

Weighted Detailed Balance and Local KMS Condition for Non-Equilibrium Stationary States

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—Dedicated to the memory of Shuichi Tasaki—

A few words of remembrance of Shuichi Tasaki by L. Accardi

Our paths with Shuichi first met in the 1990's while I was living my three year teaching experience at Nagoya University. These first meetings developed into a tradition, perpetuated for several years and leading to periodic meetings between us which took place cyclically in a few venues such as: the universities of Waseda, Nagoya, Tohoku or Tokyo University of Science, Kyoto International Institute for Advanced Studies or RIMS, in Japan; the Solvay Institute in Europe and the series of the Solvay and of the quantum probability conferences in various parts of the world.

His early scientific education took place in the framework of Prigogine's group of which he later became one of the most appreciated representatives, led in those years by our common friend Joannis Antoniou who Prigogine had selected as his successor in his later years. This experience left a permanent track in his interests for irreversibility, in particular transport and non equilibrium phenomena, which accompanied him throughout his scientific carrier.

Given this scientific horizon, it was more than natural that he developed an interest for the stochastic limit of quantum theory which in those years was asserting itself, through a large multiplicity of results and applications to different fields of physics, as the natural mathematical approach to the description of these phenomena.

This community of interests led us to organize some conferences and workshops together (see the volume [5]) and the only occasion in which we wrote a joint paper came out very naturally from our scientific works and our discussions as follows. Tasaki became interested in the C^* algebraic approach to nonequilibrium phenomena and obtained several interesting and new results in the study of a single harmonic oscillator interacting with two chains of oscillators at different temperatures in the infinite volume limit regime [27]. Stimulated by his talk at the Meijo Winter School, organized by Professor T. Hida in January 2003, Accardi, Imafuku and Lu studied, in the stochastic limit regime, the case of a single harmonic oscillator coupled to the continuous analogue of two chains of oscillators at different temperatures, ie. two free boson fields [4]. Also in this case it

was possible to compute several quantities of physical interest. However the formulas obtained were quite different and a direct comparison seemed to be impossible also because in the C^* algebraic approach case these formulas looked quite complicated. It became soon clear that the correct way to compare the two limits was to introduce, also in the C^* algebraic approach case, a weak coupling parameter and, after the infinite volume limit, letting it tend to zero possibly with appropriate rescalings. The problem was to make this idea precise and this led to introduce, also in the C^* algebraic approach, the notions of slow and fast degrees of freedom which had become familiar in the stochastic limit. To concretely realize this program took some time, but eventually it was possible to prove that, in the (appropriately rescaled) weak coupling limit, the results of the C^* algebraic approach coincide with those of the stochastic limit approach [3].

Slightly later Accardi and Imafuku, pursuing the stochastic limit approach, introduced the notions of dynamical detailed balance, of local KMS condition, computed the adjoint of the non equilibrium generator in the stationary state and several other relations of interest [2].

These notions, their mutual relationships, their generalizations are the object of the present paper.

The last letter I have from ST dates back to March 5, 2005 and concerns the final touches to our joint paper. In the final part of this letter he writes to be very interested in these new notions and asks me to send him some material about them. I did, since I have always drawn great benefit and insight from discussions with him, but I never received any feed back. Only a few years later I was able to understand that around those years he should have begun a struggle quite different from the one scientists do in their attempts to understand aspects of nature.

Abstract

We give a general definition of the local KMS condition and we prove its equivalence with a nonlinear Gibbs prescription. We discuss the irreversible (H, β) -KMS condition, its connections with the local KMS condition and we study the irreversible (H, β) -KMS condition for Markov generators of stochastic limit type. We introduce a definition of weighted detailed balance based on the notion of current decomposition and discuss invariant states with constant micro-currents. As an example, we construct a non-equilibrium steady state for a quantum spin chain coupled to two reservoirs at different temperatures and study its cycle dynamics and entropy production.

1 Introduction

1.1 Multiplicity of characterizations of equilibrium states

The notion of equilibrium states of physical systems is sufficiently well understood in the sense that there exist several characterizations of this class of states which, although based on different ideas, when applicable to the same class of systems, define the same objects. For discrete systems, i.e. with a pure point spectrum Hamiltonian H , the most explicit description of an equilibrium state at inverse temperature β is the Boltzmann–Gibbs prescription

$$\rho = \frac{e^{-\beta H}}{Z} \quad (1)$$

meant in the sense that the right hand side of (1) defines a density operator. The KMS condition (see section 2) is more general because it is not restricted to discrete systems. In addition to this there are various types of variational principles, applicable to different classes of systems,

A further, more recently discovered, kind of characterization [8], [18] relates equilibrium states with Markov evolutions and was motivated by the Friedrichs–van Hove limit of open systems ($t \mapsto t/\lambda^2$, $\lambda \rightarrow 0$). More precisely in the 1970's it was realized that, if a Markov semigroup

$$\mathcal{T}_t = e^{t\mathcal{L}} \quad ; \quad t \geq 0$$

is obtained in the limit of weak coupling of a discrete systems with Hamiltonian H with an environment (Boson field) in a state of thermal equilibrium at inverse temperature β , then under some rather general conditions on the interaction, the Gibbs state of the discrete system, at the same inverse temperature of the environment, is an invariant state for the reduced evolution (\mathcal{T}_t) and the pair $\{\rho := e^{\beta H}/Z, (\mathcal{T}_t)\}$ satisfies the following two conditions:

- (i) The Markov semigroup (\mathcal{T}_t) has a ρ -adjoint (see Definition 4) which is a Markov semigroup.
- (ii) Denoting \mathcal{L}_ρ^* the generator of the ρ -adjoint semigroup of (\mathcal{T}_t) , there exists a self-adjoint operator $\Delta = \Delta^*$ such that

$$\mathcal{L} - \mathcal{L}_\rho^* = 2i[\Delta, \cdot] \quad (2)$$

Furthermore Δ commutes with H .

Motivated by this result and since in the classical case the above conditions, with $\Delta = 0$, characterize the *detailed balance property* for the pair $\{\rho, (\mathcal{T}_t)\}$, Kossakowski, Frigerio, Gorini, and Verri [18, 19] proposed to take conditions (i) and (ii) as definition of Quantum Detailed Balance (QDB) for the pair $\{\rho, (\mathcal{T}_t)\}$. Following the pattern used in classical probability these authors did not mention the role of the Hamiltonian H in their definition of QDB, but they proved that equilibrium states of an environment can be characterized by the property of producing, in the weak coupling limit for a sufficiently large class of discrete Hamiltonians and of interactions, pairs $\{\rho, (\mathcal{T}_t)\}$ which satisfy the QDB condition.

1.2 Lack of characterization results for non-equilibrium steady states

Non equilibrium, like nonlinearity is a term that covers an infinity of totally inequivalent situations. Therefore any attempt to characterize such a variety of behaviors in terms of a few qualitative properties would be naive and probably doomed to failure.

A more realistic program is to look for some interesting candidates that, within the huge class stationary states for a given Hamiltonian, singles out some special sub-class of states with properties that are rich enough to go beyond the equilibrium situation, but concrete enough to allow explicit study and, in some

cases, explicit solutions.

We expect that the simplest classes of such states should be characterized in terms of properties that generalize the known characterizations of equilibrium states. Moreover we expect that, in analogy with the situation in the equilibrium case, different characterizations lead to the same, or at least strictly related, states.

A huge literature exists on out of equilibrium phenomena, but up to recent times principles characterizing non-trivial classes of non-equilibrium states, based on ideas comparable for generality to the KMS condition or to quantum detailed balance, do not seem to have emerged.

1.3 The stochastic limit approach to non-equilibrium steady states

The theory of open systems studies the interactions between the slow and the fast degrees of freedom of (typically infinite) dynamical systems. In many, but by far not all, concrete examples, an open system is realized by switching an interaction between a discrete quantum system and a quantum field. In these models, the slow degrees of freedom include all the observables of the discrete system, but also some *slow* observables of the field and this fact allows in particular to define the energy and quanta microcurrents, which play a crucial role in the study of non-equilibrium phenomena. In the following we only consider these kind of models. This separation between slow and fast scales is emphasized by the rescaling $t \mapsto t/\lambda^2$, $\lambda \rightarrow 0$.

