\text{Entropy production up to time } t \text{ equals } -st]} = st + o(t)$$

(2)

is an immediate consequence of the above rule (1). The LHS are expected to be linear in time $t$, the $o(t)$ term vanishes after dividing by $t$ and taking $t \uparrow \infty$. See [29] for a discussion focusing on the universality of (1).

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For our purposes, it is good to emphasize that there are two reasons to appreciate (1,2), even if those reasons are obviously intimately related:

(I) Formulas (1) and (2) can be derived on a microscopic level, starting with Hamiltonian dynamics, using its time-reversibility and identifying entropy production as the log of phase space volume. This was outlined in [30].

(II) The rules (1) and (2) do apply to a lot of effective (not purely Hamiltonian) or mesoscopic models. It is actually in effective models that the FT was observed and that it is studied most often. In [18,19,20], one treats thermostatted systems, while in e.g. [25,26,11], as well as in most later publications, one deals with stochastic models.

Note that (II) does morally, but not exactly follow from (I) since mesoscopic or effective models are merely good approximations of the Hamiltonian microscopic dynamics.

This article is concerned with the question how rules (1) and (2) extend to quantum mechanics. On the microscopic level (cfr. (I) above), there is an obvious problem with deriving (1); quantum mechanics does not have the concept of paths with associated pathwise entropy production. However, (2) still makes sense and in fact it remains true, as was pointed out in [22,24,38,35] and as we review in a streamlined version in Section 2.

As to the status of quantum FT in effective or mesoscopic models (cfr. (II)), the majority of research has focused on master equations for small systems (see recently [28]). A very explicit discussion can be found in [36], a simplified version of which is presented in Section 3.3. The ideas developed there are also implicit in [35] and [33].

The fact that not more effective or mesoscopic models have been investigated is perhaps not too surprising. With the possible exception of the master equations discussed in Section 3, there are not much Markovian models of open quantum systems which are healthy in all respects. One frequent pathology is the appearance of nonpositive density matrices. A review of this problem and a list of possible approaches is given in [12]. We should mention that these problems are not inherent to nonequilibrium models. Already the notion of detailed balance is somehow problematic for Markovian quantum models since the existing definitions [2,3] are so restrictive that the master equation in Section 3 is essentially the sole example.

Moreover, even if one has a trustworthy model, there still remains to identify the fluctuating entropy production. It should be clear from Section 3 and Remark 1 in Section 3.3 that this is not trivial.

We remark hence that in quantum mechanics, there is a practical gap between (I) and (II). This might be disconcerting, but possibly it also offers opportunities; perhaps one can improve upon some models of open quantum systems by imposing FT.

In the case of master equations which we treat in this article, not only (2) holds but there is also a convenient framework to state (1). This framework is the formalism of unraveling of master equations. Our results imply that these unravelings are rigorously linked to fluctuations of currents. This is discussed extensively in [16].

1.1. Brief summary

In Section 2, we review and sharpen the Hamiltonian approach to the FT. In Section 2.3, we give an example of a known counting formula in mesoscopic physics which satisfies FT. We introduce the master equation describing a small system in contact with different heat baths in Section 3 and we develop the necessary tools (unravelings) to identify the entropy production. Finally, in Section 4, we connect the master equation with the Hamiltonian approach and we show that fluctuations of the entropy production in the Hamiltonian model converge to fluctuations calculated by means of unravelings. The importance of this result is:

1) It shows that the FT is valid in the thermodynamic limit (at least in the weak coupling limit).
2) It rigorously justifies the technique of unravelings, which is quite popular in quantum optics.

