Steady state fluctuations of the dissipated heat for a quantum stochastic model

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Abstract: We introduce a quantum stochastic dynamics for heat conduction. A multi-level subsystem is coupled to reservoirs at different temperatures. Energy quanta are detected in the reservoirs allowing the study of steady state fluctuations of the entropy dissipation. Our main result states a symmetry in its large deviation rate function.

KEY WORDS: entropy production, fluctuation theorem, quantum stochastic calculus

1 Introduction

Steady state statistical mechanics wants to construct and to characterize the stationary distribution of a subsystem in contact with several reservoirs. By nature the required scenario is an idealization as some essential specifications of the reservoirs must be kept constant. For example, intensive quantities such as temperature or (electro-)chemical potential of the different reservoirs are defined and unchanged for an extensive amount of time, ideally ad infinitum. Reservoirs do not interact directly with each other but only via the subsystem; they remain at their same spatial location and can be identified at all times. That does not mean that nothing happens to the reservoirs; flows of energy or matter reach them and they are like sinks and sources of currents that flow through the subsystem. Concrete realizations and models of steady states vary widely depending on the type of substances and on the nature of the driving mechanism.

An old and standard problem takes the subsystem as a solid in contact at its ends with two heat reservoirs and wants to investigate properties of the energy flow. Beloved by many is a classical model consisting of a chain or an array of coupled anharmonic oscillators connected to thermal noises at the boundaries. The reservoirs are there effectively modeled by Langevin forces while the bulk of the subsystem undergoes a Hamiltonian dynamics, see e.g. \textsuperscript{[RBT02, EPRB99, MNV03]}. Our model to be specified below is a quantum

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analogue of that scenario in the sense that we also consider a combination of Hamiltonian dynamics and Markovian thermal noises.

We imagine a chain of coupled two (or multi)-level systems. The dynamics of the isolated subsystem is unitary with Hamiltonian $H_S$. Quanta of energy $\omega$ are associated to the elementary transitions between energy levels. Two physical reservoirs at inverse temperatures $\beta_k, k = 1, 2$, are now attached to the subsystem. The total dynamics is described by a quantum stochastic differential equation through which we can observe the number $N_{\omega,k}$ of quanta with energy $\omega$ that are piled up in the $k$–th reservoir. The total energy $N := H_S + \sum_{\omega,k} \omega N_{\omega,k}$ is conserved under the dynamics (Proposition 2.13). The change in the second term corresponds to the flow of energy quanta in and out of the reservoirs and specifies the dissipated heat. Our main result consists in obtaining a symmetry in the fluctuations of that dissipated heat that extends the so called steady state fluctuation theorem for the entropy production to a quantum regime (Proposition 2.14).

The quantum stochastic evolution that defines the model is a particular dilation of a semigroup dynamics that describes the weak coupling regime of our subsystem coupled to quasi-free boson fields. The dilation, a sort of quantum Langevin equation, is much richer and enables the introduction of a natural path space measure. One should remember here that a major conceptual difficulty in coming to terms with the notion of a variable entropy production for quantum steady states is to understand its path-dependence. One option is to interrupt the unitary dynamics with collapses, see e.g. [CRJ+04]. Others have proposed an entropy production operator, avoiding the problem of path-dependence. Our set-up follows a procedure that is well-known in quantum optics with thermal noises formally replacing photon detectors, see [BGM04, BMK03]. In the resulting picture we record each energy quantum that is transferred between subsystem and reservoirs. It induces a stochastic process on quanta transferrals and there remains no problem to interpret the fluctuations of the entropy production. From the mathematical point of view, the model can be analyzed via standard probabilistic techniques.

1.1 Related results

In the past decade, a lot of interest has been going to the Gallavotti-Cohen fluctuation relation [GC95b, GC95a, ECM93], see [Mae03] for more recent references. In its simplest form that relation states that the steady state probability ($\text{Prob}$) of observing a total entropy decrease $w_T = -wT$ in a time $T$, is exponentially damped with respect to the probability of observing
an increase of $w_T$ as

$$\frac{\text{Prob}(w_T = wT)}{\text{Prob}(w_T = -wT)} \approx e^{+wT} \quad (1.1)$$

at least for very large time spans $T$. The relation (1.1) is known as the steady state fluctuation theorem (SSFT) and states a symmetry in the fluctuations of the entropy dissipation in a stationary nonequilibrium state. The symmetry was first discovered in the context of dynamical systems and was applied to the phase space contraction rate in strongly chaotic dynamical systems, see [Rue99, ECM93, GC95b, GC95a]. It was first further developed for stochastic dynamics in [Kur98, LS99, Mae99]. In the present paper, we deal with the SSFT for a quantum system. The steady state condition must however be understood in a physical sense; it is about heat conduction for fixed reservoirs in the long time limit. The small system is treated in the steady state of an approximate dynamics (the weak coupling limit) while the reservoirs are kept at a fixed temperature. Yet, mathematically, we are not quite dealing with a steady or stationary state. The true total dynamics for system plus reservoirs is in fact much more complicated. We still speak about the steady state (and the SSFT) also to contrast it with transient versions of the fluctuation symmetry (1.1), see also [GC99]. Transient fluctuation theorems (TFT) start typically from a change of variables at a finite time $t$, reversing so to say the evolution, see [SEC98], and can be obtained equally well for classical as for quantum systems. That is not at all what we are doing here. We truly concentrate on the stationary heat dissipation in the reservoirs, but from a technical point of view, one could argue that our set-up is actually a “transient model of a steady state”.

The basic underlying mechanism and general unifying principles connecting SSFT and TFT with statistical mechanical entropy have been explained in [MN03, Mae03].

Monnai and Tasaki [MT03b] have investigated an exactly solvable harmonic system and found quantum corrections to both SSFT and TFT. Matsui and Tasaki [MT03a] prove a quantum TFT in a general $C^*$-algebraic setting. It is however unclear what is the meaning of their entropy production operator.

A related quantum Jarzynski relation was studied in [RM04].

Besides the fluctuation theorem, we also describe a new approach to the study of heat conduction in the quantum weak coupling limit. In [LS78], Lebowitz and Spohn studied the thermodynamics of the weak-coupling generator. They identified the mean currents, and they proved a Green-Kubo relation. At that time it was however not yet possible to conclude that these expressions are the first non-zero contributions to their counterparts at finite
coupling $\lambda$. That has recently been shown in a series of papers by Jakšić and Pillet [JP96a, JP96b, JP02b, JP02a], who used spectral techniques to study the system at finite coupling $\lambda$. It was also shown that the stationary state of the weak coupling generator is the zeroth order contribution to the system part of the so called NESS, the nonequilibrium steady state. The current fluctuations we define in our model, agree with the expressions of [LS78] as far as the mean currents and the Green-Kubo formula is concerned. Our entropy production operator is however new; it differs for example from the proposal of [MT03a]. The approach taken here also differs from the more standard route that has been followed and that was outlined by Ruelle in [Rue00]. Recently and within that approach and context of heat conduction, new results have been obtained in [JP02b, JP02a, ASF05]. To us it remains however very much unclear how to define and study in that scenario a fluctuating entropy; in contrast, that is exactly one of the things we can easily achieve via our approach but we remain in the weak coupling limit.

1.2 Basic strategies

1.2.1 Microscopic approach

In general one would like to start from a microscopic quantum dynamics. The system is then represented by a finite-dimensional Hilbert space $\mathcal{H}$ and system Hamiltonian $H_S$. The environment is made from thermal reservoirs, indexed by $k \in K$, infinitely extended quantum mechanical systems, with formal Hamiltonian,

$$H_R := \sum_{k \in K} H_{R_k}$$

The coupling between system and reservoirs is local and via some bounded interaction term $\lambda H_{S-R}$ so that the total Hamiltonian takes the form

$$H_\lambda := H_S \otimes 1 + 1 \otimes H_R + \lambda \sum_{k \in K} V_k \otimes R_k$$

where we have already inserted a specific form for the coupling $H_{S-R}$ using self-adjoint reservoir operators $R_k$ and $V_k$ acting on respectively $\mathcal{H}_{R_k}$ and $\mathcal{H}$. On the same formal level, which can however easily be made precise, the total quantum dynamics is then just

$$U_t^\lambda := e^{-iH_\lambda t}$$

We will not follow the beautiful spectral or scattering approach that has recently been exploited for that nonequilibrium problem. We refer the reader
to the specialized references such as [JP02b] [Rue00] and we only outline the main steps, totally ignoring essential assumptions and technicalities:

One starts the dynamics from an initial state

\[ \mu := \rho_S \otimes \rho_{R_1} \otimes \ldots \otimes \rho_{R_K} \]

where \( \rho_S \) stands for an initial state in the system and the \( \rho_{R_k} \) are equilibrium KMS states at inverse temperature \( \beta_k \) for the \( k \)-th reservoir. The quantum dynamics takes that initial state to the new (now coupled) state \( \mu_t \) at time \( t > 0 \). The NESS is obtained via an ergodic average

\[ \mu_{\text{NESS}} := \lim_{T \to +\infty} \frac{1}{T} \int_0^T dt \mu_t \]

(1.2)

One of the first questions (and partially solved elsewhere, see e.g. [JP02b] [Rue00] [AS06]) is then to derive the natural conditions under which the mean entropy production rate

\[ \dot{S} := i \sum_{k=1}^m \beta_k \mu_{\text{NESS}}([H_\lambda, H_{R_k}]) \]

is strictly positive. While that mean entropy production certainly coincides with conventional wisdom, we do not however believe that the operator

\[ i[H_\lambda, H_{R_k}] \]

or equivalent fluctuations which would obey the SSFT. That is not even the case for the simplest (classical) stochastic dynamics; one needs to go to path space and study current fluctuations in terms of (fluctuating) trajectories.

1.2.2 Weak coupling approach

Starting from the microscopic dynamics above, we can of course always look at the reduced dynamics \( \Lambda^\lambda_t \) on the system

\[ \Lambda^\lambda_t \rho_S = \text{Tr}_R \left[ U^\lambda_t (\rho_S \otimes \rho_{R_1} \otimes \ldots \otimes \rho_{R_K}) U^\lambda_{-t} \right] \]

for a density matrix \( \rho_S \) on the system. Obviously, the microscopic evolution couples the system with the environment and the product form of the state will in general not be preserved. One can however attempt a Boltzmann-type Ansatz or projection technique to enforce a repeated randomization. That can be made rigorous in the so called weak coupling limit. For that, one
needs the interaction picture and one keeps $\lambda^2 t = \tau$ fixed. That is the Van
Hove-Davies-limit [Hov55, Dav74]

$$\lim_{\lambda \to 0} \Lambda^0_{\tau}, \Lambda^1_{t} \rho_S := e^{\tau L^*} \rho_S$$

where $L^*$ is a linear operator acting on density matrices for the system. The
generator will be written out more explicitly in Section 2.1 but its dual $L$
acting on $B(\mathcal{H})$ is of the form, see (2.10),

$$L(\cdot) = i[H_f, \cdot] + \sum_{k \in K} L_k(\cdot)$$

where the $L_k$ can be identified with the contribution to the dissipation from
the $k$'th reservoir. $H_f$ is an effective, renormalized Hamiltonian depending
on details of the reservoirs and the coupling.

From now on, we write $\rho$ for the (assumed) unique invariant state (see also
Remark 2.1):

$$e^{\tau L^*} \rho = \rho, \quad \tau \geq 0$$

Again one can study here the mean entropy production, as for example done
in [LS78] and argue that

$$\text{Tr}[\rho L_k H_S]$$

represents the stationary heat flow into the $k$'th reservoir, at least in the
weak coupling regime. Nothing tells us here however about the physical fluc-
tuations in the heat current for which higher moments should be considered.
In fact, the reservoirs are no longer visible as the weak coupling dynamics
is really a jump process on the energy levels of the system Hamiltonian, see
further in Section 3.1. The heat flow and the energy changes in the individ-
ual reservoirs cannot be reconstructed from the changes in the system. The
present paper uses a new idea for the study of the fluctuations of the heat
dissipation in a reservoir.