The weak coupling and low density limit study the reduced (Markovian) dynamics of the slow degrees of freedom in the above mentioned limit (see [21, 9, 11]), and the references therein.

The stochastic limit extends this picture by proving that, in the above limit, the fast degrees of freedom become a quantum white noise, by constructing not only the reduced, but the full limit dynamics, proving its unitarity and deducing the white noise and stochastic differential equation satisfied by this dynamics. The reduced Markovian dynamics is obtained as a corollary through the quantum Feynman–Kac formula. Furthermore, while in the weak coupling or low density limit only vacuum or equilibrium states were considered, the stochastic limit technique can be performed starting from a general class of non-equilibrium states of the environment.

In [2] these features were applied to the study of non-equilibrium phenomena as follows. Starting from a boson field with commutation relations $[a_k, a_{k'}^\dagger] = \delta(k - k')$ (k is the momentum variable), one considers the class of mean zero gauge invariant (hence stationary under the free field evolution) Gaussian states with covariance

$$\langle a_k^\dagger a_{k'} \rangle = \frac{1}{e^{\beta(\omega(k))} - 1} \delta(k - k') \quad (3)$$

where $\omega(k) \geq 0$ is the energy density of the field and $\beta : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ is a general nonlinear function satisfying some regularity conditions (see Theorem 1). In general these are non-equilibrium states of the field. The equilibrium case (with chemical potential equal to zero) is obtained when β is a linear function $\beta(x) = \hat{\beta}x$ with $\hat{\beta} > 0$.

1.4 Non-equilibrium and time reversal: the stochastic limit approach

In section 1.1 we discussed a deep relationship between the notions of equilibrium and detailed balance. On the other hand the term *detailed balance* is used in the physical literature as an equivalent formulation of the property of *reversibility* introduced in the theory of Markov processes. In fact every classical Markov process has a canonically defined *time reversed one* and the *reversibility* of a classical Markov process amounts to be isomorphic to its time reversed process. Accardi and Mohari [7] proved that a similar picture can be constructed in the quantum case.

However the physical notion of *equilibrium* has a meaning only when referred to a specific Hamiltonian evolution, while the purely probabilistic notion of detailed balance does not involve any Hamiltonian evolution. Without such a notion it is not possible to relate in a canonical way a Markov semigroup to a Gibbs state and one has to fall back to *ad hoc* prescriptions e.g. that the Gibbs state is invariant under the Markov semigroup.

The stochastic limit provides an ideal ground to overcome this impasse because it produces Markov processes that are canonically associated with Hamiltonian evolutions. Moreover, since the stochastic limit can be performed forward and backward in time, it also provides a natural tool to compare the *physical* and the *probabilistic* time reversals. More precisely: performing the stochastic limit in the forward and

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backward directions of time one obtains two quantum Markov processes which, by construction, are one the time reversed of the other. A natural question is therefore how this duality is reflected by the structure of the generators of the associated semigroups and their invariant states.

This issue was considered in [2] for a generic Hamiltonian H (see Theorem 7.3) with the additional assumption that the susceptibility coefficients are all different from zero and led to the following conclusions:

– The invariant state (unique under the above assumptions) is common for the two semigroups (forward and backward) and has the form

$$\rho = \frac{e^{-\beta(H)H}}{Z} \quad (4)$$

where Z is a normalization factor.

– If ρ is the common invariant state, the backward generator is the ρ -adjoint of the forward one.

– In the non equilibrium case the Kossakowski, Frigerio, Gorini, Verri quantum detailed balance condition (2) must be modified by the addition of a *current operator* Π_ρ :

$$\mathcal{L} - \mathcal{L}_\rho^* = 2i[\Delta \cdot] - \Pi_\rho \quad (5)$$

The relation (5) was called in [2] *Dynamical Detailed Balance* (see equations (102), (126), (127) in [2]). The possibility to consider, in the stochastic limit, the Heisenberg evolution also of some field degrees of freedom, allowed to deduce a natural interpretation of the operator Π_ρ in terms of micro-currents, due to flows of quanta and of energy between the field and the discrete system.

For this reason it is reasonable to call the operator Π_ρ *the current operator*.

Condition (4) is clearly a non-linear generalization of the Gibbs (KMS) condition. Notice that the function β , defining the stationary state (4) of the discrete system, is the same one defining the non-equilibrium state of the field. Thus condition (4) is a non-equilibrium generalization of the situation that was discussed in section 1.1: this is the *similarity principle in the stochastic limit of quantum theory*. In [2] it was proved that condition (4) is equivalent to a *local KMS condition* (see section 2 below).

1.5 Results of the present paper

We have seen that, from the stochastic limit approach to non equilibrium phenomena three general principles characterizing, a priori different, classes of non equilibrium states emerged: the local KMS condition, the irreversible KMS condition, the dynamical detailed balance condition. The study of the mutual relationships among these conditions begun in [2] and it was proved that, for a very special class of Markov semigroups – the *generic* ones (see section 7.3), they are equivalent.

However many open problems were left open in [2]: the extension of these results to Markov semigroups of stochastic limit type (see section 7) but non generic, the possibility to include Markov semigroups not of stochastic limit type; the connections with previous approaches to non equilibrium phenomena. These problems were considered by Fagnola and Umanità in the papers [15, 16, 17] and led to the introduction of some notions, such as *privileged representation of a Markov generator with respect to a state*, which plays a crucial role in the present paper.

The content of the present paper is the following. In section 2 we formulate a general definition of the local KMS condition and we prove its equivalence with the nonlinear Gibbs prescription (4). In section 3 we discuss the irreversible (H, β) -KMS condition and its connections with the local KMS condition. In section 4 we study how the irreversible (H, β) -KMS condition for a Markov generator \mathcal{L} is related to a weaker property enjoyed by all Markov generators of stochastic limit type (i.e. the property of mapping the commutant of H into itself).

After recalling, in section 5, some known facts about the adjoint of a Markov generator with respect to a state, in section 6, we generalize the notion of dynamical detailed balance (DDB) by introducing the definition of weighted detailed balance (WDB) for general (bounded) Markov generators, which allows to get rid of the restriction, implicitly used in [2], to Markov generators of stochastic limit type. In section 7 we extend the result of [2] showing that all Markov generators of stochastic limit type with respect to an Hamiltonian H satisfy a weighted detailed balance condition.

In section 8 we establish a connection between WDB and the cycle description of Markov generators used in the Qian–Kalpazidou approach and we apply this connection, in section 8.1, to discuss invariant states with constant micro-currents. In section 9 we construct an example of a non-equilibrium steady state for a quantum spin chain coupled to two reservoirs at different temperatures, and for this model discuss cycle dynamics and entropy production (10).

Finally Appendix I and Appendix II (resp. sections 11 and 12) recall some standard notions and results of the stochastic limit frequently used in the present paper.

2 The local KMS condition

We denote $\mathcal{B}(\mathcal{H})$ the von Neumann algebra of all bounded operator on a separable Hilbert space \mathcal{H} and $\text{Tr}(\mathcal{H})$ the corresponding space of trace class operators. In the following we will be mostly concerned with bounded generators, but we try to state the main definitions and problems so that the extension to unbounded ones becomes as transparent as possible.