2. The Quantum fluctuation Theorem

To fix thoughts, we introduce a model and corresponding notation. Imagine several heat reservoirs indexed by \( k \in K \) and modeled by Hilbert spaces \( \mathcal{H}_k \) and self-adjoint Hamiltonians \( H_k \) on \( \mathcal{H}_k \). Each reservoir is in thermal equilibrium at inverse temperature \( \beta_k \). One connects all heat reservoirs with a small system \( S \), modeled by a finite-dimensional Hilbert space \( \mathcal{H}_S \) and a self-adjoint Hamiltonian \( H_S \). The connection between \( S \) and reservoir \( k \)
is through a self-adjoint coupling term $H^\lambda_{\mathcal{S} \otimes \mathcal{K}}$ on $\mathcal{H}_S \otimes \mathcal{H}_k$. The coupling is controlled by a factor $\lambda$ and the total Hamiltonian is

$$
H_\lambda = H_S + \sum_k H_k + \lambda \sum_k H^1_{\mathcal{S} \otimes \mathcal{K}}
$$

(3)

The dynamics of the full system is given by the unitary group $U^\lambda_t = e^{-itH_\lambda}$ on the Hilbert space $\mathcal{H} := \mathcal{H}_S \otimes (\otimes_k \mathcal{H}_k)$. The initial state $\rho_0$ is a product state on $\mathcal{H}$

$$
\rho_0 = \rho_0 \otimes \left( \bigotimes_k \rho_k, \beta_k \right)
$$

(4)

where the states $\rho_k, \beta_k$ are equilibrium states on $\mathcal{H}_k$ with respect to the Hamiltonians $H_k$ at inverse temperatures $\beta_k$ and $\rho_0$ is an arbitrary density matrix on $\mathcal{H}_S$.

In the thermodynamical limit, the states $\rho_k, \beta_k$ are no longer density matrices and one needs the machinery of operator algebras, see e.g. [7,14], to define these states properly. We will completely ignore this problem (since its solution belongs to standard knowledge in mathematical physics), and we avoid writing ill-defined expressions by using the notation

$$
\rho_k[A] := \text{Tr}[\rho_k A] \quad \text{with } A \text{ an operator and } \rho_k \text{ a density matrix on } \mathcal{H}_k
$$

(5)

The LHS can still be used when $\rho_k$ is no longer a density matrix, but instead a state in the sense of operator algebra. Note finally that models as (3) have received a lot of attention lately in mathematical physics. E.g. in [21] one proves the Green-Kubo relations and Onsager reciprocity in the spin-fermion model at finite $\lambda > 0$.

2.1. What do we mean by quantum fluctuations?

It is not a priori clear what one means by fluctuations of heat currents, or fluctuations of the entropy production. (See [5] for an elaboration on that question.)

One encounters at least three approaches (see however [5] for a different view),

1) Measure the energies $H_k$ in the beginning and at the end of the experiments and make statistics of the difference of both measurements. This approach yields the FT [35,22,24,37].

2) Calculate the fluctuations of the operator $U_1 H_k U_{-t} - H_k$. In [32], a deviation from the fluctuation theorem was established for the fluctuations of a related operator.

3) In [31], one studies the fluctuations of the relative modular operator - a $C^*$-algebraic concept. These fluctuations satisfy the FT, but the meaning of this relative modular operator is a priori unclear to us.

The advantage of the first approach is that it is more relevant in an experimental setup. A possible argument for the second would be that it seems better suited for taking the thermodynamic limit, since it avoids the measurements. However, by slightly reformulating the first approach, one can also meaningfully study the thermodynamical limit (see also [23]), as we point out now.

Assume for simplicity that the $H_k$ have discrete spectrum, indicating that we have not taken the thermodynamic limit and let $x \in X$ label a complete set of eigenvectors $x > 0$ of $(H_k)_{k \in K}$ with eigenvalues $(\mathcal{H}_k)_{k \in K}(x)$. Let the projectors $P_x$ stand for $1 \otimes \langle x \rvert x \rangle$ where 1 stands for identity on $\mathcal{H}_S$. The probability of measuring an entropy production $r$ is

$$
\mathbb{P}_{t,\lambda}(r) = \sum_{x,y \in X} \rho_0 \left[ P_x U^\lambda_{-t} P_y U^\lambda_t P_x \right]
$$

(6)