1.2.3 Dilation

While the weak coupling dynamics is very useful for problems of thermal
relaxation (one reservoir) and for identifying the conditions of microscopic
reversibility (detailed balance) characterizing an equilibrium dynamics, not
sufficient information is left in the weak coupling limit to identify the variable
heat dissipated in the various reservoirs. Heat is path-dependent and we need
at least a notion of energy-trajectories.\footnote{At least, if one has a stochastic or effective description of the system dynamics, as is the case in the weak-coupling limit. We do not claim at all that the trajectory-picture is microscopically fundamental.} The good news is that we can obtain
such a representation at the same time as we obtain a particular dilation of the weak coupling dynamics. The representation is basically achieved via an unraveling of the weak coupling generator $L$ and the corresponding Dyson expansion of the semigroup dynamics. That will be explained in Section 2.2.

There are many possible dilations of a quantum dissipation. It turns out that there is a dilation whose restriction to the system coincides with the Dyson representation in terms of energy-trajectories of the weak coupling dynamics. That dilation is well studied and goes under the name of a quantum stochastic dynamics. The associated quantum stochastic calculus was invented by Hudson and Parathasarathy, [HP84]. It has been extensively employed for the purpose of quantum counting processes, see e.g. [BGM04, BMK03]. Various representations and simplifications have been added, such as in [AFS7] where a (classical) Brownian motion extends the quantum dissipation. Unravelings of generators have been first employed in quantum optics in [SD81], they are further discussed in [Car93].

1.2.4 Results

We prove a symmetry in the large deviation generating function of the dissipated heat (Proposition 2.8). This function is analytic and this implies the large deviation principle. The symmetry is recognized as the fluctuation theorem for the entropy production. The precise form of the fluctuation theorem depends on whether the model has been derived from a reversible or an irreversible (e.g. because of the presence of magnetic fields) dynamics. This point was clarified in [Mae04]. By a theorem of Bryc [Bry93], analyticity of the generating function implies the central limit theorem for the currents. We do not stress this point but it is implicitly used in deriving a Green-Kubo relation and Onsager reciprocity (Proposition 2.10), or modifications of these, again depending on the reversibility of the original model. In all cases, the fluctuation symmetry helps to establish strict positivity of the entropy production (Proposition 2.9). Let us stress that our main result, Proposition 2.8, depends on an interpretation, as described above under Section 1.2.3. However, the consequences of our main result, Propositions 2.9 and 2.10, do not depend on this interpretation. This will be further discussed in Section 3.

1.2.5 Comparison with earlier results

Technically, our fluctuation theorem is very close to the results obtained in [Kur98] or [LS99]. The Green-Kubo relations and Onsager reciprocity have been established recently in e.g. [JOP05] for the spin-fermion model. In the
weak-coupling limit they were discussed already in [LS78], however there the authors did not distinguish between reversible and irreversible models (this is commented upon in Remark 2.6). The strict positivity in the weak-coupling limit was proven in [JP02b] (for the spin-fermion model) and in [AS06] (under general conditions). Our theorem on strict positivity is however slightly more general: Assuming the existence of a unique, faithful stationary state, we formulate a necessary and sufficient condition for strict positivity.

1.3 Outline of the paper

In Section 2, we introduce the quantum stochastic model and state the result. In Section 3 follows a discussion where the main points and novelties are emphasized. Proofs are postponed to Section 4.

2 The Model

2.1 Weak Coupling

We briefly introduce here the weak coupling dynamics without speaking about its derivation, which is not relevant for the discussion here. Some of that was briefly addressed in Sections 1.2.1-1.2.2 and it is covered in detail in [Dav74] and [LS78].

Let $\mathcal{H}$ be a finite-dimensional Hilbert space assigned to a small subsystem, called system in what follows. Let $H_S$ be a self-adjoint Hamiltonian on $\mathcal{H}$. Introduce the set of Bohr frequencies

$$F := \{\omega \in \mathbb{R} \mid \exists e, e' \in \text{sp}H_S : \omega = e - e'\}$$

(2.1)

Remark that $F$ is the set of eigenvalues of the derivation $-i[H_S, \cdot]$. We label by $k \in K$ (a finite number of) different heat reservoirs at inverse temperatures $\beta_k < \infty$. To each reservoir $k$ is assigned a self-adjoint operator $V_k \in \mathcal{B}(\mathcal{H})$ and for each $k \in K, \omega \in F$, we put

$$V_{\omega,k} = \sum_{e, e' \in \text{sp}H_S, \omega = e - e'} 1_e(H_S)V_k1_{e'}(H_S)$$

(2.2)

where $1_e(H_S)$ for $e \in \text{sp}(H_S)$ is the spectral projection on $e$ associated to $H_S$.

\[4\]Besides, from [JP02b], it follows that the strict positivity remains true at small nonzero coupling, without taking the weak coupling limit.
Fix for $k \in K$, nonnegative functions $\eta_k \in L^1(\mathbb{R})$ and assume them to be Hölder continuous in $F \subset \mathbb{R}$ and satisfying the condition

$$\eta_k(x) = e^{-\beta_k x} \eta_k(-x) \geq 0, \quad x \in \mathbb{R}$$  \hspace{1cm} (2.3)

which is related to the KMS equilibrium conditions in the reservoir $k \in K$, see further under remark 2.5. Write also for $\omega \in F, k \in K$

$$s_k(\omega) = \lim_{\epsilon \downarrow 0} \int_{\mathbb{R} \setminus [\omega - \epsilon, \omega + \epsilon]} \frac{\eta_k(x)}{\omega - x}$$  \hspace{1cm} (2.4)

which is well defined by the assumption of Hölder continuity for $\eta_{k \in K}$. From now on, we simply write the indices $\omega, k$ for $\omega \in F, k \in K$. We consider the self-adjoint Hamiltonian

$$H_f := \sum_{\omega, k} s_k(\omega) V_{\omega, k}^* V_{\omega, k}$$  \hspace{1cm} (2.5)

satisfying by construction

$$[H_f, H_S] = 0$$  \hspace{1cm} (2.6)

We work with the following generator $\mathcal{L}$ on $\mathcal{B}(\mathcal{H})$

$$\mathcal{L}(\cdot) = i[H_f, \cdot] + \sum_{\omega, k} \eta_k(\omega)(V_{\omega, k}^* \cdot V_{\omega, k} - \frac{1}{2}(V_{\omega, k}^* V_{\omega, k}, \cdot))$$  \hspace{1cm} (2.7)

Putting $\mathcal{T}(\mathcal{H}) \subset \mathcal{B}(\mathcal{H})$ the set of all density matrices on $\mathcal{H}$, i.e:

$$\mu \in \mathcal{T}(\mathcal{H}) \iff \text{Tr}[\mu] = 1, \quad \mu \geq 0$$  \hspace{1cm} (2.8)

one introduces the dual generator $\mathcal{L}^*$ on $\mathcal{T}(\mathcal{H})$, defined through

$$\text{Tr}[A \mathcal{L}^* \mu] = \text{Tr}[\mu \mathcal{L} A], \quad A \in \mathcal{B}(\mathcal{H}), \mu \in \mathcal{T}(\mathcal{H})$$  \hspace{1cm} (2.9)

By grouping all terms with the same $k$ in (2.7), we can also write

$$\mathcal{L}(\cdot) = -i[H_f, \cdot] + \sum_{k \in K} \mathcal{L}_k(\cdot)$$  \hspace{1cm} (2.10)

Both $\mathcal{L}$ and $\mathcal{L}_{k \in K}$ are of the Lindblad form \cite{Lin75} and hence they generate completely positive semigroups $e^{t\mathcal{L}}$ and $e^{t\mathcal{L}_k}$. A $\rho \in \mathcal{T}(\mathcal{H})$ is a stationary state for the semigroup $e^{t\mathcal{L}}$ iff

$$\mathcal{L}^* \rho = 0 \quad \text{or, equivalently,} \quad e^{t\mathcal{L}^*} \rho = \rho$$  \hspace{1cm} (2.11)
We fix an anti-unitary operator $T$ on $\mathcal{H}$, which has to be thought of as playing the role of time reversal. Let

$$H^\theta_S := TH^\theta_S, \quad V^\theta_k := TV^\theta_k$$

(2.12)

That defines a new model, satisfying all necessary requirements. This model can be thought of as the time-reversal of the original one.

We will need the following assumptions:

**Assumption A1**

*We ask triviality of the commutant*

$$\{\eta_{k}^{1/2}(\omega)V_{\omega,k} \mid k \in K, \omega \in F\}' = C1$$

where for $A \subset B(\mathcal{H})$,

$$B \in A' \iff \forall A \in A : [A, B] = 0$$

(2.14)

That ensures the existence of a unique stationary state, as stated in Remark 2.4

**Assumption A2**

*We ask that the system can complete a closed cycle in which the entropy production is nonzero.* More precisely, there are sequences $\omega_1, \ldots, \omega_n$ in $F$ and $k_1, \ldots, k_n$ in $K$ such that

1. $$\sum_{i=1}^{n} \beta_k \omega_i \neq 0$$

(2.15)

2. *There is a one-dimensional projection $P \in B(\mathcal{H})$ such that*

$$\text{Tr} [PV_{\omega_n,k_n} \ldots V_{\omega_2,k_2}V_{\omega_1,k_1}P] \neq 0$$

(2.16)

**Assumption A3**

*This assumption expresses that our model is time-reversal invariant. It will be used in deriving the full fluctuation theorem, the Green-Kubo relations and Onsager reciprocity.*

$$H^\theta_S = H_S, \quad \forall k \in K : V^\theta_k = V_k$$

(2.17)
Remark 2.1. If Assumption \textbf{A1} holds, then, by a theorem of Frigerio (Theorem 3.2 in [Fri78]) and the fact that $\beta_k \in K < \infty$, the semigroup $e^{t\mathcal{L}}$ has a unique stationary state $\rho$. This state is faithful, i.e. for all nonzero projections $P \neq 0 \in \mathcal{B}(\mathcal{H})$:

$$\text{Tr}[\rho P] > 0$$

(2.18)

Assumption \textbf{A1} is actually a necessary condition for the existence of a unique stationary state.

Remark 2.2. Assumption \textbf{A2} comprises the intuitive assumption that the system does not break up in independent subsystems which are coupled separately to the reservoirs. If that would be the case, then most of our results still hold but they become trivial. For example, the rate function $\mathcal{E}$ from Proposition 2.8 satisfies

$$\forall \kappa \in \mathbb{C} : \mathcal{E}(\kappa) = 0.$$

Remark 2.3. If for all $k \in K$, $\beta_k = \beta$ for some $\beta$, then

$$\rho_\beta := \exp(-\beta H_S)/\text{Tr}[\exp(-\beta H_S)]$$

is a stationary state for $e^{t\mathcal{L}}$, as follows from the condition (2.3) and the explicit form (2.7).

Remark 2.4. If \textbf{A1} holds (assuring the uniqueness of the stationary state), then one easily checks

$$\forall A \in \mathcal{B}(\mathcal{H}), \forall e \neq e' \in \text{sp} H_S : \lim_{t \to +\infty} e^{t\mathcal{L}}(1_e(H_S)A1_{e'}(H_S)) = 0$$

(2.20)

which is usually called “decoherence”. As a consequence of (2.20), the stationary state $\rho \in \mathcal{T}(\mathcal{H})$ of $e^{t\mathcal{L}}$ satisfies,

$$\sum_{e \in \text{sp} H_S} 1_e(H_S) \rho 1_e(H_S) = \rho$$

(2.21)

Remark 2.5. If one would derive the model from a microscopic setup, then we can be more specific. Let $\mathcal{H}_{R_k}$ be the Hilbert space of the $k$’th reservoir and $\rho_k$ a thermal equilibrium state at $\beta_k$ on (a subalgebra of) $\mathcal{B}(\mathcal{H}_{R_k})$. Assume the coupling is given by

$$\sum_{k \in K} V_k \otimes R_k, \quad R_k = R_k^* \in \mathcal{B}(\mathcal{H}_{R_k})$$

(2.22)

Then the functions $\eta_k$ are fourier transforms of the autocorrelation function of $R_k$ and the KMS conditions imply (2.3). All this is discussed at length in [LS99].

The restriction to couplings of the form \textbf{(2.22)}, where each term is self-adjoint by itself, is not necessary. Besides, one can also have multiple couplings per reservoir. Since this complicates our notation without introducing any novelty, we adhere to the simple form \textbf{(2.22)}. 