Definition 1. Let be given a von Neumann algebra \mathcal{A} acting on a Hilbert space \mathcal{H} , a self-adjoint operator H affiliated with \mathcal{A} and a Borel function

$$\beta : \mathbb{R}_+ \rightarrow \mathbb{R}_+$$

Denote

$$u_t : \mathcal{A} \ni x \rightarrow u_t(x) := e^{itH} x e^{-itH} =: x(t) \in \mathcal{A} \quad (6)$$

the 1-parameter automorphism group of \mathcal{A} generated by H (Heisenberg evolution). A normal state φ on \mathcal{A} is said to satisfy the local KMS condition with respect to the function β and the Heisenberg dynamics (6) (simply the (H, β) -KMS condition, or the local KMS condition, if no confusion is possible), if, for each $x, y \in \mathcal{A}$:

(i) The map

$$\mathbb{R} + i\beta(\text{spec}(H)) \ni t + i\beta(\lambda) \mapsto \varphi(xy(t + i\beta(\lambda))) \quad (7)$$

is well defined by analytic continuation of the map $t \in \mathbb{R} \mapsto \varphi(xy(t))$.

(ii) Denoting $E_H(\cdot)$ the spectral measure of H and introducing the complex valued measure

$$\mathbb{R}_+ \times \mathbb{R}_+ \supseteq I \times J \mapsto \varphi_{x,y,H}(I, J) := \varphi_{x,y,H}(xE_H(I)yE_H(J)) \quad (8)$$

for each $t \in \mathbb{R}$ the integral

$$\int_{\mathbb{R}_+ \times \mathbb{R}_+} e^{it(\lambda-\mu)} e^{\beta(\mu)\mu - \beta(\lambda)\lambda} \varphi_{x,y,H}(d\lambda, d\mu) =: \varphi(xy(t + i\beta(H))) \quad (9)$$

exists.

(iii) In the notations (6), (9) for all $t \in \mathbb{R}$ the following identity holds:

$$\varphi(xy(t + i\beta(H))) = \varphi(y(t)x) \quad (10)$$

Remark. If H is bounded and β is a locally bounded function (bounded on bounded sets), then the operator $\exp(\beta(H)H)$ is bounded and for all $x \in \mathcal{A}$ and $t \in \mathbb{R}$ one has:

$$\begin{aligned} y(t + i\beta(H)) &= e^{i(t+i\beta(H))H} x e^{-i(t+i\beta(H))H} = e^{-\beta(H)H} e^{itH} x e^{-itH} e^{\beta(H)H} \\ &= e^{-\beta(H)H} x(t) e^{\beta(H)H}. \end{aligned} \quad (11)$$

In the general case the operator $\exp(\beta(H)H)$ is well defined by the spectral theorem and affiliated with \mathcal{A} . Moreover both linear multiplicative maps on $\mathcal{B}(\mathcal{H})$

$$\mathcal{B}(\mathcal{H}) \ni x \mapsto e^{-\beta(H)H} x e^{\beta(H)H} \quad ; \quad \mathcal{B}(\mathcal{H}) \ni x \mapsto e^{\beta(H)H} x e^{-\beta(H)H} \quad (12)$$

can be shown to preserve the trace on $\mathcal{B}(\mathcal{H})$ (and also on \mathcal{A} , if \mathcal{A} is semi-finite). Therefore the maps (12) are densely defined on $\mathcal{B}(\mathcal{H})$ and, in the following, whenever these maps will be used, it will always be

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understood that their arguments are in their domains.

With these notations the local KMS condition (10) can be re-written in the more intuitive form:

$$\varphi \left(x e^{-\beta(H)H} y(t) e^{\beta(H)H} \right) = \varphi (y(t)x) ; \forall x, y \in \mathcal{B}(\mathcal{H}), \forall t \in \mathbb{R} \quad (13)$$

Differentiating (13) at $t = 0$ one finds

$$\varphi \left(x e^{-\beta(H)H} \delta(y) e^{\beta(H)H} \right) = \varphi (\delta(y)x) \quad (14)$$

where

$$\delta(y) := i[H, y] \quad ; \quad y \in \mathcal{B}(\mathcal{H}) \cap \text{Domain}(i[H, \cdot])$$

is the infinitesimal generator of the Heisenberg dynamics.

The identity (14) gives the infinitesimal form of the local KMS condition.

Let $H = H^* \in \mathcal{B}(\mathcal{H})$ be a positive self-adjoint operator (Hamiltonian) with discrete spectral decomposition

$$H = \sum_{\epsilon \in \text{Spec}(H)} \epsilon P_\epsilon = \sum_{m \in \mathbb{N}} \epsilon_m P_m \quad (15)$$

and let $\beta : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ be a Borel function such that $e^{-\beta(H)H} \in \text{Tr}(\mathcal{H})$. For a density operator $\rho \in \text{Tr}(\mathcal{H})$ with corresponding normal state on $\mathcal{B}(\mathcal{H})$

$$\tilde{\rho}(\cdot) := \text{Tr}(\rho(\cdot)), \quad (16)$$

one can define $\tilde{\rho}(xy(t + i\beta(H)))$ by means of (9). Here the spectral resolution of H is atomic, hence the integral is reduced to a double series.

Theorem 1. *The following are equivalent:*

(i) ρ satisfies the local (H, β) -KMS condition

$$\tilde{\rho}(xy(t + i\beta(H))) = \tilde{\rho}(y(t)x), \quad \forall x, y \in \mathcal{B}(\mathcal{H}), \forall t \in \mathbb{R} \quad (17)$$

(ii) $e^{-\beta(H)H}$ is trace class and

$$\rho = \rho_{\beta, H} := Z_\beta^{-1} e^{-\beta(H)H}, \quad Z_\beta := \text{tr} \left(e^{-\beta(H)H} \right) \quad (18)$$

Proof. (i) \Rightarrow (ii). We observed (see (13) and the remark before it) that (17) can be more explicitly written in the form:

$$\text{tr} \left(\rho x e^{-\beta(H)H} y(t) e^{\beta(H)H} \right) = \text{tr}(\rho y(t)x) ; \forall x, y \in \mathcal{B}(\mathcal{H}), \forall t \in \mathbb{R} \quad (19)$$

Putting $t = 0$ and using the cyclicity of the trace we find

$$\text{tr} \left(x e^{-\beta(H)H} y e^{\beta(H)H} \rho \right) = \text{tr}(x\rho y) \quad ; \quad \forall x, y \in \mathcal{B}(\mathcal{H})$$

Since $x \in \mathcal{B}(\mathcal{H})$ is arbitrary, this is equivalent to

$$e^{-\beta(H)H} y e^{\beta(H)H} \rho = \rho y, \quad (20)$$

which holds if and only if

$$y e^{\beta(H)H} \rho = e^{\beta(H)H} \rho y \quad ; \quad \forall y \in \mathcal{B}(\mathcal{H}), \quad (21)$$

and this implies that, for some scalar $\lambda (\neq 0$ because $\text{tr}(\rho) = 1$), one has:

$$e^{\beta(H)H} \rho = \lambda 1 \quad (22)$$

In particular ρ is invertible and the condition $\text{tr}(\rho) = 1$ implies (18).

Thus condition (ii) is necessary for the validity of (i).

Let us prove that it is also sufficient, i.e. that (ii) \Rightarrow (i).

This follows because the identity (17), given (13) and (18), can be rewritten in the form:

$$\begin{aligned}\tilde{\rho}(xy(t + i\beta(H))) &= \text{tr} \left(\rho x e^{-\beta(H)H} y(t) e^{\beta(H)H} \right) \\ &= Z_\beta^{-1} \text{tr} \left(x e^{-\beta(H)H} y(t) \right) = \text{tr} (\rho y(t)x) = \tilde{\rho}(y(t)x)\end{aligned}\tag{23}$$

□

Remark.