The idea behind the formula is clear: measure (thereby projecting on the eigenstates $x$), then switch on the time evolution $U^\lambda_t$, finally measure again (projecting on the eigenstates $y$). For later convenience, instead of studying the probability distribution $\mathbb{P}_{t,\lambda}(r)$, we focus on the Laplace transform.

$$
F(k, t, \lambda, \rho_0) := \int_\mathbb{R} d\mathbb{P}_{t,\lambda}(r) e^{-kr}
$$

(7)

In fact, the situation is even more complicated. For fermions, one can indeed find a subalgebra of $\mathcal{B}(\mathcal{H}_k)$ - the Weyl-$C^*$-algebra - on which the state $\rho_k, \beta_k$ can be appropriately defined. For bosons, one has to invoke $W^*$-algebra’s and the Araki-Woods representation to give rigorous meaning to the model.
which, in the case when $P_{t,\lambda}(r)$ is given by (6), reads

$$F(\kappa, t, \lambda, \rho_0) := \sum_{x,y \in X} \rho_0 \left[ P_x U_{\lambda,\kappa} P_y U_{\lambda,\kappa}^* P_x \right] e^{-\kappa} \sum_k \beta_k (H_k(y) - H_k(x))$$

(8)

We now use that the initial state $\rho_0$ is diagonal in the basis $|x>$ to rewrite (8) into

$$F(\kappa, t, \lambda, \rho_0) = \rho_0 \left[ U_{\lambda,\kappa}^* e^{-\kappa} \sum_k \beta_k H_k U_{\lambda,\kappa} e^{\kappa} \sum_k \beta_k H_k \right]$$

(9)

This last expression is perfectly suited for taking the thermodynamic limit, since it remains well-defined when the operators $H_k$ have continuous spectrum and the state $\rho_0$ is not given by a density matrix. (Which does not mean that the expression (9) is necessarily finite. After all, the physics could be such that the Laplace transform is infinite for some $\kappa$.)

2.2. Derivation of the quantum fluctuation theorem

If one defines the fluctuations through (9), FT is easily derived. Assume that the initial state $\rho_0$ is given by

$$\rho_0 = \frac{1}{d} \otimes \left[ \otimes_k \frac{e^{-\beta_k H_k}}{Z_k} \right], \quad Z_k := \text{Tr} e^{-\beta_k H_k}, \quad d := \dim \mathcal{H}_S,$$

(10)

hence the initial state on the small system is the trace state, or infinite temperature state. Assume further that the dynamics is reversible, i.e. there is an anti-unitary time-reversal involution $T$ which commutes with both the free and interacting Hamiltonians

$$[T, H_k] = 0 \quad [T, H_\lambda] = 0 \quad TT = 1 \quadTU_{\kappa}^* T = U_{\kappa}^\lambda$$

(11)

Abbreviating $W = \sum_k \beta_k H_k$, using the above relations and cyclicity of the trace, one calculates

$$F(\kappa, t, \lambda, \rho_0) = \text{Tr} \left[ e^{-W} TU_{\kappa}^\lambda TT e^{-\lambda W} TTU_{\kappa}^\lambda TT e^{\lambda W} \right] (d \prod_k Z_k)^{-1}$$

$$= \text{Tr} \left[ e^{-\lambda W} U_{\kappa}^\lambda e^{-(1-\kappa)W} U_{\kappa}^\lambda e^{(1-\kappa)W} \right] (d \prod_k Z_k)^{-1} = F(1 - \kappa, t, \lambda, \rho_0)$$

(12)

(13)

which is equivalent to (2) without the $o(t)$-correction term. The above derivation relies on a particular initial state for the small system. It is known as a transient FT. Obviously, for large $t$, one expects the initial state of the small system to be irrelevant and (2) follows under some additional ergodicity assumptions.