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Remark 2.6. If $H_S$ is nondegenerate, one can choose $T$ as follows: Let $\psi_e, e \in \text{sp} H_S$ be a complete set of eigenvectors for $H_S$ and put

$$T\left(\sum_{e \in \text{sp} H_S} c_e \psi_e\right) = \sum_{e \in \text{sp} H_S} \bar{c}_e \psi_e, \quad c_e \in \text{sp} H_S \subset \mathbb{C}$$ (2.23)

Although this does not necessarily imply Assumption A3, it does imply

$$H^\theta_S = H_S, \quad V_{\omega,k}A V^*_\omega,k = V^\theta_{\omega,k} A (V^\theta_{\omega,k})^* \quad A \in \mathcal{B}(\mathcal{H})$$ (2.24)

which, as one can check from the proofs, can replace A3 for all purposes of this paper. Hence, a nondegenerate model is automatically time-reversal invariant. This explains why in LS78 the Green-Kubo relations were derived for nondegenerate Hamiltonians without speaking about microscopic time-reversal. It also explains why time-reversal does not appear naturally in the framework of classical Markov jump processes.

2.2 Unraveling the generator

We associate to that semigroup dynamics, generated by (2.7), a pathspace measure by a procedure which is known as “unraveling the generator”. Basically, we will introduce $|F| \times |K|$ Poissonian clocks, one for each reservoir and each Bohr frequency. Whenever clock $(\omega, k)$ ticks, our system will make a transition with Bohr frequency $\omega$, induced by reservoir $k$. This will be our ‘a priori’ measure $d\sigma$ (see further). If $H_S$ is nondegenerate, then it is very easy to upgrade $d\sigma$ to the appropriate pathspace measure: one multiplies $d\sigma$ with a certain factor for each jump and with factors for the waiting times, obtaining something of the form

$$d\mathbb{P}_{\rho_0}(\sigma) = e^{-(t-t_n)c_n}\ldots e^{-(t_2-t_1)c_1}e^{-t_1r_1}d\sigma$$ (2.25)

for some positive numbers $c_1, \ldots, c_n$ and $r_1, \ldots, r_{n+1}$ and initial state $\rho_0$.

When $H_S$ is degenerate, one has to do things more carefully, leading to the expression (2.42) in Lemma 2.7. The technical difference between degenerate and non-degenerate $H_S$ is further discussed in Section 3.

2.2.1 Preliminaries

Put

$$\Omega^1_t := \{\sigma \subset [0, t] | |\sigma| < \infty\}, \quad \Omega^1 := \{\sigma \subset \mathbb{R}^+ | |\sigma| < \infty\}$$ (2.26)
where \(|\sigma|\) is the cardinality of the set \(\sigma \subset \mathbb{R}\). Let \((\Omega^1_t)_{\omega,k}, \Omega^1_{\omega,k}\) stand for identical copies of \(\Omega^1_t, \Omega^1_{\omega,k}\) and put

\[
\Omega := \times_{\omega,k} \Omega^1_{\omega,k}, \quad \Omega_t := \times_{\omega,k} (\Omega^1_t)_{\omega,k}
\]

(2.27)

\(\Omega\) and \(\Omega_t\) are called Guichardet spaces, see [Gui72]. An element \(\sigma \in \Omega\) looks like

\[
\sigma = (\omega_1, k_1, t_1; \ldots; \omega_n, k_n, t_n) \text{ with } 0 < t_1 < t_2 < \ldots < t_n < +\infty
\]

(2.28)

Alternatively, and corresponding to the product in (2.27):

\[
\sigma = (\sigma_{\omega,k})_{\omega,k} \text{ with } \sigma_{\omega,k} \in \Omega^1_{\omega,k}, \quad |\sigma| := \sum_{\omega,k} |\sigma_{\omega,k}|
\]

(2.29)

We define integration on \(\Omega_t\) and \(\Omega\), by putting for any sequence of functions \(g = (g_n)_{n \in \mathbb{N}}\) with \(g_n\) a measurable function on \(F^n \times K^n \times (\mathbb{R}^+)^n\) for all \(n \in \mathbb{N}\),

\[
\int_{\Omega_t} d\sigma g(\sigma) := \sum_{n=0}^{\infty} \sum_{k_1, \ldots, k_n \in K^n_{\omega_1, \ldots, \omega_n} \in F^n} \int_{\Delta^n_t} dt_1 \ldots dt_ng_n((\omega_1, k_1, t_1; \ldots; \omega_n, k_n, t_n))
\]

(2.30)

where \(\Delta^n_t \subset \mathbb{R}^n\) is the simplex

\[
(t_1, \ldots, t_n) \in \Delta^n_t \iff 0 < t_1 < \ldots < t_n < t
\]

(2.31)

The equality (2.30) defines the symbol “\(d\sigma\)" and the notion of measurable sets in \(\Omega_t\) or \(\Omega\) (for the latter, take \(t = \infty\) in the above definitions).

For future use, we introduce 'number functions’ \(n^t_{\omega,k}\), defined as

\[
n^t_{\omega,k}(\sigma) := |\sigma_{\omega,k} \cap [0,t]|, \quad n_{\omega,k}(\sigma) := |\sigma_{\omega,k}|
\]

(2.32)

and the abbreviations \(\sigma \cup \tau\) and \(\tau \setminus \sigma\) for elements of \(\Omega\), defined by

\[
(\sigma \cup \tau)_{\omega,k} := \sigma_{\omega,k} \cup \tau_{\omega,k}, \quad \sigma = \xi \setminus \tau \iff \sigma \cup \tau = \xi
\]

(2.33)

If \(\sigma \in \Omega_s\) and \(\tau \in \Omega_u\), we also need \(\sigma \tau \in \Omega_{s+u}\), defined by

\[
(\sigma \tau)_{\omega,k} := \sigma_{\omega,k} \cup (s + \tau_{\omega,k}) \quad \text{where } q \in s + \tau_{\omega,k} \iff q - s \in \tau_{\omega,k}
\]

(2.34)

Remark that a function \(g\) on \(\Omega_s\) is naturally made into a function on \(\Omega_{s+u}\) by, using the notation (2.33),

\[
g(\sigma \tau) := g(\sigma), \quad \sigma \in \Omega_s, \tau \in \Omega_u
\]

(2.35)
2.2.2 Constructing a pathspace measure

Write the weak coupling generator (2.7) as
\[ \mathcal{L} = \mathcal{L}_0 + \sum_{\omega,k} J_{\omega,k} \]  
with
\[ J_{\omega,k}(\cdot) := \eta_k(\omega) V_{\omega,k}^* \cdot V_{\omega,k} \]  
and
\[ \mathcal{L}_0(\cdot) := i[H_f, \cdot] - \frac{1}{2} \sum_{\omega,k} \eta_k(\omega) \{ V_{\omega,k}^* V_{\omega,k}, \cdot \} \]  
Consider \( W_t(\sigma) : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H}) \) as the completely positive map depending on \( \sigma \in \Omega \)
\[ W_t(\sigma) := I_{\Omega_t}(\sigma) e^{t_1 \mathcal{L}_0} J_{\omega_1,k_1} e^{(t_2-t_1) \mathcal{L}_0} \ldots e^{(t_{|\sigma|}-t_{|\sigma|}-1) \mathcal{L}_0} J_{\omega_{|\sigma|},k_{|\sigma|}} e^{(t-t_{|\sigma|}) \mathcal{L}_0} \]  
with \( I_{\Omega_t} \) the indicator function of \( \Omega_t \subset \Omega \) and with the indices \((\omega_i, k_i), i = 1, \ldots, |\sigma|\) referring to the representation (2.28) of \( \sigma \). To verify the complete positivity of (2.38), rewrite \( \mathcal{L}_0 \) as
\[ \mathcal{L}_0(\cdot) = S \cdot + S^*, \quad S = iH_f - \frac{1}{2} \sum_{\omega,k} \eta_k(\omega) V_{\omega,k}^* V_{\omega,k} \]  
which yields,
\[ e^{t \mathcal{L}_0}(\cdot) = e^{tS} \cdot (e^{tS})^* \]  
Complete positivity of (2.37) is obvious from its definition. The Dyson expansion of \( e^{t\mathcal{L}} \), corresponding to the splitting (2.36), reads
\[ e^{t\mathcal{L}} = \int_{\Omega_t} d\sigma \mathcal{W}_t(\sigma) \]  
That expression induces a ‘path space measure’, or a notion of ‘quantum trajectories’ on \( \Omega \).

**Lemma 2.7.** Choose \( \mu \in \mathcal{T}(\mathcal{H}) \). Let \( E \subset \Omega_t \) be measurable and define
\[ \mathbb{P}_{\mu,t}(E) := \int_E d\sigma \text{Tr} [\mu \mathcal{W}_t(\sigma)] \]  
Then \( (\mathbb{P}_{\mu,t})_{t \in \mathbb{R}^+} \) are a consistent family of probability measures on \( (\Omega_t)_{t \in \mathbb{R}^+} \), i.e. for a measurable function \( g \) on \( \Omega_t \),
\[ \int_{\Omega_t} d\mathbb{P}_{\mu,t}(\sigma) g(\sigma) = \int_{\Omega_s} d\mathbb{P}_{\mu,s}(\sigma) g(\sigma), \quad s \geq t \]  
where \( g \) is extended to \( \Omega_s \) as in (2.35).
Thus we obtain a new probability measure \( P_{\mu} \) on \( \Omega \) by the Kolmogorov extension theorem, for \( t > 0 \) and a function \( g \) on \( \Omega_t \),

\[
\int_{\Omega} dP_{\mu}(\sigma) g(\sigma) = \int_{\Omega_t} dP_{\mu,t}(\sigma) g(\sigma) \tag{2.44}
\]

where we used again the extension as in (2.35). The expectation with respect to these measures is denoted

\[
E_{\mu,t} \text{ on } \Omega_t, \quad E_{\mu} \text{ on } \Omega \tag{2.45}
\]

These probability measures are often called ‘quantum counting processes’, see [BGM04, BMK03].

### 2.3 Results

We define the integrated entropy current \( w^t \) up to time \( t \) as a function on \( \Omega \):

\[
w^t(\sigma) = -\sum_{\omega,k} \beta_k \omega n^t_{\omega,k}(\sigma) \tag{2.46}
\]

with \( n^t_{\omega,k} \) as in (2.32). In what follows, we denote by \( \rho \) the stationary state for \( e^{t\kappa} \), which is unique by Assumption A1. For \( \kappa \in \mathbb{C} \), we write

\[
e(\kappa) := \lim_{t \to +\infty} \frac{1}{t} \log E_{\rho}[e^{-\kappa w^t}] \tag{2.47}
\]

if it exists. Then, \( e(\kappa) \) of course depends on all model parameters, i.e. on \( H_S, V_k, \eta_k \). We introduce \( e^{\theta}(\kappa) \) which is derived from the model with new parameters \( H_{\theta}^S, V_k^\theta, \eta_k^\theta = \eta_k \), see (2.12).

Now we can already formulate the main result of the paper:

**Proposition 2.8. Fluctuation Theorem**

Assume A1. Let \( w^t \) be defined by (2.46). There is an open set \( \mathcal{U} \subset \mathbb{C} \) containing the real line, \( \mathbb{R} \subset \mathcal{U} \), such that for all \( \kappa \in \mathcal{U} \), the limit

\[
e(\kappa) := \lim_{t \to +\infty} \frac{1}{t} \log E_{\rho}[e^{-\kappa w^t}] \tag{2.48}
\]

exists and the function \( \kappa \to e(\kappa) \) is analytic on \( \mathcal{U} \). Moreover,

\[
e(\kappa) = e^\theta(1 - \kappa) \tag{2.49}
\]

If also A3 holds, then \( e(\kappa) = e^\theta(\kappa) \) and

\[
e(\kappa) = e(1 - \kappa) \tag{2.50}
\]
We list some consequences of the fluctuation relations (2.49) and (2.50).