- (i) Notice that when $\beta(H) = \beta$ (constant), the state (18) is the usual Gibbs state at inverse temperature β .
- (ii) Our condition that $\beta : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ excludes the case that some value of β could be $+\infty$. This means that every state of the form (18) is faithful. We will see that some equivalent formulations of the KMS condition are meaningful also for non faithful states. However in the present paper we will restrict our attention to faithful states.
- (iii) Since $H \geq 0$ and adding a constant to H does not change the dynamics, one can suppose that $H > 0$, i.e. that H is invertible. With this convention, if ρ is any invertible density operator which is a function of the Hamiltonian then, for some function

$$\begin{aligned}F : \mathbb{R}_+ &\rightarrow \mathbb{R}_+ \\ \rho &= Z^{-1} e^{-F(H)} = Z^{-1} e^{-\frac{F(H)}{H} H}\end{aligned}$$

So that, defining $\beta(H) := F(H)H^{-1}$ ρ has the form (18). Thus the local KMS condition distinguishes, among the faithful invariant states of a dynamics, those which are functions of the dynamics, i.e. in $\{H\}''$.

3 The irreversible (H, β) -KMS condition

In the following, by a *Markov semigroup* (resp. *Markov generator*) we mean a weak*-continuous semigroup (resp. generator) of completely positive (resp. conditionally completely positive), normal, identity preserving maps on $\mathcal{B}(\mathcal{H})$. We will freely use the convention introduced in the remark after Definition 1.

In the present section we introduce an irreversible generalization of the local KMS condition, relating a Markov semigroup with a state (see the identity (41) of [2]). We prove that, under general additional conditions on the Markov generator the two conditions characterize the same family of states.

We start by the following proposition motivating our definition of irreversible (H, β) -KMS condition.

Proposition 1. *Suppose that the Hamiltonian H given by (15) is non degenerate, namely eigenvectors ϵ_n are distinct and their eigenspaces are one-dimensional, then the infinitesimal local (H, β) -KMS condition (14) is equivalent to the local (H, β) -KMS condition (13).*

Proof. Let $|\epsilon_m\rangle$ and $|\epsilon_n\rangle$ be the eigenvalues corresponding to the eigenvectors ϵ_m and ϵ_n . The rank-one operator $|\epsilon_m\rangle\langle\epsilon_n|$ satisfies

$\delta(|\epsilon_m\rangle\langle\epsilon_n|) = i(\epsilon_m - \epsilon_n)|\epsilon_m\rangle\langle\epsilon_n|$. It follows that the range of the map δ contains all rank-one operators $|\epsilon_m\rangle\langle\epsilon_n|$ with $n \neq m$.

By the arbitrariness of $x \in \mathcal{B}(\mathcal{H})$, the infinitesimal local (H, β) -KMS condition (14) yields as in the proof of Theorem 1 (formula (20))

$$|\epsilon_m\rangle\langle\epsilon_n| e^{\beta(H)H} \rho = e^{\beta(H)H} \rho |\epsilon_m\rangle\langle\epsilon_n|.$$

It follows that $e^{\beta(H)H} \rho \epsilon_m = e^{\beta(H)H} \rho \epsilon_n$ for all $n \neq m$, namely $e^{\beta(H)H} \rho$ is a multiple of the identity operator and the conclusion follows as in the proof of Theorem 1. □

We now introduce the irreversible KMS condition in infinitesimal form.

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Definition 2. Let \mathcal{L} be a Markov generator, ρ a state on $\mathcal{B}(\mathcal{H})$, and (H, β) as in section (2). The pair (ρ, \mathcal{L}) is said to satisfy the infinitesimal form of the irreversible (H, β) -KMS condition

$$\mathrm{tr}(\rho x e^{-\beta(H)H} \mathcal{L}(y) e^{\beta(H)H}) = \mathrm{tr}(\rho \mathcal{L}(y)x) \quad (24)$$

for all $x \in \mathcal{B}(\mathcal{H})$ and $y \in \mathrm{Domain}(\mathcal{L})$ for which the left hand side of (24) is well defined.

Remark. In the notation (16), (24) becomes

$$\tilde{\rho} \left(x e^{-\beta(H)H} \mathcal{L}(y) e^{\beta(H)H} \right) = \tilde{\rho}(\mathcal{L}(y)x) \quad (25)$$

Comparing this with (14) we see that (24) (or (25)) is a natural irreversible generalization of the infinitesimal form of the local KMS condition which is equivalent to the local KMS condition in generic cases described in Proposition 1. Denoting

$$\mathcal{T}_t := e^{t\mathcal{L}} \quad ; \quad t \geq 0$$

the Markov semigroup generated by \mathcal{L} and with the notation

$$y(t) := \mathcal{T}_t(y) \quad ; \quad y \in \mathcal{B}(\mathcal{H}) \quad (26)$$

With this notations the integral form of condition (24), called in the following the *irreversible (H, β) -KMS condition for the pair (ρ, \mathcal{T}_t)* , is:

$$\tilde{\rho} \left(x e^{-\beta(H)H} y(t) e^{\beta(H)H} \right) = \tilde{\rho}(y(t)x) \quad ; \quad t \geq 0, \forall x, y \in \mathcal{B}(\mathcal{H}) \quad (27)$$

which is clearly a generalization, to irreversible evolutions, of the local KMS condition in its formulation (13).

Taking derivative at $t = 0$ shows that (27) implies (24).

Remark. Condition (27) with $t = 0$, implies that the state ρ has the form $\rho = Z^{-1} e^{-\beta(H)H}$. This is an immediate consequence of the proof of (i) \Rightarrow (ii) in Theorem 1. Hence, by replacing $\rho = Z^{-1} e^{-\beta(H)H}$ in the right-hand side of (27), we get $\mathrm{tr}(Z^{-1} e^{-\beta(H)H} x e^{-\beta(H)H} y(t) e^{\beta(H)H}) = \mathrm{tr}(Z^{-1} x e^{-\beta(H)H} y(t)) = (\rho y(t)x)$, $t \geq 0 \forall x, y \in \mathcal{B}(\mathcal{H})$. Therefore (27) does not impose any condition on the pair (ρ, \mathcal{T}_t) for $t > 0$. As a consequence the irreversible (H, β) -KMS condition, introduced in infinitesimal form in Definition 2, is *not* equivalent to (27).

4 Markov generators associated with a given Hamiltonian

The irreversible (H, β) -KMS condition, in infinitesimal form of Definition 2, implies a strong connection of the Markov semigroup (\mathcal{T}_t) (and of its generator) with H : it must be in some sense *associated* with H . The stochastic limit of quantum theory (in absence of external forces) gives rise to such a class of Markov semigroups: they have the property to leave invariant the commutant algebra of an Hamiltonian operator H (which in the stochastic limit is interpreted as the Hamiltonian of the *small* system coupled to the environment).

Recall that the commutant algebra $\{H\}'$ of a self-adjoint operator H is, by definition, the commutant of the (abelian) von Neumann algebra generated by the spectral projections of H .

In fact the property of leaving $\{H\}'$ invariant is a consequence of a very detailed structure of the above mentioned class of Markov semigroups which implies several other properties and which will be described in section 12 below. In the present section we concentrate our analysis on the connections between this property and the irreversible (H, β) -KMS condition.

In the following, operators commuting with a self-adjoint operator H will be called *H-diagonal* (simply diagonal if no confusion is possible).

Definition 3. Let H be a self-adjoint operator. A Markov semigroup (\mathcal{T}_t) with generator \mathcal{L} is called *associated to H* if:

$$\mathcal{T}_t(\{H\}') \subseteq \{H\}' \quad \forall t \geq 0 \quad (28)$$

or, in infinitesimal form:

$$\mathcal{L}(\mathrm{Domain}(\mathcal{L}) \cap \{H\}') \subseteq \{H\}' \quad (29)$$

We now fix the Hamiltonian (15). Since it has discrete spectrum the map

$$\mathcal{B}(\mathcal{H}) \ni x \mapsto E_0(x) := \sum_{n \in \mathbb{N}} P_n x P_n$$

is a normal Umegaki conditional expectation (completely positive norm one projection) onto the commutant of H , i.e. the *diagonal algebra*. Therefore:

$$\{H\}' = \{x \in \mathcal{B}(\mathcal{H}) : [x, H] = 0\} = \{x \in \mathcal{B}(\mathcal{H}) : E_0(x) = x\} \quad (30)$$

The elements of the operator space

$$\begin{aligned} \mathcal{B}(\mathcal{H})_{off} &:= \{x - E_0(x) : x \in \mathcal{B}(\mathcal{H})\} = \{x \in \mathcal{B}(\mathcal{H}) : E_0(x) = 0\} \\ &= \{x \in \mathcal{B}(\mathcal{H}) : x = \sum_{m \neq n} P_m x P_n\} \end{aligned} \quad (31)$$

will be called the *off-diagonal space*.