2.3. Example: counting statistics for charge transport

As argued in Section 1, it is interesting to investigate to what extent the fluctuation symmetry is actually present in known expressions for current statistics. We briefly discuss the Lesovik-Levitov formula [27] for electronic transport between leads. We base our treatment on a neat version of the formula presented in [23] wherein the electrons do not interact and the formula (16) can be derived without any approximation. It is also assumed that all Hilbert spaces are finite-dimensional (see [6] for a discussion of the thermodynamical limit).

Let $\mathfrak{h}$ be the Hilbert space of one electron. The presence of two leads is made explicit by splitting $\mathfrak{h} = \mathfrak{h}_1 \oplus \mathfrak{h}_2$ where the spaces $\mathfrak{h}_1, \mathfrak{h}_2$ contain all the states in respectively lead 1, 2. The projectors on $\mathfrak{h}_1, \mathfrak{h}_2$ are denoted $1_{\mathfrak{h}_1}, 1_{\mathfrak{h}_2}$ and the decoupled one-particle Hamiltonian is $H_1 \oplus H_2$. Let the inverse temperature be $\beta$ and let the leads have respective chemical potentials $\mu_1, \mu_2$. Let $n$ be the occupation number operator (dictated by Fermi-Dirac statistics)

$$n = \left( e^{\beta(H_1 - \mu_1 + 1)} + e^{\beta(H_2 - \mu_2 + 1)} \right)^{-1}$$

(14)

The contact between the leads is modeled by a scattering process with unitary scattering matrix $S$. We assume, that the scattering process conserves total energy and that both scattering process and decoupled evolution are reversible

$$[S, \mathfrak{h}_1 \oplus \mathfrak{h}_2] = 0 \quad TH_{1,2} = H_{1,2} \quad TST = S^*$$

(15)
for some anti-unitary operator $T$ modeling time-reversal.

At time $t = 0$ and $t = \tau$, one measures the total charge in, say, lead 1 (For simplicity, we set the charge to unity, so that ‘charge’ just means ‘number of particles’). Let $F(\kappa)$ be the laplace transform of the distribution of transported charge $F(\kappa) = \sum_{q=-\infty}^{\infty} p(q) e^{-\kappa q}$ where $p(q)$ is the probability to find at time $t = \tau$ an excess charge $q$, as compared to $t = 0$.

The Lesovik-Levitov formula reads (see [23], where the formula is given for the Fourier transform, hence for $\kappa \in i\mathbb{R}$):

$$F(\kappa) = \det (1 + n(S^* e^{-\kappa S_1} S e^{\kappa S_1} - 1))$$

The entropy production in this scenario is just $-\beta(\mu_1 - \mu_2) q$ and hence one expects that FT implies the following symmetry (cfr. (12-13))

$$F(-\kappa \beta(\mu_1 - \mu_2)) = F(-(1 - \kappa) \beta(\mu_1 - \mu_2))$$

That relation is easily verified by starting from (16), using (15) and the fact that $\det(AB) = \det(A)\det(B)$ for matrices $A, B$ (Recall that our one-fermion space is finite-dimensional).

3. A good effective model: the master equation

3.1. Construction of the master equation

Having in mind the Hamiltonian model introduced in Section 2, we can construct a master equation that approximates the evolution of a general density matrix $\rho_0$ on the small system $\mathcal{H}_S$. This master equation describes essentially two effects:

1) Decoherence: non-diagonal elements in the eigenbasis of $\mathcal{H}_S$ vanish

2) The fluctuations of the diagonal elements, which evolve independently of the off-diagonal elements.

In view of this behavior, we choose to restrict attention to diagonal elements. This allows for a less technical presentation, as we can replace the Lindblad master equation by a classical Markov process.

Let $e, e', \ldots$ be the eigenvalues of the system Hamiltonian $\mathcal{H}_S$ and let $P_e, P_{e'}, \ldots$ be the projectors on the corresponding eigenspaces which we assume one-dimensional.