**Proposition 2.9. Strict Positivity of the Entropy Production**

Assume $A_1$, then

\[ A_2 \text{ holds } \iff \lim_{t \to +\infty} \frac{1}{t} \mathbb{E}_\rho[w^t] > 0 \] (2.51)

For the next proposition we introduce energy functions $n^t_k$ on $\Omega$;

\[ n^t_k := - \sum_{\omega \in F} \omega n^t_{\omega,k} \] (2.52)

**Proposition 2.10. Green-Kubo Relations**

Assume $A_1$ and fix some $\beta > 0$. Let for $k, k' \in K$:

\[ L_{k,k'}(\beta) := \frac{\partial}{\partial \beta} \lim_{t \to +\infty} \frac{1}{t} \mathbb{E}_\rho[n^t_k] \big|_{\beta_1 = \ldots = \beta_{|K|} = \beta} \] (2.53)

and similarly the time-reversed coefficient $L^0_{k,k'}$, obtained by starting with $H^\theta_S$ and $V^\theta_k$. Then,

\[ L_{k,k'}(\beta) + L^0_{k,k'}(\beta) = \beta \lim_{t \to +\infty} \frac{1}{t} \mathbb{E}_\rho[n^t_k n^t_{k'}] \] (2.54)

If also $A_3$ holds, then

\[ L_{k,k'} = \frac{1}{2} \beta \lim_{t \to +\infty} \frac{1}{t} \mathbb{E}_\rho[n^t_k n^t_{k'}] \] (2.55)

with Onsager reciprocity

\[ L_{k,k'} = L_{k',k} \] (2.56)

### 2.4 The quantum model: a dilation of the semigroup $e^{t\mathcal{L}}$

#### 2.4.1 Heuristics

In the next section we construct a unitary evolution, which is our basic quantum model. This type of unitary evolutions is generally known as solutions of quantum stochastic differential equations, introduced in [HP84].

For the readers who are familiar with stochastic calculus, we briefly state how our evolution would look in traditional notation. Recommended references are [Par92, Att03] for quantum stochastic calculus and [Der03] for the formalism of second quantization.
For all $\omega \in F$ and $k \in K$, let $(L^2(\mathbb{R}^+))_{\omega,k}$ be a copy of $L^2(\mathbb{R}^+)$. We consider the bosonic Fock space ($\Gamma_s$ denotes symmetrized second quantization)

$$\mathcal{R} = \Gamma_s \left[ \bigoplus_{\omega,k} (L^2(\mathbb{R}^+))_{\omega,k} \right] = \bigotimes_{\omega,k} \Gamma_s \left[ (L^2(\mathbb{R}^+))_{\omega,k} \right]$$  \hspace{1cm} (2.57)

and think of $dA^*_{\omega,k,t}$ with $t \in \mathbb{R}^+$ as the creation operator on $\Gamma_s \left[ (L^2(\mathbb{R}^+))_{\omega,k} \right]$ creating the “wavefunction” $\chi_{[t,t+dt]}$ (the indicator function of the interval $[t,t+dt]$). We now write a Quantum Stochastic Differential Equation (QSDE) on $\mathcal{B}(\mathcal{H} \otimes \mathcal{R})$:

$$dU_t = \sum_{\omega,k} \eta_k^{1/2}(\omega) \left( V_{\omega,k} dA^*_{\omega,k,t} - V^*_{\omega,k} dA_{\omega,k,t} \right) U_t$$  \hspace{1cm} (2.58)

$$- \left( iH_d dt - \frac{1}{2} \sum_{\omega,k} \eta_k(\omega) V^*_{\omega,k} V_{\omega,k} dt \right) U_t, \quad U_0 = 1 \otimes 1$$

Of course, the intuitive definitions given here, do not suffice to give meaning to this expression. We content ourselves with stating that (2.58) defines a unitary evolution $U_t$, which we will now rigourously construct by using Maassen’s approach of integral kernels [Maa84].

### 2.4.2 Construction of the unitary evolution $U_t$

Recall the Guichardet spaces $\Omega_t$ and $\Omega$, introduced in section 2.2 and define for $(\sigma, \tau) \in \Omega \times \Omega$ the ordered sequence of times $(t_1, \ldots, t_n)$ as

$$\{t_1, \ldots, t_n\} = \bigcup_{\omega,k} (\sigma_{\omega,k} \cup \tau_{\omega,k}) \text{ and } 0 < t_1 < \ldots < t_n \quad n = |\sigma| + |\tau|$$  \hspace{1cm} (2.59)

We define the integral kernel $u_t : \Omega \times \Omega \mapsto \mathcal{B}(\mathcal{H})$:

$$u_t(\sigma, \tau) = I_{\Omega_t \times \Omega_t} (\sigma, \tau) e^{(t-t_n)_{K}} Z_{n \in (l-\tau_{n-1})_{K}} Z_{n-1} \ldots Z_{2} e^{(t_2-t_1)_{K}} Z_{1} e^{t_{1}K}$$  \hspace{1cm} (2.60)

with $I_{\Omega_t \times \Omega_t}$ the indicator function of $\Omega_t \times \Omega_t$, $S \in \mathcal{B}(\mathcal{H})$ as in (2.39) and for $j = 1, \ldots, n$

$$Z_j = \begin{cases} 
\eta_k^{1/2}(\omega) V_{\omega,k} & \text{if } t_j \in \sigma_{\omega,k} \\
-\eta_k^{1/2}(\omega) V^*_{\omega,k} & \text{if } t_j \in \tau_{\omega,k}
\end{cases}$$  \hspace{1cm} (2.61)

Finally, let

$$\mathcal{F} := L^2(\Omega, \mathcal{H}, d\sigma) \simeq \mathcal{H} \otimes L^2(\Omega, d\sigma)$$  \hspace{1cm} (2.62)

Remark that in a natural way, we have $\mathcal{F} \simeq \mathcal{H} \otimes \mathcal{R}$ with $\mathcal{R}$ as defined in (2.57). Take $f \in L^2(\Omega, \mathcal{H}, d\sigma)$ and define

$$(U_t f)(\xi) = \sum_{\sigma \subseteq \xi} \int_\Omega u_t(\sigma, \tau) f((\xi \setminus \sigma) \cup \tau) d\tau$$  \hspace{1cm} (2.63)
In [Maa84], one proves that this $U_t$ is unitary and that it solves the QSDE (2.58).

The unitary family $U_t$, thus defined, is not a group, but a so-called cocycle; physically this corresponds to an interaction picture and it can be made into a group by multiplying it with a well chosen ‘free evolution’. Note that by taking each $V_{\omega,k} = 0$ or $V_k = 0$ in (2.2) the subsystem decouples from the reservoir and (2.63) reduces to

$$U_t = 1 \otimes 1$$

(2.64)

This follows since the kernel $u_t(\sigma, \tau)$ in (2.60) vanishes except for $\sigma = \tau = \emptyset$ and $S$ reduces to 0.

Remark that in (2.58) or (2.63), the reservoirs are now not only labeled by $k \in K$, as in the original physical picture, but also by $\omega \in F$; each transition has its own mathematical reservoir. To formulate our results, we also need to specify the state. Define the one-dimensional vacuum projection $1_{\emptyset} \in \mathcal{B}(\mathcal{F})$

$$(1_{\emptyset}f)(\sigma) = \begin{cases} f(\emptyset) & \text{when } \sigma = \emptyset \\ 0 & \text{when } \sigma \neq \emptyset \end{cases}$$

(2.65)

Our reference state is

$$\rho \otimes 1_{\emptyset} \text{ on } \mathcal{H} \otimes \mathcal{F}$$

(2.66)

where $\rho$ is the unique stationary state of $e^{tL}$, see Remark 2.1.

Note that the state $\rho \otimes 1_{\emptyset}$ is not invariant under the dynamics, only its restriction to $\mathcal{H}$ is invariant (see also (2.74)). Hence, technically, it is quite different from a NESS as in (1.2).

We will abbreviate the Heisenberg dynamics as

$$j_t(G) := U_t^\dagger GU_t, \quad G \in \mathcal{B}(\mathcal{H} \otimes \mathcal{F})$$

(2.67)

with $U_t$ as in (2.63). Let for each $k \in K, t \geq 0$, $N^t_k \in \mathcal{B}(\mathcal{F})$ be the energy operators

$$(N^t_k f)(\sigma) = n^t_k(\sigma)f(\sigma)$$

(2.68)

with $n^t_k \sigma$ defined in (2.52).

We also define a quantity which we interpret as the total energy of subsystem plus reservoirs

$$N^t := H_S + \sum_{\omega,k} N^t_k, \quad N^t \in \mathcal{B}(\mathcal{H} \otimes \mathcal{F})$$

(2.69)

This interpretation is backed by Proposition 2.13.
These ‘energies’ should be understood as renormalized quantities, of which the (infinite) equilibrium energy of the reservoirs was subtracted. This interpretation is confirmed by remarking that at time $s = 0$, these ‘energies’ equal 0: for all continuous functions $g$,
\[
\text{Tr} \left[ 1_\emptyset g(j_{s=0}(N^t_k)) \right] = \text{Tr} \left[ 1_\emptyset g(N^t_k) \right] = g(0) \text{ for all } k \in K, t \geq 0 \quad (2.70)
\]

### 2.4.3 Connection of the QSDE with the counting process

The connection of the QSDE with the ‘quantum trajectories’ is provided by the following lemma, which we will not prove. It can be found for example in [BMK03, BGM04] and it is easy to derive starting from (2.63) and remarking that
\[
W_t(\sigma)(\cdot) = u_t^*(\sigma, \emptyset) \cdot u_t(\sigma, \emptyset) \quad (2.71)
\]

**Lemma 2.11.** Let $E \subset \Omega$ be measurable (as for 2.30). Denote by $1_E$ the orthogonal projection
\[
1_E : L^2(\Omega) \rightarrow L^2(E) \quad (2.72)
\]
and recall $1_\emptyset$ from (2.65). Then, for all $A \in B(H)$
\[
\text{Tr}_F \left[ 1_\emptyset j_t(A \otimes 1_E) \right] = \int_E d\sigma \, W_t(\sigma)A \quad (2.73)
\]
where $\text{Tr}_F$ denotes the partial trace over $F$.

The formula (2.63) actually defines a dilation of the semigroup $e^{t \mathcal{L}}$. To see this, take $E = \Omega$, then (2.73) reads
\[
\text{Tr}_F \left[ 1_\emptyset j_t(A \otimes 1) \right] = \int_\Omega d\sigma \, W_t(\sigma)A = e^{t \mathcal{L}}A \quad (2.74)
\]

Another useful consequence of lemma 2.11 is the connection between the energy operators in (2.68) and the functions (2.52).

**Proposition 2.12.** Let $k_1, \ldots, k_\ell, t_1, \ldots, t_\ell$ and $g_1, \ldots, g_\ell$ be finite ($\ell < \infty$) sequences of, respectively, elements of $K$, $\mathbb{R}^+$ and continuous functions, and let $\mu \in T(H)$, then
\[
\text{Tr} \left[ (\mu \otimes 1_\emptyset) \prod_{i=1}^\ell g_i(j_{t_i}(N^{t_i}_{k_i})) \right] = \mathbb{E}_\mu \left[ g_\ell(\prod_{i=1}^\ell n^{t_i}_{k_i}) \right] \quad (2.75)
\]

Again, we do not give a complete proof and we refer to [BGM04, BMK03]. Proposition 2.12 follows from lemma 2.11 by using that for all $t \geq s$ and $k \in K$
\[
\dot{j}_t(N^t_k) = j_s(N^s_k) \quad (2.76)
\]
and that the family $\{N^t_k \mid t > 0, k \in K\}$ is commutative.
2.5 Results within the quantum picture

First, we show that the energy (see (2.69)) is conserved.

**Proposition 2.13.** Let $N^t$ be as in (2.69). For all continuous functions $g$:

$$\text{Tr} \left[ (\rho \otimes 1_{\emptyset}) g(j_t(N^t)) \right] = \text{Tr} \left[ (\rho \otimes 1_{\emptyset}) g(N^t) \right] = \text{Tr} \left[ \rho g(H_S) \right]$$ (2.77)

The change of entropy in the environment up to time $t$ is

$$W^t := \sum_{k \in K} \beta_k j_t(N^t_k)$$ (2.78)

and its ‘steady state expectation’ is the entropy production. Our main result is a fluctuation theorem for $W^t$.