A Markov generator \mathcal{L} is associated with H if and only if:

$$\mathcal{L} \circ E_0 = E_0 \circ \mathcal{L} = E_0 \circ \mathcal{L} \circ E_0 \quad (32)$$

and one easily verifies that this is equivalent to say that

$$x \in \text{Domain}(\mathcal{L}) \Leftrightarrow E_0(x), x - E_0(x) \in \text{Domain}(\mathcal{L})$$

and

$$\mathcal{L}(\text{Domain}(\mathcal{L}) \cap \mathcal{B}(\mathcal{H})_{off}) \subseteq \mathcal{B}(\mathcal{H})_{off} \quad (33)$$

Lemma 1. *Let H and β be as in Theorem (1) and suppose that:*

(i) \mathcal{L} be a Markov generator satisfying (32).

(ii) ρ is a function of H .

Then, if either x or y are diagonal, the identity (24) (infinitesimal form of the irreversible (H, β) -KMS condition) holds for any choice of the function β .

Proof. If $y \in \{H\}'$, (32) implies that also $\mathcal{L}(y) \in \{H\}'$. Therefore, taking the traspose in a base diagonalising H ,

$$\text{tr}(\rho x e^{-\beta(H)H} \mathcal{L}(y) e^{\beta(H)H}) = \text{tr}(\rho e^{\beta(H)H} \mathcal{L}(y) e^{-\beta(H)H} x) = \text{tr}(\rho \mathcal{L}(y) x)$$

Since ρ is a function of H and $\mathcal{L}(y) \in \{H\}'$ we conclude that:

$$\text{tr}(\rho e^{\beta(H)H} \mathcal{L}(y) e^{-\beta(H)H} x) = \text{tr}(\mathcal{L}(y) \rho x) = \text{tr}(\rho x \mathcal{L}(y))$$

which is (24).

If $x \in \{H\}'$, since ρ is a function of H , we have:

$$\text{tr}(\rho e^{\beta(H)H} \mathcal{L}(y) e^{-\beta(H)H} x) = \text{tr}(\rho e^{\beta(H)H} x \mathcal{L}(y) e^{-\beta(H)H}) = \text{tr}(\rho x \mathcal{L}(y))$$

which is again (24).

Remark. Notice that the above proof of Lemma 1 cannot be applied in general if, instead of assuming that ρ is a function of H , one only assumes that $\rho \in \{H\}'$.

Lemma 2. *In the assumptions of Lemma 1, the identity (24) holds for any choice of the function β whenever x and y are in the off-diagonal space.*

Proof. Suppose that $x, y \in \mathcal{B}(\mathcal{H})_{off}$. Then

$$\begin{aligned} \text{tr}(\rho e^{\beta(H)H} \mathcal{L}(y) e^{-\beta(H)H} x) &= \sum_{m \neq n} \sum_{h \neq k} \text{tr}(\rho e^{\beta(H)H} P_m \mathcal{L}(y) P_n P_h e^{-\beta(H)H} x P_k) \\ &= \sum_{m \neq n} \sum_{n \neq k} \text{tr}(\rho e^{\beta(H)H} P_m \mathcal{L}(y) P_n e^{-\beta(H)H} x P_k) \\ &= \sum_n \sum_{m \neq n} \sum_{k \neq n} \text{tr}(\rho e^{\beta(H)H} P_m \mathcal{L}(y) P_n e^{-\beta(H)H} x P_k) \end{aligned}$$

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Since ρ is a function of H this is equal to

$$\begin{aligned} & \sum_n \sum_{m \neq n} \sum_{k \neq n} \delta_{m,k} \text{tr}(\rho e^{\beta(H)H} P_m \mathcal{L}(y) P_n e^{-\beta(H)H} x) \\ &= \sum_{n \neq k} \text{tr}(\rho e^{\beta(H)H} P_k \mathcal{L}(y) P_n e^{-\beta(H)H} x) \end{aligned}$$

Since y , hence $\mathcal{L}(y)$, is off-diagonal, this is equal to

$$\text{tr}(\rho e^{\beta(H)H} \mathcal{L}(y) e^{-\beta(H)H} x)$$

and the identity (24) becomes equivalent to:

$$\text{tr}(\rho e^{\beta(H)H} \mathcal{L}(y) e^{-\beta(H)H} x) = \text{tr}(e^{\beta(H)H} \rho \mathcal{L}(y) e^{-\beta(H)H} x) = \text{tr}(\rho \mathcal{L}(y) x) \quad (34)$$

where the first identity in (34) holds because ρ is a function of H .

Now notice that, if $z \in \{H\}'$, then

$$\text{tr}(e^{\beta(H)H} \rho \mathcal{L}(y) e^{-\beta(H)H} z) = \text{tr}(e^{\beta(H)H} \rho \mathcal{L}(y) z e^{-\beta(H)H}) = \text{tr}(\rho \mathcal{L}(y) z)$$

Therefore, for any $z \in \{H\}'$, (34) is equivalent to

$$\text{tr}(e^{\beta(H)H} \rho \mathcal{L}(y) e^{-\beta(H)H} (x + z)) = \text{tr}(\rho \mathcal{L}(y) (x + z)) \quad (35)$$

But, since x is arbitrary off-diagonal and z is arbitrary diagonal, $x + z$ is arbitrary in $\mathcal{B}(\mathcal{H})$. Therefore (35) is equivalent to:

$$e^{\beta(H)H} \rho \mathcal{L}(y) e^{-\beta(H)H} = \rho \mathcal{L}(y)$$

for every off-diagonal y . But, under this condition, it is clear that the identity (34), and therefore (24), is satisfied. This proves the statement.

Theorem 2. Let H and β be as in Theorem (1) and let be given:

- (i) a Markov generator \mathcal{L} associated with H , i.e. satisfying (32),
- (ii) a density operator ρ which is a function of H .

Then (24) (infinitesimal form of the (H, β) -DDB condition) holds for any choice of the function β .

Remark.

- (i) It should be emphasized that the above theorem does not require the invertibility of ρ : any function of the Hamiltonian H would do.
- (ii) Since any element of $\mathcal{B}(\mathcal{H})$ can be written in a unique way as a sum of a diagonal and an off diagonal part, Lemma (1) allows to reduce the proof of (24) to the case in which both x and y are in the off-diagonal space and, in this case the validity of (24) is guaranteed by Lemma 2.
- (iii) Theorem 2 says that, if \mathcal{L} is a Markov generator associated with H , then for any density operator ρ , which is a function of H i.e. such that $\rho \in \{H\}''$, the pair (ρ, \mathcal{L}) satisfies the infinitesimal form of the irreversible (H, β) -KMS condition. It is therefore natural to ask oneself if, under the same condition on \mathcal{L} , there exist other density operators with the same property.

The following theorem answers this question.

Theorem 3. Let H, β be as in Theorem 2 and let ρ be a state on $\mathcal{B}(\mathcal{H})$ and \mathcal{L} a Markov generator (not necessarily associated with H).