Define transition probabilities for each separate $k \in K$ as

$$p_k(e, e') := \int_{\mathbb{R}} dt ~ e^{i(t' - t)} (1 \otimes \rho_k, \beta_k) \left[ e^{\mathcal{H} k} P_{e'} H_{\mathcal{S} - k}^1 P_k e^{-i \mathcal{H} k} \right]$$

where 1 is the (unnormalized) density matrix 1 on $\mathcal{H}_S$. The total transition probabilities are hence given as

$$p(e, e') = \sum_k p_k(e, e')$$

The information about the temperatures $\beta_k$ is encoded into the RHS of (18) through the state $\rho_k$ and in fact one can show

$$\text{Reservoir } k \text{ is at thermal equilibrium at } \beta_k \Rightarrow p_k(e, e') / p_k(e', e) = e^{\beta_k (e - e')}$$

As said, the density matrix of the system is diagonal. We denote the time-dependent diagonal elements by $\mu_e(t)$. The (Pauli) master equation now reads

$$\frac{d\mu_e(t)}{dt} = \sum_{e'} (\mu_{e'}(t) p(e', e) - \mu_e(t) p(e, e'))$$

That is, if we assume $\mathcal{H}_S$ to be nondegenerate. If it is degenerate, the picture is slightly more complicated but the results still hold, see [36].
3.2. Derivation of the master equation

The only information missing is in what sense this master equation (21) approximates the true dynamics generated by (3). Physically, one needs to perform the Born-Markov approximation and the rotating wave approximation, on which we will not comment here (see instead [4,8]). Mathematically, one can make the convergence generated by (3). Physically, one needs to perform the Born-Markov approximation and the rotating wave approximation in Section 4, is

\[
\mu^\lambda(t) = \text{Tr}_R \left[ U_t^\lambda \mu_0 \otimes [\otimes_k \rho_{k,\beta_k}] \right] U_{-t}^\lambda
\]

(22)

where Tr\_R is a conditional expectation. (If \( \rho \) is a state on \( \mathcal{H}_S \otimes \mathcal{H}_R \), then \( \text{Tr}_R \rho \) is a state on \( \mathcal{H}_S \) such that for any operator \( A \) on \( \mathcal{H}_S \): \( \rho(A) = (\text{Tr}_R \rho)(A) \). If \( \rho \) is a density matrix, then \( \text{Tr}_R \) is just the partial trace over the reservoirs.) The statement, rigorously proven in [13] under mild assumptions (about which we will be more explicit in Section 4), is

\[
P_{\lambda} \mu^\lambda(\lambda^{-2}) P_{\lambda} \xrightarrow{\lambda \to 0} \mu_e(t)
\]

(23)

As is clear from the scaling and the expression (18), the master equation emerges in second-order perturbation theory. Hence we require that \( \text{Tr}_R (H_{S\beta_k}) = 0 \) such that the first order term perturbation term vanishes (which can always be achieved by redefining \( H_S \)).

3.3. Guessing path-wise entropy production

Given the very suggestive form of the transition probabilities (18), one is inclined to supplement the master equation in the following way: The paths \( \sigma \) of the markov process defined by formula (21) are sequences of energy levels \( e_i \), with transition times \( t_i \) (jump from \( e_{i-1} \) to \( e_i \)) with \( P^e_{\sigma_0} \) the path probabilities up to time \( t \)

\[
\sigma = (e_0; t_1, e_1; t_2, e_2; \ldots; t_n, e_n)
\]

\[
P^e_{\sigma_0}(\sigma) = e^{-\lambda_0 t_1} p(e_0, e_1) e^{-\lambda_1 (t_2-t_1)} \ldots p(e_{j-1}, e_j) e^{-\lambda_j (t-t_j)}
\]

(24)

where \( j \) is the highest index such that \( t_j < t \) and \( \lambda_k = \sum_{e'} p(e, e') \) are the escape rates. The subscript \( e_0 \) in \( P^e_{\sigma_0} \) indicates the the process has been started from \( e_0 \).