**Proposition 2.14.** Assume $A_1$. Let $W^t$ be defined as in (2.78). There is an open set $U \in \mathbb{C}$ containing the real line, $\mathbb{R} \subset U$, such that for all $\kappa \in U$, the limit

$$\hat{\varepsilon}(\kappa) := \lim_{t \uparrow +\infty} \frac{1}{t} \log \text{Tr} \left[ (\rho \otimes 1_{\emptyset}) e^{-\kappa W^t} \right]$$ (2.79)

exists and the function $\kappa \rightarrow \hat{\varepsilon}(\kappa)$ is analytic on $U$. Let $e(\kappa)$ by defined as in (2.48). Then,

$$\hat{\varepsilon}(\kappa) = e(\kappa)$$ (2.80)

on $U$ and thus all statements in Proposition 2.8 carry over to $\hat{\varepsilon}(\kappa)$.

From $\rho \otimes 1_{\emptyset}$ we deduce probability measures $T_t$ on $\mathbb{R}$. Let $A \subset \mathbb{R}$ be measurable, then

$$T_t(A) = \text{Tr} \left[ (\rho \otimes 1_{\emptyset}) 1_A(W^t) \right]$$ (2.81)

where $1_A(W^t)$ is the spectral projection on $A$ associated to $W^t$. Via Legendre-transformation (2.50) implies

$$- \lim_{t \uparrow +\infty} \frac{1}{t} \log \frac{dT_t(-a)}{dT_t(a)} = a$$ (2.82)

which is (1.1).

In the same way as in Proposition 2.13, Propositions (2.10) and (2.9) carry over the quantum picture; for concreteness we give the analogue of Proposition 2.10.

**Proposition 2.15.** Assume $A_1$ and fix some $\beta > 0$. Let for $k, k' \in K$:

$$L_{k,k'}(\beta) := \frac{\partial}{\partial \beta_k} \lim_{t \uparrow +\infty} \frac{1}{t} \text{Tr} \left[ (\rho \otimes 1_{\emptyset}) N^t_k \right] \bigg|_{\beta_1 = \ldots = \beta_{|K|} = \beta}$$ (2.83)
and similarly the time-reversed coefficient \( \bar{L}_{k,k'}^\theta \), obtained by starting with \( H_S^\theta \) and \( V_k^\theta \).

\[
\bar{L}_{k,k'}(\beta) + \bar{L}_{k,k'}^\theta(\beta) = \beta \lim_{t \to +\infty} \frac{1}{t} \text{Tr} \left[ (\rho \otimes 1_\emptyset) N_{k}^t N_{k'}^t \right] \quad (2.84)
\]

If also \( A_3 \) holds, then

\[
\bar{L}_{k,k'} = \frac{1}{2} \beta \lim_{t \to +\infty} \frac{1}{t} \text{Tr} \left[ (\rho \otimes 1_\emptyset) N_{k}^t N_{k'}^t \right] \quad (2.85)
\]

with Onsager reciprocity

\[
\bar{L}_{k,k'} = \bar{L}_{k',k} \quad (2.86)
\]

Recall \( L_{k,k'} \) from Proposition 2.10. Then for all \( k \in K \),

\[
\bar{L}_{k,k'} = L_{k,k'} \quad (2.87)
\]

Remark that Propositions 2.14 and 2.15 follow immediately from Propositions 2.8 and 2.10 by application of Proposition 2.12.

3 Discussion

3.1 Entropy production for Markov processes

It is well known that the weak coupling generator is ‘classical’ in the sense that the commutant algebra \( A_{cl} := \{ A \in \mathcal{B}(\mathcal{H}) \mid [A, H_S^\theta] = 0 \} \) is invariant. In case the Hamiltonian \( H_S^\theta \) is non-degenerate and only then, \( A_{cl} \) is a commutative algebra. Then we can construct a Markov process with state space \( \Lambda \) which is the restriction of (the dual of) the semigroup \( e^{tL} \) to \( A_{cl} \simeq \mathcal{C}(\Lambda) \). Loosely speaking, let \( \rho \) be the stationary state, \( \Omega^t := \Lambda^{[0,t]} \) the pathspace up to time \( t \), and \( \mathcal{P}_\rho^t \) the pathspace measure (starting from \( \rho \)) of this Markov process. The time reversal operation \( \Theta \) acts on \( \Omega^t \) as \( (\Omega^t \xi)(u) = \xi(t - u) \) for \( \xi \in \Omega^t \) and \( 0 \leq u \leq t \).

For such Markov processes describing a nonequilibrium dynamics, we dispose of a general strategy for identifying the entropy production. It turns out in a lot of interesting cases [Mae04, MNV03, Mae99] that

\[
\log \frac{d\mathcal{P}^t_\rho}{d\Theta \mathcal{P}^t_\rho}(\xi) = S_t(\xi) + \mathcal{O}(1) \quad (3.1)
\]

where \( S_t(\xi) \) is the random variable that one physically identifies as the entropy production. The second term in the right-hand side is non-extensive in
time. The algorithm allows to derive \((1.1)\) from \((3.1)\).

Since we also have a Markov generator, we can apply the same scheme to our setup. To evaluate the result, we however need a physical notion of entropy production in our model. As mentioned earlier, such a notion is rather unambiguous here, see also [LS78, JP02b]:

\[
\langle \text{current into } k\text{'th reservoir} \rangle = \text{Tr} [\rho L_k H_S] \quad (3.2)
\]

But the mean entropy production based on these currents is \textbf{not} equal to the expectation value of \((3.1)\):

\[
\sum_{k \in K} \beta_k \text{Tr} [\rho L_k H_S] \neq \lim_{t \to \infty} \frac{1}{t} \text{E}_{\mathcal{P}_\rho} \left[ \ln \frac{d\mathcal{P}_\rho^t}{d\Theta \mathcal{P}_\rho^t} \right] \quad (3.3)
\]

For example, take two reservoirs \((k = L(\text{left}), R(\text{right}))\) and let \(\text{Refl} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})\) stand for the involution which models left-right reflection. Assume that \(H_S\) is non-degenerate and that for all \(x \in \mathbb{R}\),

\[
\text{Refl} H_S = H_S, \quad \text{Refl} V_L = V_R, \quad e^{\beta_L x/2} \eta_L(x) = e^{\beta_R x/2} \eta_R(x) \quad (3.4)
\]

Hence all parameters are left-right symmetric, except the inverse temperatures \(\beta_L, \beta_R\). (Actually, these assumptions are inconsistent; if \(H_S\) is left-right symmetric, then it must be degenerate. However, one can introduce an arbitrarily small symmetry breaking which will generically lift the degeneracy, such that the our reasoning still applies.) One checks that

\[
\log \frac{d\mathcal{P}_\rho^t}{d\Theta \mathcal{P}_\rho^t}(\xi) = \log \sum_{e_0 \in A_0 \subset \text{sp} H_S} \rho [1_{e_0}(H_S)] + \sum_{e_m \in A_m \subset \text{sp} H_S} \rho [1_{e_m}(H_S)] + \sum_{i=1}^m \log \frac{e^{-\beta_L \omega_i} + e^{-\beta_R \omega_i}}{e^{-\beta_L \omega_i} + e^{-\beta_R \omega_i}}
\]

\[
= \mathcal{O}(1) - (\beta_L + \beta_R) \sum_{i=1}^m \omega_i \quad (3.5)
\]

where the sets \(A_0, A_m\) and the sequence \(\omega_i^m\) of energy jumps are derived from \(\xi\), and moreover \(|\sum_{i=1}^m \omega_i| \leq \|H_S\|\). This means that in this particular left-right symmetric case, \((3.5)\) is bounded, independently of \(t\) for every \(\xi\), and hence the RHS of \((3.3)\) vanishes, which disqualifies it as “entropy production”.

\(^5\)Very recently, a paper [EM06] appeared where exactly this is done: one derives a fluctuation theorem for \(\log \frac{d\mathcal{P}_\rho^t}{d\Theta \mathcal{P}_\rho^t}\) as in \((3.1)\). Since the authors consider mainly examples involving one reservoir, they do not run into the difficulty described here.
This trivial remark shows that it is not enough to look at the semigroup \(e^{t\mathcal{L}}\) to identify the entropy production. Instead we use more input: we certainly use the fact that \(\mathcal{L} = \sum_{k \in K} \mathcal{L}_k\) where the index \(k\) runs over the different reservoirs but moreover, with the unraveling of the generator, Section 2.2 comes an intuitive interpretation of the various terms. That can be contrasted with results by V. Jakšić and C. A. Pillet, where one actually proves that quantities like \(\text{Tr} [\rho \mathcal{L}_k H_S]\), cfr. (3.2) are limits of currents in the original microscopic Hamiltonian model. Of course, we take care that our choices are consistent with that result. However, for the higher-order fluctuations, we do not know; we just make a choice which looks very natural. At present, we do not give arguments that for a class of reasonable functions \(g\)

\[
\mathbb{E}_\rho \left[ g(w') \right] \tag{3.6}
\]

is indeed the limit of some fluctuation of dissipated heat in the microscopic model. (Although [DR06] points in that direction, see also point 2 in section 3.3)

Another choice for the higher order fluctuations is discussed in Section 3.2. It is exactly here that lies the role of the dilation with quantum stochastic evolutions. If one takes that quantum model as a starting point, then one can derive that (3.6) is a fluctuation of the dissipated heat. To our knowledge, that is the only quantum model in which one can study the fluctuations of the dissipated heat.

On the other hand, one can also make a classical dilation of the semigroup and in fact, this is exactly what we do in Section 2.2. Yet, there is a technical difference between the cases of degenerate and non-degenerate system Hamiltonians \(H_S\). If \(1_e(H_S)\) is one-dimensional for \(e \in \text{sp}H_S\), and in addition, for a nonzero \(\omega \in F\), \(e\) is the unique element of \(\text{sp}H_S\) such that \(e - \omega \in \text{sp}H_S\), then we have the following form of Markovianness: If a \(\sigma \in \Omega\) contains \(\omega\), i.e.

\[
\sigma = \sigma_0 \tau \sigma_1, \quad \sigma_0 \in \Omega_{t_0}, \sigma_1 \in \Omega_{t_1}, \tau = (t_0, \omega, k) \text{ for some } k \in K, t_0, t_1 \geq 0 \tag{3.7}
\]

then

\[
\text{d}\mathbb{P}_\rho(\sigma) = \text{Tr} [\rho \mathcal{W}_{t_0+t_1}(\sigma)1] \\
= \text{Tr} [\rho \mathcal{W}_{t_0}(\sigma_0 \tau)1] \text{d}\sigma_0 \text{d}\tau \times \text{Tr} [1_e(H_S) \mathcal{W}_{t_1}(\sigma_1)1] \text{d}\sigma_1 \\
= \text{d}\mathbb{P}_\rho(\sigma_0 \tau) \text{d}\mathbb{P}_{1_e(H_S)}(\sigma_1) \tag{3.8}
\]

In words, a one-dimensional spectral subspace erases memory. That does not work in the degenerate case.

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3.2 Integrated currents within the semigroup approach

Starting from (3.2) one could define the integrated currents \( \hat{J}_{k,t} \in B(H) \) as

\[
\hat{J}_{k,t} = \int_0^t du e^{u\mathcal{L}}(\mathcal{L}_k(H_S)) \tag{3.9}
\]

and study their fluctuations. One can ask whether these fluctuations coincide with those in our model? The answer is partially positive because

**Proposition 3.1.** Take for all \( k \in K : \beta_k = \beta \) for a certain \( \beta \) and let \( \rho_\beta \) be the stationary state for \( e^{t\mathcal{L}} \) as in Remark 2.3. For all \( k, k' \in K \) and all \( u \geq 0 \),

\[
\frac{\partial^2}{\partial v_1 \partial v_2} \mathbb{E}_{\rho_\beta}\left[n_{k'}^{v_1} n_k^{v_2}\right]_{v_1=0, v_2=u} = - \text{Tr} \left[ \rho_\beta \mathcal{L}_{k'}(H_S)e^{u\mathcal{L}}(\mathcal{L}_k(H_S)) \right] \tag{3.10}
\]

which gives a relation between Proposition 2.10 and the Green-Kubo relation in [LS99]. Also the averages coincide, leading to (3.2). However it is not true that for a reasonable class of functions \( g \)

\[
\mathbb{E}_\rho[g(n_k^t)] = \text{Tr}[\rho g(\hat{J}_{k,t})] \tag{3.11}
\]

So the mean entropy production and the Green-Kubo-formula can correctly be expressed in terms of the operators \( \hat{J}_{k,t} \), but higher order fluctuations of the dissipated heat cannot.