Then the pair (ρ, \mathcal{L}) satisfies the infinitesimal form (24), of the irreversible (H, β) -KMS condition, if and only if:

$$e^{\beta(H)H} \rho \in \{\text{Range}(\mathcal{L})\}' \quad (36)$$

Proof. Since the pair (ρ, \mathcal{L}) satisfies the infinitesimal form (24), one has for all $x, y \in \mathcal{B}(\mathcal{H})$:

$$\mathrm{tr}(e^{\beta(H)H} \rho x e^{-\beta(H)H} \mathcal{L}(y)) = \mathrm{tr}(\rho \mathcal{L}(y)x)$$

if and only if

$$\mathrm{tr}(e^{-\beta(H)H} \mathcal{L}(y) e^{\beta(H)H} \rho x) = \mathrm{tr}(\rho \mathcal{L}(y)x).$$

Since $x \in \mathcal{B}(\mathcal{H})$ is arbitrary, this is equivalent to:

$$e^{-\beta(H)H} \mathcal{L}(y) e^{\beta(H)H} \rho = \rho \mathcal{L}(y) \quad \text{if and only if} \quad \mathcal{L}(y) e^{\beta(H)H} \rho = e^{\beta(H)H} \rho \mathcal{L}(y)$$

Since $y \in \mathcal{B}(\mathcal{H})$ is arbitrary, this is equivalent to (36).

Corollary 1. *If the Markov generator \mathcal{L} satisfies (24) and the commutant of the range of \mathcal{L} is trivial, i.e.*

$$\{\mathrm{Range}(\mathcal{L})\}' = \mathbb{C} \cdot 1 \tag{37}$$

then ρ has the form (18).

Proof. The thesis follows because (36) implies that $e^{\beta(H)H} \rho$ is a multiple of the identity and we have seen that this implies that ρ has the form (18).

5 Time reversed and adjoints of a Markov generator

The theory of stochastic limit allows us to associate in a canonical way to a system with free Hamiltonian H , interacting with an *environment*, two Markov processes: the *forward* and the *backward* process, obtained by taking the stochastic limit respectively in the forward and backward time direction.

Like all Markov processes also these ones are canonically associated to Markov semigroups, the forward and the backward (or *time reversed*) semigroup, whose structure depends not only on H but also on the free Hamiltonian of the environment, on the interaction and on the initial state of the environment. The generators of the forward and the backward semigroup are related by a kind of duality relation introduced in [2] and called *dynamical detailed balance condition*. If the initial state of the environment is an equilibrium one, this reduces to Kossakowski, Frigerio, Gorini, Verri detailed balance.

In the following sections we will analyze the connections between the above mentioned duality and some known operator-theoretical duality notions between Markov semigroups or their generators. For this reason, in the present section, we recall some of these duality notions and their properties.

If $\mathcal{L} : \mathcal{D} \subseteq \mathcal{B}(\mathcal{H}) \rightarrow \mathcal{B}(\mathcal{H})$ is any linear operator, with a dense domain \mathcal{D} , the *trace dual* of \mathcal{L} is by definition the linear operator $\mathcal{L}_* : \mathcal{D}_* \subseteq \mathrm{Tr}(\mathcal{H}) \rightarrow \mathrm{Tr}(\mathcal{H})$, with domain \mathcal{D}_* , defined by the relation

$$\mathrm{tr}(\omega \mathcal{L}(x)) = \mathrm{tr}(\mathcal{L}_*(\omega)x) \quad ; \quad \omega \in \mathcal{D}_*, x \in \mathcal{D}. \tag{38}$$

A density operator $\rho \in \mathcal{D}_*$ is called \mathcal{L} -stationary if

$$\mathcal{L}_*(\rho) = 0 \tag{39}$$

For Markov generators the following notions of duality with respect to a fixed state ρ is often used.

Definition 4. *Given a densely defined linear operator Φ on $\mathrm{Dom}(\Phi) \subseteq \mathcal{B}(\mathcal{H})$ and a normal state ρ on $\mathcal{B}(\mathcal{H})$, the linear operator $(\Phi_\rho^*, \mathrm{Dom}(\Phi_\rho^*))$ is the adjoint of Φ with respect to the scalar product induced by ρ on $\mathcal{B}(\mathcal{H})$, i.e.*

$$\langle x, y \rangle_\rho =: \mathrm{tr}(\rho x^* y) \quad ; \quad x, y \in \mathcal{B}(\mathcal{H}) \tag{40}$$

More explicitly, the pair $(\Phi_\rho^*, \mathrm{Dom}(\Phi_\rho^*))$, where $\mathrm{Dom}(\Phi_\rho^*)$ is

$$\{x \in \mathcal{B}(\mathcal{H}) : \exists z \in \mathcal{B}(\mathcal{H}), \forall y \in \mathrm{Dom}(\Phi), \mathrm{tr}(\rho zy) = \mathrm{tr}(\rho x \Phi(y))\}$$

and

$$\mathrm{tr}(\rho \Phi_\rho^*(x)y) = \mathrm{tr}(\rho x \Phi(y)), \quad \forall y \in \mathrm{Dom}(\Phi), \tag{41}$$

is called the ρ -adjoint of Φ and we denote it simply by Φ_ρ^* .

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Remark.

- (i) Due to the non-commutativity, there are other choices for a scalar product on $\mathcal{B}(\mathcal{H})$ induced by ρ . In fact for every real parameter $s \in [0, 1]$ one can define a s -scalar product by means of $\langle x, y \rangle_s = \text{tr}(\rho^{1-s} x \rho^s y)$. Fagnola and Umanità have shown that, concerning detailed balance, there are two prototype cases: $s = 0$, (that we consider in this work) and $s = 1/2$, see [16, 17].
- (ii) If \mathcal{L} is a Markov generator written in the standard GKSL form:

$$\mathcal{L}(x) = \sum_k \left(L_k^* x L_k - \frac{1}{2} \{L_k^* L_k, x\} \right) \quad (42)$$

and ρ is invertible, then the formal expression for \mathcal{L}_ρ^* is

$$\mathcal{L}_\rho^*(x) = \sum_k \left(\rho^{-1} L_k \rho x L_k^* - \frac{1}{2} (x L_k^* L_k + \rho^{-1} L_k^* L_k \rho x) \right); \quad x \in \mathcal{B}(\mathcal{H})$$

From this it is clear that, even if \mathcal{L} is Markov generator, in general its ρ -adjoint does not need to be densely defined or to map the bounded operators into themselves. Furthermore, even if either of these properties holds, in general it will not be a Markov generator.

- (iii) Putting $x = 1$ in (41) one finds that

$$\text{tr}(\rho \mathcal{L}_\rho^*(y)) = \text{tr}(\rho \mathcal{L}(1)y) = 0 \quad ; \quad \forall y \in \text{Dom}(\mathcal{L}_\rho^*)$$

If $\text{Dom}(\mathcal{L}_\rho^*)$ is dense, this is equivalent to say that $\rho \in \text{Dom}((\mathcal{L}_\rho^*)^*)$ and $(\mathcal{L}_\rho^*)^*(\rho) = 0$. In any case, for $x = 1$, this implies that ρ is \mathcal{L}_ρ^* -stationary even if \mathcal{L}_ρ^* is not a generator.

From now on we assume that $\text{Dom}(\mathcal{L}_\rho^*)$ is dense.

Lemma 3. *Suppose that $\text{Dom}(\mathcal{L})$ is dense and consider the following statements:*

- (i) ρ is \mathcal{L} -stationary
(ii) \mathcal{L}_ρ^* satisfies

$$\mathcal{L}_\rho^*(1) = 0 \quad (43)$$

Then

- (ii) implies (i)
- if ρ is invertible, (i.e., it has a dense range, therefore its inverse is densely defined, but not necessarily bounded), then (i) implies (ii).

Proof. (41) implies the following identities:

$$\text{tr}(\mathcal{L}_\rho^*(1)y\rho) = \text{tr}(\rho \mathcal{L}_\rho^*(1)y) = \text{tr}(\rho \mathcal{L}(y)) = \text{tr}(\mathcal{L}_*(\rho)y); \quad \forall y \in \text{Dom}(\mathcal{L})$$

Thus if (ii) holds then, for all $y \in \text{Dom}(\mathcal{L})$, $\text{tr}(\mathcal{L}_*(\rho)y) = 0$ and (i) follows from the density of $\text{Dom}(\mathcal{L})$. Conversely if (i) holds then, with $x = 1$ (41) implies that

$$\text{tr}(\rho \mathcal{L}_\rho^*(1)y) = \text{tr}(\rho \mathcal{L}(y)) = \text{tr}(\mathcal{L}_*(\rho)y) = 0$$

for all $y \in \text{Dom}(\mathcal{L})$.