Clearly, to speak about currents and entropy production, we need more information; we need to know which bath \( k \) triggered the transition. Hence, we need a process with paths \( \tilde{\sigma} \) and probabilities \( \tilde{P}^e_{\sigma_0}(\tilde{\sigma}) \):

\[
\tilde{\sigma} = (e_0; t_1, k_1, e_1; t_2, k_2, e_2; \ldots; t_n, k_n, e_n)
\]

\[
\tilde{P}^e_{\sigma_0}(\tilde{\sigma}) = e^{-\lambda_0 t_1} p_{k_1}(e_0, e_1) e^{-\lambda_1 (t_2-t_1)} \ldots p_{k_j}(e_{j-1}, e_j) e^{-\lambda_j (t-t_j)}
\]

(25)

We simply define a new process corresponding to the pathspace measure (25). Remark that obviously,

\[
\sum_{\tilde{\sigma} \to \sigma} \tilde{P}^e_{\sigma_0}(\tilde{\sigma}) = P^e_{\sigma_0}(\sigma)
\]

(26)

where the sum is over all \( \tilde{\sigma} \) which reduce to \( \sigma \) by omitting all \( k_i \).

One can just as well calculate the matrix elements \( \mu_e(t) \) from the path probabilites \( \tilde{P} \) as from \( P \):

\[
\mu_e(t) = \sum_{\tilde{\sigma}, e_n(\tilde{\sigma}) = e} \tilde{P}^t_{\mu_0(0)}(\tilde{\sigma}) = \sum_{\sigma, e_n(\sigma) = e} P^t_{\mu_0(0)}(\sigma)
\]

(27)

where

\[
\tilde{P}^t_{\mu_0(0)} = \sum_{e_0} \mu_{e_0}(0) \tilde{P}^t_{e_0}, \quad P^t_{\mu_0(0)} = \sum_{e_0} \mu_{e_0}(0) P^t_{e_0}
\]

(28)

and with \( n(\tilde{\sigma}), n(\sigma) \) being the number of jumps in the paths \( \tilde{\sigma}, \sigma \). Hence, we have extended our pathspace probability measure \( P^t \) into a pathspace probability measure \( \tilde{P}^t \). In the theory of open quantum systems, one calls such an extension an unraveling and the paths \( \tilde{\sigma} \) are called quantum trajectories, see [9,8] for an overview and [10] for similar reasoning.
Having the pathspace probability measure \( \tilde{\mathcal{P}} \) at our disposal, we can do all the manipulations which are familiar from classical markov processes. The function on paths \( \tilde{\sigma} \)

\[
w^t(\tilde{\sigma}) = -\sum_{i=1}^{n} \beta_{k_i}(e_i - e_{i-1})
\]

which we identify as the path dependent entropy production, is equal to the ratio of probabilities of forward and backward paths;

\[
w^t(\tilde{\sigma}) = \log \left( \frac{d\tilde{\mathcal{P}}_{\mu}(\tilde{\sigma})}{d\mathcal{P}_{\mu}(\theta\tilde{\sigma})} \right) \quad \text{with} \quad \theta\tilde{\sigma} = (e_n; t - t_n, k_n, e_{n-1}; \ldots; t - t_2, k_2, e_2; t - t_1, k_1, e_0)
\]

as follows from (20). From (30), we retrieve the FT (2), or its Laplace-transformed version

\[
\log \int d\tilde{\mathcal{P}}_{\mu}(\tilde{\sigma}) e^{-\kappa w^t(\sigma)} = \log \int d\mathcal{P}_{\mu}(\tilde{\sigma}) e^{-(1-\kappa)w^t(\sigma) + o(t)}
\]

Obviously, one can push on and prove the Green-Kubo relations, Onsager reciprocity and strict positivity of the entropy production from (31). This is discussed at length in [36].

At this point, one should note that this unraveling and the construction of the pathspace measure \( \tilde{\mathcal{P}} \) was a product of our intuition. Hence, it not a priori clear whether the fluctuations of entropy production which we can calculate through formula (29) and the measure \( \tilde{\mathcal{P}} \) coincide with the entropy fluctuations in the original model. This problem motivates the following section.