3.3 Connection to microscopic dynamics

We know of three derivations in the literature of the stochastic evolution (2.63) or (2.58) from a microscopic setup:

**1 Stochastic Limit**

Accardi et al. prove in [AFL90] that the weak coupling limit can be extended to the total evolution of subsystem observables. Let \( \mathcal{U}_t^\lambda \) be the evolution (in the interaction picture) on the total system with \( \lambda \) the coupling between subsystem and reservoirs. Then, in a certain sense,

\[
\mathcal{U}_{-t/\lambda^2}(S \otimes 1)\mathcal{U}_{t/\lambda^2}^\lambda \to U_t^\lambda(S \otimes 1)U_t^\lambda \tag{3.12}
\]

whereas the traditional weak coupling limit only speaks about convergence in expectation of the left-hand side. The unitary \( U_t^\lambda \) is the solution of (2.58).
2 Stochastic Limit Revisited

In [DR06], the approach of [AFL90] (mentioned above) was simplified. By introducing a unitary map $J_{\lambda}$ acting on the reservoirs, we get for all continuous functions $g$

\[
\lim_{\lambda \downarrow 0} J_{\lambda}^* U_{\lambda-t} J_{\lambda} = U_t, \quad \lim_{\lambda \downarrow 0} J_{\lambda}^* g(H_k) J_{\lambda} = g(N_k)
\] (3.13)

where $\lim$ denotes strong operator convergence and $H_k$ is the generator of the dynamics in the uncoupled $k$th reservoir. This suggests that one can study the fluctuations of the reservoir energies by looking at the number operators $N_k$ in the model reservoirs, exactly as we do in the present paper.

3 Repeated Interactions

In [AP03], Attal and Pautrat describe a subsystem with Hilbertspace $\mathcal{H}$ interacting repeatedly for a time $h$ with a small reservoir with Hilbertspace $\mathcal{R}$. After each time $h$, $\mathcal{R}$ is replaced by an identical copy. This procedure ensures that at any time, the subsystem sees a ‘fresh’ reservoir. In the limit $h \to 0$ the dynamics (in the interaction picture) converges in a certain sense to the solution of a QSDE. One can choose a particular QSDE by tuning the parameters of the interaction. Assume that

\[
\mathcal{R} = \otimes_{\omega,k} \mathcal{R}_{\omega,k}
\] (3.14)

Each $\mathcal{R}_{\omega,k}$ is 2-dimensional with basevectors $(\theta, \omega)$. Define $a_{\omega,k}$ on $\mathcal{R}_{\omega,k}$ by

\[
a_{\omega,k}(\omega) = \theta, \quad a_{\omega,k} \theta = 0
\] (3.15)

Choose the dynamics on $\mathcal{H} \otimes \mathcal{R}$ as $e^{-iH(h)}$ for $0 \leq t \leq h$ with

\[
H(h) = H_f + \frac{1}{\sqrt{h}} \sum_{\omega,k} \left( V_{\omega,k} a_{\omega,k}^* + V_{\omega,k}^* a_{\omega,k} \right)
\] (3.16)

Then, through the limiting procedure of [AP03], equation (2.58) obtains.

4 Proofs

4.1 Proof of Lemma 2.7

From

\[
\int_{\Omega_t} d\sigma \mathcal{W}_t(\sigma) 1 = e^{tE} 1 = 1, \quad \forall \sigma \in \Omega : \mathcal{W}_t(\sigma) 1 \geq 0
\] (4.1)

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for all $t \geq 0$, it follows that $(P_{\mu,t})_{t \in \mathbb{R}^+}$ is indeed a family of probability measures for all $\mu \in \mathcal{T}(\mathcal{H})$. Further, for $s,u \geq 0$, we have

$$W_t(\sigma)W_t(\tau) = W_t(\sigma \tau), \quad \sigma \in \Omega_s, \tau \in \Omega_u \quad (4.2)$$

Together with (4.1), this yields consistency of the family $(P_{\mu,t})_{t \in \mathbb{R}^+}$.

### 4.2 Proof of Proposition 2.8

Define for $\kappa \in C_{|K|}$ and $t > 0$,

$$M_{t,\kappa} : \Omega \mapsto C, \quad M_{t,\kappa}(\sigma) = \sum_{k \in K} \kappa_k \beta_k n_k^t(\sigma) \quad (4.3)$$

Our results rely on the following lemma

**Lemma 4.1.** Assume A1 and let $\mu \in \mathcal{T}(\mathcal{H})$. There is an open set $U \subset C_{|K|}$, with $\mathbb{R}^{|K|} \subset U$ such that

$$e(\kappa) := \lim_{t \uparrow +\infty} \frac{1}{t} \log \mathbb{E}_\mu \left[ e^{M_{t,\kappa}} \right] \quad (4.4)$$

is an analytic function on $U$ which does not depend on $\mu$. Moreover, for any sequence $k_1, \ldots, k_\ell \in K$,

$$\lim_{t \uparrow +\infty} \frac{\partial}{\partial \kappa_1} \cdots \frac{\partial}{\partial \kappa_\ell} \frac{1}{t} \log \mathbb{E}_\mu \left[ e^{M_{t,\kappa}} \right] = \frac{\partial}{\partial \kappa_1} \cdots \frac{\partial}{\partial \kappa_\ell} e(\kappa) \quad (4.5)$$

uniformly on compacts.

**Proof.** We apply the generalized Perron-Frobenius Theorem 4.3 of the Appendix with

$$\Lambda = \int_{\Omega} d\sigma \mathcal{W}_{t_\epsilon}(\sigma)e^{M_{t_\epsilon,\kappa}(\sigma)} \quad (4.6)$$

for well chosen $t_\epsilon$ and $\kappa \in \mathbb{R}^{|K|}$. Since for $\kappa \in \mathbb{R}^{|K|}$, $M_{t,\kappa}$ is a real function, the map $\Lambda$ is completely positive as a linear combination of completely positive maps with positive coefficients.

Below we choose $t_\epsilon$ so as to satisfy the non-degeneracy requirement (A-2) of the Appendix.

By faithfulness of the stationary state $\rho$,

$$\epsilon := \inf_{0 < P \in \mathcal{B}(\mathcal{H}), P^2 = P} \text{Tr} [\rho P] > 0 \quad (4.7)$$

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Since the semigroup is ergodic, it follows that there is \( t_\epsilon \) such that for all \( t > t_\epsilon \),

\[
\sup_{\mu \in \mathcal{T}(\mathcal{H})} \| \rho - e^{tL^*} \mu \| \leq \frac{\epsilon}{3(\dim \mathcal{H})^2}
\]

(4.8)

Since \( \|L\|, \|L_0\| < +\infty \), with \( \| \cdot \| \) being the operator norm in \( B(B(\mathcal{H})) \), the Dyson expansion (2.41) is absolutely convergent. Hence, we can find \( n \in \mathbb{N} \) such that

\[
\| \int_{|\sigma| \leq n} d\sigma \mathcal{W}_{t_\epsilon}(\sigma) - e^{tL} \| \leq \frac{\epsilon}{3 \dim \mathcal{H}}
\]

(4.9)

Let \( m := \inf_{|\sigma| \leq n} M_{t_\epsilon, \tau}(\sigma) \). For each \( \tau \in \mathbb{R}^{|K|} \), decompose

\[
\int_{\Omega} d\sigma \mathcal{W}_{t_\epsilon}(\sigma)e^{M_{t\epsilon} \tau} = e^m \int_{|\sigma| \leq n} d\sigma \mathcal{W}_{t_\epsilon}(\sigma)
\]

(4.10)

and for each pair of non-zero projections \( P \neq 0, P' \neq 0 \in B(\mathcal{H}) \), we have

\[
\text{Tr} \left[ P \int \mathcal{W}_{t_\epsilon}(\sigma)e^{M_{t\epsilon} \tau} P' \right] \geq e^m \int_{|\sigma| \leq n} d\sigma \text{ Tr} [PW_{t_\epsilon}(\sigma)P']
\]

\[
\geq e^m \left( \text{Tr} [Pe^{tL}P'] - \frac{\epsilon}{3} \right)
\]

\[
\geq e^m \left( \text{Tr} [P' \rho] - \frac{\epsilon}{3} - \frac{\epsilon}{3} \right) \geq e^m \frac{\epsilon}{3}
\]

(4.11)

This shows that one can apply Theorem 4.3 with \( \Lambda \) as in (4.6). Call the dominant eigenvalue of \( \Lambda \), \( \lambda(\tau, t_\epsilon) \) and the corresponding strictly positive eigenvector \( v(\tau) \). Remark that for each \( \tau \in \mathbb{C}^{|K|} \) and \( t \in \mathbb{R}^+ \),

\[
\int_{\Omega} d\sigma \mathcal{W}_{t}(\sigma)e^{M_{t} \tau(\sigma)} = e^{tL\tau}
\]

(4.12)

where

\[
L\tau(\cdot) = L_0(\cdot) + \sum_{\omega,k} \eta_k(\omega)e^{-\kappa_k \beta_k \omega}V^*_{\omega,k} \cdot V_{\omega,k}
\]

(4.13)

This follows by comparing the Dyson expansions (in the same sense as for (2.41)) corresponding to the left-hand and the right-hand side of (4.12). As a consequence, for all \( \tau \in \mathbb{R}^{|K|} \), \( L\tau \) has a non-degenerate maximal eigenvalue \( \lambda(\tau) = \frac{1}{t_\epsilon} \ln \lambda(\tau, t_\epsilon) \) corresponding to the eigenvector \( v(\tau) \). Since \( v(\tau) \) is strictly positive, we have \( \text{Tr} [v(\tau)] > 0 \), and, for any \( \mu \in \mathcal{T}(\mathcal{H}) \), \( \text{Tr} [v(\tau)\mu] > 0 \). This implies

\[
\lim_{t \uparrow +\infty} \frac{1}{t} \log \text{Tr} [\mu e^{tL\tau}1] = \lambda(\tau)
\]

(4.14)
and hence, again by (4.12)
\[ e(\mathbf{r}) = \lambda(\mathbf{r}) \] (4.15)

Since for all \( \mathbf{r} \in C^{|K|} \), \( \mathbf{L}_\mathbf{r} \) depends analytically on \( \mathbf{r} \), perturbation theory for isolated eigenvalues gives us for all \( \mathbf{r} \in \mathbb{R}^{|K|} \) an open set \( U_\mathbf{r} \ni \mathbf{r} \) such that for all \( \mathbf{r} \in U_\mathbf{r} \):

1. There is a unique \( \lambda(\mathbf{r}) \in \text{sp}\mathbf{L}_\mathbf{r} \) such that
\[
\inf\{\Re\lambda(\mathbf{r}) - |p| \mid p \in \text{sp}\mathbf{L}_\mathbf{r} \setminus \lambda(\mathbf{r})\} > 0
\] (4.16)

2. The eigenvector \( \mathbf{v}(\mathbf{r}) \), corresponding to \( \lambda(\mathbf{r}) \) satisfies
\[
\inf_{\mu \in \mathcal{T}(\mathcal{H})} (\Re \text{Tr}[\mu \mathbf{v}(\mathbf{r})]) > 0
\] (4.17)

It follows that (4.14) holds for all \( \mathbf{r} \in \bigcup_{\mathbf{r} \in \mathbb{R}^{|K|}} U_\mathbf{r} \).

\[ e(\mathbf{r}) = \lim_{t \to \infty} \frac{1}{t} \log \text{Tr}[\mu e^{t\mathbf{L}_\mathbf{r}}] = \lambda(\mathbf{r}) \] (4.18)

Summarizing, we have for all \( \mathbf{r} \in \mathbb{R}^{|K|} \) and \( \mu \in \mathcal{T}(\mathcal{H}) \) a family of analytic functions
\[ F(t, \mathbf{r}) := \frac{1}{t} \log \text{Tr}[\mu e^{t\mathbf{L}_\mathbf{r}}] \] (4.19)

converging pointwise in \( U_\mathbf{r} \) to the function \( e(\mathbf{r}) \) as \( t \uparrow +\infty \).