Since $\text{Dom}(\mathcal{L})$ is dense and the map $y \mapsto y\rho$ is invertible and bounded because such is ρ , this implies that also $\rho \text{Dom}(\mathcal{L})$ is dense and therefore (43) holds.

The pairs (ρ, \mathcal{L}) such that \mathcal{L}_ρ^* is a Markov generator can be characterized, if \mathcal{L} is uniformly bounded, as follows (see e.g. [15] Theorem 3.1 p. 341).

Theorem 4. If \mathcal{L} is uniformly bounded and ρ is faithful, then the following statements are equivalent:

- (i) \mathcal{L}_ρ^* is a Markov generator (in this case it is uniformly bounded),
- (ii) denoting

$$\sigma_t(a) = \rho^{it} a \rho^{-it}$$

the modular group of ρ , \mathcal{L} commutes with σ_t , i.e. $\mathcal{L} \sigma_t = \sigma_t \mathcal{L}$, $\forall t \geq 0$,

- (iii) \mathcal{L} commutes with σ_{-i} , i.e. $\mathcal{L} \sigma_{-i} = \sigma_{-i} \mathcal{L}$.

6 Weighted detailed balance for Markov generators

In the paper [2] it was shown that the dynamical detailed balance condition implies a very special relation, which is a natural generalization of the quantum detailed balance condition of Frigerio, Kossakowski, Gorini, Verri ([18]), between a Markov generator with an invariant measure ρ and its ρ -adjoint.

In this section we introduce the notion of *weighted detailed balance*, which generalizes the dynamical detailed balance condition.

For simplicity, from now on we work with bounded Markov generators \mathcal{L} . These Markov generators can be written in the standard Gorini-Kossakowski-Sudarshan and Lindblad (GKSL) form

$$\mathcal{L}(x) = i[H, x] - \frac{1}{2} \sum_{k \geq 1} (L_k^* L_k x - 2L_k^* x L_k + x L_k^* L_k), \quad (44)$$

where $H, L_k \in \mathcal{B}(\mathcal{H})$ with $H = H^*$ and the series $\sum_{k \geq 1} L_k^* L_k$ is strongly convergent. We shall consider special GKSL representations of these generators. The following theorem (see [24] Theorem 30.16 for the proof), describes these representations.

Theorem 5. Let \mathcal{L} be the generator of a norm-continuous QMS on $\mathcal{B}(\mathcal{H})$ and let ρ be a normal state on $\mathcal{B}(\mathcal{H})$. There exists a bounded self-adjoint operator H and a finite or infinite sequence $(L_k)_{k \geq 1}$ of elements of $\mathcal{B}(\mathcal{H})$ such that:

- (i) $\text{tr}(\rho L_k) = 0$ for each $k \geq 1$,
- (ii) $\sum_{k \geq 1} L_k^* L_k$ is a strongly convergent sum,
- (iii) if $\sum_{k \geq 0} |c_k|^2 < \infty$ and $c_0 + \sum_{k \geq 1} c_k L_k = 0$ for complex scalars $(c_k)_{k \geq 0}$, then $c_k = 0$ for every $k \geq 0$,
- (iv) the GKSL representation (44) holds.

If \tilde{H} , $(\tilde{L}_k)_{k \geq 1}$ is another family of bounded operators in $\mathcal{B}(\mathcal{H})$ with \tilde{H} self-adjoint and the sequence $(\tilde{L}_k)_{k \geq 1}$ is finite or infinite then the conditions (i) – (iv) are fulfilled with H , $(L_k)_{k \geq 1}$ replaced by \tilde{H} , $(\tilde{L}_k)_{k \geq 1}$ respectively if and only if the lengths of the sequences $(L_k)_{k \geq 1}$, $(\tilde{L}_k)_{k \geq 1}$ are equal and for some scalar $c \in \mathbb{R}$ and a unitary matrix $(u_{ij})_{i,j}$ we have

$$\tilde{H} = H + c, \quad \tilde{L}_j = \sum_j u_{ij} L_j.$$

Let k be a Hilbert space with Hilbertian dimension equal to the length of the sequence $(L_k)_k$, with (f_k) an orthonormal basis of k . This Hilbert space is called the multiplicity space of the completely positive (CP) part of \mathcal{L} . We can identify the unitary matrix $(u_{jk})_{j,k \geq 1}$ in the above basis $(f_k)_{k \geq 1}$ with a unitary operator on k .

Following the terminology in [15], a special representation of a bounded Markov \mathcal{L} with respect to an invariant faithful state ρ by means of operators H, L_k is called *privileged* if H commutes with ρ and $\rho L_k = \lambda_k L_k \rho$ for some $\lambda_k > 0$.

Privileged representations characterize those bounded GKSL generators whose ρ -adjoint \mathcal{L}_ρ^* is also the generator of a uniformly continuous QMS, see Theorem 4.3 in [15].

Theorem 6. The ρ -adjoint \mathcal{L}_ρ^* of a GKSL bounded generator \mathcal{L} is the generator of a uniformly continuous QMS if and only if there exists a privileged GKSL representation of \mathcal{L} with respect to ρ .

With every privileged, representation of a GKSL generator \mathcal{L} corresponds a privileged representation of its adjoint \mathcal{L}_ρ^* , see Theorem 4.4 in [15].

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Theorem 7. *If the ρ -adjoint \mathcal{L}_ρ^* is a GKSL generator, for every privileged GKSL representations of \mathcal{L} by means of operators H, L_k as in (44), there exists a privileged GKSL representation of \mathcal{L}_ρ^* by means of operators \tilde{H}, \tilde{L}_k such that:*

- (i) $\tilde{H} = -H - \alpha$ for some $\alpha \in \mathbb{R}$,
- (ii) $\tilde{L}_k = \lambda_k^{-\frac{1}{2}} L_k^*$ for some $\lambda_k > 0$.

Theorem 8. *Given a special GKSL representation by means of operators H, L_k , of a bounded Markov generator \mathcal{L} of a norm continuous QMS $(\mathcal{T}_t)_{t \geq 0}$ with faithful invariant state ρ , then the following are equivalent:*

- (i) *There exists a sequence of positive weights $q := (q_k)_k$ and operators H', L'_k of a (possibly another) special representation of \mathcal{L} such that the difference $\mathcal{L}_\rho^* - \mathcal{L}$ has the structure*

$$\mathcal{L}_\rho^* - \mathcal{L} = -2i[K, \cdot] + \Pi, \tag{45}$$

where $K = K^*$ is bounded and

$$\Pi(x) = \sum_k (q_k - 1) L_k'^* x L_k'. \tag{46}$$

- (ii) *\mathcal{L}_ρ^* is a bounded GKSL generator, the operators H, L_k yield a privileged representation of \mathcal{L} with \tilde{H}, \tilde{L}_k the operators in the corresponding privileged GKSL representation of \mathcal{L}_ρ^* , given by Theorem 7, and there exists a sequence of positive weights $q := (q_k)$ and operators H'', L''_k of a (possibly another) special representation of \mathcal{L} such that,*

$$\tilde{L}_k = q_k^{\frac{1}{2}} L''_k, \quad \forall k \geq 1. \tag{47}$$

Proof. Let us prove that (i) implies (ii). Any Π of the form (46) is a $*$ -map, i.e. $\Pi(x)^* = \Pi(x^*)$. It follows that \mathcal{L}_ρ^* is also a $*$ -map, being a sum of maps with these properties. Since, by assumption, \mathcal{L} , Π and K are bounded and ρ is faithful, we can apply a result of Majewski and Streater (see Theorem 6, p. 7985 in [22]) and conclude that $\tilde{\mathcal{L}}$ is a GKSL generator. Hence, by Theorem 6, we can assume that H, L_k are operators of a privileged representation of \mathcal{L} . Then we have that H and $\sum_k L_k^* L_k$ commutes with ρ and (45), (46) imply that

$$\sum_k \tilde{L}_k^* x \tilde{L}_k = \sum_k L_k^* y L_k + \sum_k (q_k - 1) L_k'^* x L_k', \tag{48}$$

with L'_k operators of a special representation of \mathcal{L} . By Theorem 5, we can write $L'_k = \sum_l u_{kl} L_l$ with $u = (u_{kl})$ unitary operator on k . Now a direct computation shows that

$$\sum_k L_k'^* x L_k' = \sum_{j,\ell} \left(\sum_k \bar{u}_{kj} u_{kl} \right) L_j^* x L_l = \sum_j L_j^* x L_j.$$