**Remark 1** However intuitive the above reasoning, one should keep in mind that we have used more information than is contained in the bare master equation (21). In particular, we used (19). To put things even sharper: given a master equation without any additional information, one could associate to it baths in different ways, thereby obtaining completely different expressions for the entropy production.

### 4. Linking the microscopic fluctuations with the quantum trajectory fluctuations

The idea of this section is to justify the guesses in Section 3.3. We do this by connecting fluctuations of the entropy production in the Hamiltonian model, in expression (9) to the fluctuations calculated by the probability measure \( \tilde{\mathcal{P}}_{\mu} \). This connection is made sharp in the regime in which the master equation is derived, i.e. in the weak coupling limit. To be as concrete as possible, we make explicit the model which was outlined in the beginning of Section 2.

Let for each \( k \), \( \mathcal{H}_k \) be a fermionic Fock space, i.e.

\[
\mathcal{H}_k := \mathcal{C} \oplus L^2(\mathbb{R}^d) \oplus L^2(\mathbb{R}^d) \otimes \mathcal{C} \oplus L^2(\mathbb{R}^d) \oplus \ldots
\]

where the \( \otimes \) denotes the anti-symmetrized tensor product, which accounts for the fermion statistics. Let the Hamiltonian \( H_k \) describe free fermions with one-particle dispersion relations \( h_k(q) = h_k(|q|) \) where \( q \in \mathbb{R}^d \) is the momentum, i.e.

\[
H_k = \int_{\mathbb{R}^d} dq h_k(|q|) a_k^*(q) a_k(q)
\]

with \( a_k(q), a_k^*(q) \) creators/annihilators of fermions in reservoir \( k \) with momentum \( q \), that is

\[
\{ a_k(q), a_{k'}(q') \} = \delta_{k,k'} \delta(q - q')
\]

Let now the interaction \( H^I_{S-k} \) be given as

\[
H^I_{S-k} = \int_{\mathbb{R}^d} dq f_s(q) D_k \otimes a_k^*(q) + \bar{f}_s(q) D_k^* \otimes a_k(q)
\]

---

4 One could just as well take bosons here, but then formulas like (37) need more elaboration to get rigorous meaning, see also the footnote in the introduction to Section 2.
for some operators $D_k$ on $\mathcal{H}_S$ and coupling functions $f_k \in L^2(\mathbb{R}^d)$. The thermal states $\rho_{k, \beta\omega}$ on $\mathcal{H}_k$ are defined as quasi-free states determined by their two-point correlation function (determined by the Fermi-Dirac distribution)
\[ \rho_{k, \beta\omega}[a^* g a] = (g, (1 + e^{\beta\omega H_k})^{-1} g) \quad (36) \]

We recall the definition of $F(\kappa, t, \lambda, \rho_0)$ in (9) as the Laplace transform of the distribution of entropy production;
\[ F(\kappa, t, \lambda, \rho_0) = \rho_0 \left[ U_\lambda^{-t} e^{-\kappa \sum_k \beta_k H_k} U_\lambda^t e^{\kappa \sum_k \beta_k H_k} \right] \quad (37) \]

where again, as in (4), $\rho_0 = \rho_0 \otimes [\otimes_k \rho_{k, \beta\omega}]$ with $\mu_0$ an arbitrary density matrix on $\mathcal{H}_S$.
We can now state the main message of this paper.

5. Conclusion

We investigated the question of generalization of FT to quantum systems. We remarked in Section 2.2 that in a microscopic (=Hamiltonian) framework, one can unambiguously state FT. In practice, it is more common to
start from a mesoscopic (=effective, nonhamiltonian) description of an open quantum system. In Section 3.3, we discussed a very straightforward and successful approach for the dynamics given by a specific master equation; one can guess what are fluctuations of entropy production and one can state FT. Finally, in Section 4, we state the link between fluctuations of the entropy production, defined in the microscopic model in Section 2 and the fluctuations which are the result of the guess-work in Section 3, which hence turns out to be good guess-work.

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