We recall Montel’s Theorem, see e.g. p. 153 of [Con78]:

**Theorem 4.2.** Let \( G \subset \mathbb{C} \) be open and let \( (f_n)_{n \in \mathbb{N}} \) be a sequence of analytic functions \( G \mapsto \mathbb{C} \), then \( (f_n)_{n \in \mathbb{N}} \) contains a uniformly convergent on compacts subsequence iff the set \( (f_n)_{n \in \mathbb{N}} \) is locally bounded, i.e., that for each \( z \in G \) there is a \( r > 0 \) and \( M > 0 \), such that
\[
|z' - z| \leq r \Rightarrow \forall n \in \mathbb{N} : |f_n(z')| \leq M
\] (4.20)

For all \( \mathbf{r} \in \mathbb{R}^{|K|} \), the family \( (F(t, \mathbf{r}))_{t \geq t_0} \) is locally bounded on \( U_\mathbf{r} \) for large enough \( t_0 \geq 0 \). This follows from analyticity of \( \mathbf{L}_\mathbf{r} \) and from the condition (4.17). Consequently, one can apply Theorem 4.2 for each component of \( \mathbf{r} \) separately. A standard result, e.g. Theorem 2.1, p. 151 in [Con78] states that the uniform limit of a sequence of analytic functions is analytic and that all derivatives converge. Since this generalizes to the multidimensional variable \( \mathbf{r} \), e.g. by Hartog’s theorem, Lemma 4.1 is proven. \( \square \)
Referring again to the representation (2.28), we introduce for $\sigma \in \Omega$ the factor

\[ \eta(\sigma) := \prod_{i=1}^{[\sigma]} \eta_{k_i}(\omega_i) \quad (4.21) \]

Recall the definition of $S$ in (2.40), introduce the time-reversed maps $L^0_{\theta}$ and, for $t \geq 0$, $\mathcal{W}^\theta_t$ (i.e., these maps are derived from $H^\theta_S$ and $V^\theta_k$) and remark, (see also (2.40))

\[ e^{t L^0_{\theta}(\cdot)} = e^{t S} \cdot e^{t S^*} \quad e^{t L^0_{\theta}^*(\cdot)} = e^{t S^* T} \cdot e^{T S T} \quad (4.22) \]

Define the operation $\theta_t$ on $\Omega_t$ as

\[ \theta_t(\omega_1, k_1, t_1; \ldots; \omega_n, k_n, t_n) := (-\omega_n, k_n, t - t_n; \ldots; -\omega_1, k_1, t - t_1) \quad (4.23) \]

Calculate

\[ \eta^{-1}(\sigma) \Tr[\mathcal{W}_t(\sigma)1] = \Tr\left[ \cdots V^*_{\omega_1,k_1}e^{(t_1+1-t_i)}S^*V^*_{\omega_i+1,k_i+1} \cdots V^*_{\omega_t,k_t}e^{(t_t+1-t_i)}S^*V^*_{\omega_t,k_t} \cdots \right] \]

\[ = \Tr\left[ \cdots TV^*_{\omega_1+1,k_1+1}T e^{(t_1+1-t_i)}S^*TTV^*_{\omega_1,k_1}T \cdots TV^*_{\omega_t,k_t}T e^{(t_t+1-t_i)}S^*TTV^*_{\omega_t,k_t}T \cdots \right] \]

\[ = \Tr\left[ \cdots TV^*_{\omega_1+1,k_1+1} T e^{(t_1+1-t_i)}S^*TTV^*_{\omega_1,k_1} T \cdots TV^*_{\omega_t,k_t} T e^{(t_t+1-t_i)}S^*TTV^*_{\omega_t,k_t} T \cdots \right] \]

\[ = \eta^{-1}(\theta_t \sigma) \Tr[\mathcal{W}^\theta_t(\theta_t \sigma)1] = \eta^{-1}(\sigma) e^{\omega_t(\sigma)} \Tr[\mathcal{W}^\theta_t(\theta_t \sigma)1] \]

In the last equality the KMS-condition (2.3) was used. The previous equalities follow from cyclicity of the trace, $TT = 1$, $V^*_{\omega,k} = V_{-\omega,k}$ and (4.22). Using (4.21), we calculate by change of integration variables (putting $I := \frac{1}{\dim \mathcal{H}} \in \mathcal{T}(\mathcal{H})$,)

\[ \mathbb{E}_I [e^{M_t, \sigma}] = \int_\Omega d\sigma \Tr[I \mathcal{W}_t(\sigma)1] e^{M_t, \sigma} = \int_\Omega d\sigma \Tr[I \mathcal{W}^\theta_t(\sigma)1] e^{-\omega^t(\sigma)} e^{-M_t, \sigma} \]

Since in the limit $t \uparrow \infty$, one can replace the initial state $I$ by $\rho$, as in (4.13), the formula (4.25) yields for all $\pi \in \mathcal{U}$ as in Lemma 4.1

\[ e(\pi) = e^{\vartheta}(1 - \pi) \text{ with } 1 - \pi := (1 - \kappa_1, \ldots, 1 - \kappa_{\mid K\mid}) \quad (4.26) \]

Finally, Proposition 2.8 follows from (4.26) by putting for some $\kappa \in \mathbb{C}$,

\[ \kappa_i := \kappa \quad i = 1, \ldots, \mid K\mid \]

thus obtaining $M_{t, \pi} = \kappa w^t$.
4.3 Proof of Proposition 2.9

The nonnegativity of the entropy production follows from Proposition 2.8 by Jensen’s inequality. To get the strict positivity from \(A2\), we first need to introduce more notation.

Let \(\rho\) be the unique stationary state of \(e^{tL}\). We decompose the states \(\rho\) and \(T\rho T\) in one-dimensional unnormalized states as

\[
\rho^* = \sum_{i \in D} \rho_i^*, \quad \rho_i^* \rho_j^* = \delta_{i,j} \|\rho_i^*\|^2, \quad \rho_i^* > 0, \quad i, j \in D
\]

(4.28)

where \(\rho^*\) can stand for \(\rho\) or \(T\rho T\) and \(D := \{1, \ldots, \dim \mathcal{H}\}\). The decomposition (4.28) differs from the spectral decomposition when \(\rho\) is degenerate. Remark that there is an arbitrariness in labeling the unnormalized states, as well as a possible arbitrariness stemming from degeneracies in \(\rho^*\). We partially fix this arbitrariness by asking that

\[
T(T\rho^*T)_j T = \rho_j^*
\]

(4.29)

This is always possible because the set \(T(T\rho^*T)_j T, j \in D\) satisfies all the requirements of (4.28) as a decomposition of \(\rho^*\). Let \(\tilde{\Omega}_t = \Omega_t \times D \times D\) for a \(t \geq 0\) and define the measure \(\tilde{P}_t\) by (letting \(g\) be a measurable function):

\[
\int_{\tilde{\Omega}_t} d\tilde{P}_t(\tilde{\sigma}) g(\tilde{\sigma}) = \sum_{i,j} \int_{\Omega_t} d\sigma \operatorname{Tr} \left[ \rho_i \mathcal{W}_t(\sigma) \frac{(T\rho T)_j}{\| (T\rho T)_j \|} \right] g(\sigma, i, j), \quad \tilde{\sigma} = (\sigma, i, j) \in \tilde{\Omega}_t
\]

(4.30)

where it is understood that \(\sigma \in \Omega_t\) and \(i, j \in D\). In the rest of this section we will use this notation without further comments. Positivity of \(\tilde{P}_t\) is obvious and normalization follows by

\[
\sum_{i,j} \int_{\Omega_t} d\sigma \operatorname{Tr} \left[ \rho_i \mathcal{W}_t(\sigma) \frac{(T\rho T)_j}{\| (T\rho T)_j \|} \right] = \sum_i \int_{\Omega_t} d\sigma \operatorname{Tr} [\rho_i \mathcal{W}_t(\sigma) 1] = \int d\rho_{\rho,t}(\sigma) = 1
\]

(4.31)

We call \(\tilde{P}^\theta_t\) the measure, constructed as above, but with \(\mathcal{W}^\theta_t\) replacing \(\mathcal{W}_t\). Remark that this is not the measure one would obtain by starting from \(H^\theta_S, V^\theta_k\) instead of \(H_S, V_k\), because then one would also replace \(\rho\) in (4.30) by \(\rho^\theta\), the stationary state of \(L^\theta\).

Define again the operation \(\theta_t\) on \(\tilde{\Omega}_t\) as

\[
\theta_t(\sigma, i, j) = (\theta_t \sigma, j, i)
\]

(4.32)
where the action of $\theta_t$ on $\Omega_t$ was defined in (4.23).

Consider the function

$$S^t : \tilde{\Omega}_t \mapsto \mathbb{R} \quad S^t(\tilde{\sigma}) = -\log \frac{d\tilde{P}^\theta(\theta \tilde{\sigma})}{d\tilde{P}(\tilde{\sigma})}$$ (4.33)

We upgrade the function $w^t$ on $\Omega_t$ to a function on $\tilde{\Omega}_t$ as

$$w^t(\tilde{\sigma}) = w^t(\sigma), \quad \tilde{\sigma} = (\sigma, i, j)$$ (4.34)

Our strategy will be to prove (Section 4.3.1) that for some $u > 0$

$$\int_{\tilde{\Omega}_t} d\tilde{P}_u(\tilde{\sigma}) S^u(\tilde{\sigma}) > 0$$ (4.35)

and then (Section 4.3.2) that for all $t \geq 0$

$$\int_{\tilde{\Omega}_t} d\tilde{P}_t(\tilde{\sigma})(S^t(\tilde{\sigma}) - w^t(\tilde{\sigma})) \leq 0$$ (4.36)

which will lead to the conclusion that for a certain $u \in \mathbb{R}^+$,

$$\int_{\Omega} d\tilde{P}_u(\sigma) w^u(\sigma) = \int_{\Omega} d\tilde{P}_u(\tilde{\sigma}) w^u(\tilde{\sigma}) > 0$$ (4.37)

where the first equality is checked by arguing as in (4.31). The converse statement is proven in Section 4.3.3.

4.3.1 Positivity of $S^t$

Looking back at the calculation (4.24), one immediately checks that for $t \geq 0$ and $\sigma \in \Omega$,

$$\text{Tr} \left[ \frac{\rho_i}{\|\rho_i\|} W_i(\sigma) \frac{(T \rho T)_j}{\|(T \rho T)_j\|} \right] = e^{w^t(\sigma)} \text{Tr} \left[ \frac{\rho_j}{\|\rho_j\|} W^\theta(\theta \sigma) \frac{(T \rho T)_i}{\|(T \rho T)_i\|} \right]$$ (4.38)

and hence

$$S^t(\tilde{\sigma}) = w^t(\tilde{\sigma}) - \log(\|\rho_j\|) + \log(\|\rho_i\|), \quad \tilde{\sigma} = (\sigma, i, j)$$ (4.39)

Note, using (4.33) and $S^t(\tilde{\sigma}) = -S^t(\theta \tilde{\sigma})$, that $S^t$ satisfies an exact fluctuation symmetry, for $t \geq 0$ and $\kappa \in \mathbb{C}$:

$$\int_{\tilde{\Omega}_t} d\tilde{P}_t(\tilde{\sigma}) e^{-\kappa S^t(\tilde{\sigma})} = \int_{\tilde{\Omega}_t} d\tilde{P}^\theta_t(\tilde{\sigma}) e^{-(1-\kappa)S^t(\tilde{\sigma})}$$ (4.40)
Remark that \( f : \mathbb{R} \to \mathbb{R} : x \to e^{-x} + x - 1 \) is positive for all \( x \), increasing for \( x \geq 0 \) and decreasing for \( x \leq 0 \). A Chebyshev inequality with \( \delta > 0 \) yields
\[
\int_{\tilde{\Omega}_t} d\tilde{P}_t(\tilde{\sigma}) S^t(\tilde{\sigma}) = \int_{\tilde{\Omega}_t} d\tilde{P}_t(\tilde{\sigma})(e^{-S^t} + S^t - 1)(\tilde{\sigma}) \geq (e^{-\delta} + \delta - 1)\tilde{P}_t(|S^t| \geq \delta)
\]
(4.41)
Rephrasing (2.15)-(2.16), there is for \( u > 0 \), a \( E \subset \Omega_u \), and one-dimensional projection \( P \in \mathcal{B}(\mathcal{H}) \) such that
\[
\int_{E} d\sigma \text{Tr} [P\mathcal{W}_u(\sigma)P] > 0, \quad w^u(E) = w \neq 0
\]
(4.42)
For any \( k \in \mathbb{N} \), we construct
\[
\Omega_{ku} \supset E^k := \{ \sigma_1 \sigma_2 \ldots \sigma_k, \mid \sigma_1, \ldots, \sigma_k \in E \}
\]
(4.43)
where the notation \( \sigma_1 \sigma_2 \), and consequently also \( \sigma_1 \sigma_2 \ldots \sigma_k \) was defined in (2.34). We have
\[
w^t(E^k) = kw, \quad \int_{E^k} d\sigma \text{Tr} [P\mathcal{W}_u(\sigma)P] > 0
\]
(4.44)
Since \( \rho \) is faithful, there are \( i, j \in \{1, \ldots, \dim \mathcal{H} \} \) such that
\[
\int_{E^k} d\sigma \text{Tr} [\rho_i \mathcal{W}_{ku}(\sigma)\rho_j] > 0
\]
(4.45)
Since the function \( S^u - w^u \) is bounded uniformly in \( u \in \mathbb{R}^+ \) (this follows e.g. from (4.39)), one can choose \( k \in \mathbb{N} \) and \( i, j \in \{1, \ldots, \dim \mathcal{H} \} \) such that
\[
\text{Tr} [\rho_i \mathcal{W}_{ku}(\sigma)\rho_j] = kw + \log \|\rho_i\| - \log \|\rho_j\| > 0, \quad \sigma \in E^k
\]
(4.46)
This proves that the last expression in (4.41) is not zero (after replacing \( t \) by \( ku \)). Hence, (4.35) is proven.

### 4.3.2 Difference between \( S^t \) and \( w^t \)

Calculate for \( t \geq 0 \)
\[
\int_{\tilde{\Omega}_t} d\tilde{P}_t(\tilde{\sigma}) \log \|\rho_j\| = \sum_{i,j \in D} \int_{\tilde{\Omega}_t} d\sigma \text{Tr} \left[ \rho_i \mathcal{W}_t(\sigma) \frac{(T\rho T)j}{\|\rho_j\|} \right] \log \|\rho_j\|
= \text{Tr} [\rho e^{t\mathcal{L}} \log T \rho T] = \text{Tr} [\rho \log T \rho T]
\]
(4.47)
and
\[ \int_{\tilde{\Omega}_t} d\tilde{\mathbb{P}}(\tilde{\sigma}) \log \|\rho_i\| = \sum_{i,j \in D} \int_{\tilde{\Omega}_t} d\sigma \text{Tr} \left[ \rho_i \mathcal{W}_i(\sigma) \frac{T_{\rho_j T}}{\|\rho_j\|} \right] \log \|\rho_i\| \]
\[ = \sum_{i \in D} \text{Tr} \left[ \rho_i e^{tC} 1 \right] \log \|\rho_i\| = \text{Tr} [\rho \log \rho] \quad (4.48) \]
where we used \( \rho e^{tC} = \rho \) and \( e^{tC} 1 = 1 \).
Hence one gets
\[ \int_{\tilde{\Omega}_t} d\tilde{\mathbb{P}}(\tilde{\sigma}) \left( \log((T\rho T)_i) - \log(\rho_j) \right) = \text{Tr} [\rho (\log \rho - \log T\rho T)] \leq 0 \quad (4.49) \]
where the last inequality follows from the nonnegativity of the relative entropy.

### 4.3.3 Strict positivity implies Assumption A2

We prove that \textbf{A2} is a necessary condition for a nonzero entropy production. First remark that
\[ \int_{\tilde{\Omega}_t} d\tilde{\mathbb{P}}(\tilde{\sigma}) w^t(\sigma) \quad (4.50) \]
is extensive in \( t > 0 \). This follows from translation invariance (in \( t \)) of \( w^t \) and stationarity of \( \mathbb{P}_\rho \). Hence we can fix \( t > 0 \) such that
\[ \left| \int_{\tilde{\Omega}_t} d\tilde{\mathbb{P}}(\tilde{\sigma}) w^t(\sigma) \right| > 2 \dim \mathcal{H} \max_{\omega,k} |\beta_k \omega| \quad (4.51) \]
Take \( \sigma \in \Omega_t \) satisfying \( \mathcal{W}_i(\sigma) \neq 0 \). It follows that one can split \( t = \sum_{i=1}^3 t_i \) and
\( \sigma = \tau_3 \tau_2 \tau_1, \quad \tau_i \in \Omega_i, \quad i = 1, 2, 3 \quad (4.52) \)
(again the notation (2.34) was used) such that
1. There is a one-dimensional projection \( P \) such that
\[ \text{Tr} [P \mathcal{W}_{t_2}(\tau_2) P] > 0 \quad (4.53) \]
2. \[ |\tau_1| \leq \dim \mathcal{H}, \quad |\tau_3| \leq \dim \mathcal{H} \quad (4.54) \]
Assume that \textbf{A2} does not hold. It follows that \( w^{t_2}(\tau_2) = 0 \). Hence, by (4.51),
\[ |w^t(\sigma)| = |w^{t_1}(\tau_1) + w^{t_3}(\tau_3)| \leq 2 \dim \mathcal{H} \max_{\omega,k} |\beta_k \omega| \quad (4.55) \]
which is in obvious contradiction with (4.51).
4.4 Proof of Proposition 2.10

This proof is by now quite standard, it can be found e.g. in [LS78]. We recall from (4.5) in Lemma 4.1 that we can interchange the limit $t \uparrow \infty$ and differentiation of $\pi \mapsto \epsilon(\pi)$. By differentiating relation (4.26) with respect to $\kappa_k$ and to $\beta_k'$ in $\pi = 0$ and $\beta_{k \in K} = \beta$, and interchanging limits and derivatives, we arrive at the modified Green-Kubo relation:

$$L_{k,l} + L^g_{k,l} = \beta \lim_{t \uparrow \infty} \frac{1}{t} \mathbb{E}_\rho [n^t_k n^t_{k'}]$$

(4.56)

from which the other statements in Proposition 2.10 easily follow.

4.5 Proof of proposition 2.13

Choose $v \in \mathcal{H}$ and $\phi \in L^2(\Omega_t)$ such that

$$H_S v = m_S v \quad \forall k \in K : \mathcal{N}_k^t \phi = m_k \phi \quad m_S, m_{k \in K} \in \mathbb{R}$$

(4.57)

By the definition of $U_t$,

$$U_t (v \otimes \phi)(\xi) = \sum_{\sigma \subset \xi} \int_{\Omega} d\tau \ u_t(\sigma, \tau) v \phi((\xi \setminus \sigma) \cup \tau), \quad \xi \in \Omega_t$$

(4.58)

Using $[S, H_S] = 0$, one checks that $u_t(\sigma, \tau)v$ either vanishes or

$$H_S (u_t(\sigma, \tau)v - v) = \sum_{\omega, k} \omega(\omega, k)(u_t(\sigma, \tau)v - v)$$

(4.59)

By (4.57), it follows that $\phi((\xi \setminus \sigma) \cup \tau) = 0$ in (4.58), unless for all $k \in K$

$$\sum_\omega \omega \omega(\omega, k) + \sigma_{\omega, k} = m_k$$

(4.60)

Together with (4.59), this implies

$$\mathcal{N}^t U_t (v \otimes \phi) = \mathcal{N}^t (v \otimes \phi) = (m_S + \sum_{k \in K} m_k)(v \otimes \phi)$$

(4.61)

Since the operators $H_S, \mathcal{N}_{k \in K}$ mutually commute, vectors like $v \otimes \phi$ as in (4.57) furnish a complete set of eigenvectors. This proves the proposition.
4.6 Proof of Proposition 3.1

By expanding the left-hand side of (3.10) in a Dyson expansion, as in (2.41), one can evaluate the derivatives, leading to

\[
\frac{\partial^2}{\partial v_1 \partial v_2} \mathbb{E}_\rho [n_k^1 n_k^2] | v_1 = 0, v_2 = u = \sum_{\omega_1, \omega_2} \omega_1 \omega_2 \text{Tr} [\rho \mathcal{J}_{\omega_1, k_1} e^{u\mathcal{L}} \mathcal{J}_{\omega_2, k_2}(1)]
\]

Putting \( \rho = \rho_\beta \), yields \( \rho_\beta V_{\omega, k} = V_{\omega, k} \rho_\beta e^{-\beta \omega} \). Now (3.10) follows after some reshuffling, using

\[
V_{\omega, k}^* = V_{-\omega, k}, \quad \eta_k(\omega) = e^{-\beta_k \omega} \eta_k(-\omega), \quad \sum_{\omega} \omega \eta_k(\omega) V_{\omega, k}^* V_{\omega, k} = \mathcal{L}_k(H_S)
\]

APPENDIX

Let \( \mathcal{A} \) be the matrix algebra \( M_n(\mathbb{C}) \) for some \( n \in \mathbb{N} \), and denote by \( \mathcal{A}^+ \) its positive cone, i.e,

\[
\mathcal{A}^+ = \{ x^* x \mid x \in \mathcal{A} \}
\]

An element \( x \in \mathcal{A}^+ \) is called strictly positive (notation: \( x > 0 \)) if it is invertible.

**Theorem 4.3.** Let \( \Lambda : \mathcal{A} \to \mathcal{A} \) be a completely positive linear map, satisfying

\[
\text{Tr} [x \Lambda y] > 0, \quad x, y \in \mathcal{A}^+, x \neq 0, y \neq 0
\]

Then, \( \Lambda \) has a positive eigenvalue \( \lambda \), such that if \( \mu \) is another eigenvalue, then \( |\mu| < \lambda \). The eigenvector \( v \in \mathcal{A} \) corresponding to \( \lambda \) can be chosen strictly positive. The eigenvalue \( \lambda \) is simple, i.e., as a root of the characteristic equation of \( \Lambda \) it has multiplicity 1.

The theorem was proven almost in the above form in [EHK78], (see Theorem 4.2 therein). We state (a simplified version of) that theorem and we show that the above statement follows from it. We call a positive map \( \phi \) on \( \mathcal{A} \) irreducible if

\[
\forall x \neq 0, y \neq 0 \in \mathcal{A}^+, \exists k \in \mathbb{N} : \text{Tr} [x \phi^k y] > 0
\]

**Theorem 4.4.** Let \( \phi \) be a positive map such that

1. \( \phi \) preserves the unit \( 1 \in \mathcal{A} : \phi(1) = 1 \)
2. $\phi$ satisfies the two-positivity inequality:

$$\phi(x^*x) \geq \phi(x)^*\phi(x) \text{ for all } x \in \mathcal{A} \quad (A-4)$$

3. For all $k = 1, 2, \ldots$, $\phi^k$ is irreducible

Then, $\phi$ has a positive, simple eigenvalue $\lambda$, such that if $\mu$ is another eigenvalue, then $|\mu| < \lambda$. The eigenvector $v \in \mathcal{A}$ corresponding to $\lambda$ can be chosen strictly positive.

Another theorem in [EHK78] is (Theorem 2.4, combined with the sentences following it):

**Theorem 4.5.** Let $\phi$ be an irreducible positive linear map on $\mathcal{A}$ and let $r$ be the spectral radius

$$r := \sup\{|c| \mid c \in \text{sp}\phi\} \quad (A-5)$$

then there is a unique eigenvector $v \in \mathcal{A}^+$ with eigenvalue $r$.

To prove Theorem 4.3, we remark that $\Lambda$ has the same spectral properties as a well-chosen map $\phi$ that satisfies the conditions of Theorem 4.4. Since $\Lambda$ is irreducible, one can apply Theorem 4.5 to find an eigenvector $v$. Because of $A-2$, we conclude that $v > 0$. Let now the map $\phi$ be defined as

$$\phi(x) = \frac{1}{r}v^{-1/2}\Lambda(v^{1/2}xv^{1/2})v^{-1/2}, \quad x \in \mathcal{A} \quad (A-6)$$

It is clear that

1. $\phi$ is completely positive and $\phi$ still satisfies $A-2$

2. $\phi(1) = 1$

3. $\text{sp}\phi = \frac{1}{r}\text{sp}\Lambda$ and also the multiplicities of the eigenvalues are equal

Hence $\phi$ satisfies the conditions of Theorem 4.4, since unity-preserving completely positive maps satisfy the two-positivity inequality $(A-4)$. Theorem 4.3 follows.

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