Therefore we can simplify the right-hand side of (48) and find

$$\sum_k \tilde{L}_k^* x \tilde{L}_k = \sum_k q_k L_k'^* x L_k' = \sum_k \left(q_k^{1/2} L_k' \right)^* x \left(q_k^{1/2} L_k' \right)$$

Then we can apply Theorem 30.16 in [24] on Kraus' representations of normal completely positive maps to conclude that there exists a unitary operator $v = (v_{kl})$ on k such that

$$\tilde{L}_k = q_k^{\frac{1}{2}} \sum_j v_{kj} L_j' = q_k^{\frac{1}{2}} L''_k,$$

with $L''_k = \sum_j v_{kj} L_j'$. This proves (ii).

Conversely, assume (ii) holds and let us compute the ρ -adjoint of $\Phi(x) = \sum_k L_k^* x L_k$, the CP part of \mathcal{L} . Since the GKSL representation of \mathcal{L} by means of the operators H , L_k is privileged, by Theorem 7 the ρ -adjoint of the CP part $\Phi(x) = \sum_k L_k^* x L_k$ of \mathcal{L} is

$$\tilde{\Phi}(x) = \sum_k \tilde{L}_k^* x \tilde{L}_k,$$

where $\tilde{L}_k = \lambda_k^{-\frac{1}{2}} L_k^*$. A direct computation using (47) with $L_k'' = \sum_l u_{kl} L_l$ yields

$$\begin{aligned} \tilde{\Phi}(x) &= \sum_k \tilde{L}_k^* x \tilde{L}_k = \sum_k q_k L_k''^* x L_k'' \\ &= \sum_k \tilde{L}_k''^* x L_k'' + \sum_k (q_k - 1) L_k''^* x L_k'' \\ &= \Phi(x) + \sum_k (q_k - 1) L_k''^* x L_k''. \end{aligned}$$

Since H and $\sum_k L_k^* L_k$ commute with ρ , we obtain (45) and (46) with $L_k' = L_k''$. This proves (i).

Definition 5. A uniformly continuous quantum Markov semigroup $(\mathcal{T}_t)_{t \geq 0}$ satisfies a **weighted detailed balance condition** with respect to a faithful invariant state ρ , if its generator \mathcal{L} satisfies any one of the two equivalent conditions in Theorem 8.

Corollary 2. Assume that H , L_k are operators of a privileged representation of the bounded Markov generator \mathcal{L} with respect to a faithful invariant state ρ . Then the following are equivalent:

(i) the generator \mathcal{L} satisfies the quantum detailed balance condition of Frigerio, Kossakowski, Gorini, Verri [18]

$$\mathcal{L} - \mathcal{L}_\rho^* = 2i[H, \cdot] \quad (49)$$

(ii) \mathcal{L} satisfies a weighted detailed balance condition with respect to the faithful invariant state ρ with weights

$$q = (1, 1, \dots)$$

i.e., $q_k = 1, \forall k$.

Proof. The thesis is an immediate consequence of Theorem 8 combined with Theorem 5.1 in [15].

Remark.

- (i) Roughly speaking, according to condition (ii) in Theorem 8 and Corollary 2, detailed balance holds if and only if each operator \tilde{L}_k of a privileged representation of \mathcal{L}_ρ^* coincide with some operator L_k'' in a privileged representation of \mathcal{L} . Weighted detailed balance allows deviations from this equilibrium situation by associating with each operator \tilde{L}_k of a privileged representation of \mathcal{L}_ρ^* , a positive multiple $q_k^{\frac{1}{2}} L_k''$ of some operator L_k'' of a privileged representation of \mathcal{L} .
- (ii) The connection of the notion of weighted detailed balance with dynamical detailed balance, as well as an intuitive idea of the meaning of the correspondence $\tilde{L}_k \leftrightarrow q_k^{\frac{1}{2}} L_k''$ entering in the weighted detailed balance condition, is given by the physical models considered in Theorems 9 and 11, which correspond to the situation originally considered in [2] and give rise to simple unitaries permutating each operator L_j with its adjoint.

To finish this section let us consider a simple example.

Example 1. (A quantum 3-level system). Consider the QMS on $\mathcal{B}(\mathbb{C}^3)$ generated by

$$\mathcal{L}(x) = \alpha S^* x S + (1 - \alpha) S x S^* - x,$$

where S is the unitary right shift defined on the orthonormal basis $(e_j)_{0 \leq j \leq 2}$ of \mathbb{C}^3 by $S e_j = e_{j+1}$, the sum must be understood modulo 3, and $\alpha \in (0, 1)$.

This QMS arises in the stochastic limit of a three-level system dipole-type interacting with two reservoirs

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under the generalized rotating wave approximation. One can easily see that the normalised trace $\rho = I/3$ is a faithful invariant state, i.e., $\mathcal{L}_*(\rho) = 0$, where \mathcal{L}_* is the pre-dual generator:

$$\mathcal{L}_*(\rho) = \alpha S \rho S^* + (1 - \alpha) S^* \rho S - \rho.$$

Clearly the ρ -adjoint is $\mathcal{L}_\rho^* = \mathcal{L}_*$. Moreover, the above GKSL representations of \mathcal{L} and \mathcal{L}_ρ^* by means of operators $H = 0$; $L_1 = \alpha^{\frac{1}{2}} S$, $L_2 = (1 - \alpha)^{\frac{1}{2}} S^*$ and $\tilde{H} = 0$; $\tilde{L}_1 = \alpha^{\frac{1}{2}} S^*$, $\tilde{L}_2 = (1 - \alpha)^{\frac{1}{2}} S$, respectively, are privileged. Indeed, this representation are special since $\text{tr}(S) = \text{tr}(S^*) = 0$ and I, S, S^* are linearly independent. Moreover, $\tilde{L}_1 = \frac{\alpha^{\frac{1}{2}}}{(1-\alpha)^{\frac{1}{2}}} L_2$, $\tilde{L}_2 = \frac{(1-\alpha)^{\frac{1}{2}}}{\alpha^{\frac{1}{2}}} L_1$. Weighted detailed balance holds since $\tilde{L}_1 = q_1^{\frac{1}{2}} L_1''$, $\tilde{L}_2 = q_2^{\frac{1}{2}} L_2''$ with $L_1'' = L_2$, $L_2'' = L_1$ and $q_1 = \frac{\alpha}{1-\alpha}$, $q_2 = \frac{1-\alpha}{\alpha}$. Hence, quantum detailed balance holds if and only if $\alpha = 1/2$. Fagnola and Rebolledo proved in [14] that for $\alpha \neq \frac{1}{2}$ this system has non-zero entropy production, that characterizes non-equilibrium systems.

7 Markov generators of stochastic limit type with respect to an Hamiltonian H

The origins, from the stochastic limit approach, of the special class of generators described in the present section are briefly outlined in Appendix II (see section (12)). In the following we will freely use the notations introduced in Appendix I (see section (11)). Let $H \in \mathcal{B}(\mathcal{H})$ be a self-adjoint operator (Hamiltonian) with discrete spectral decomposition

$$H = \sum_{\epsilon_m \in \text{Spec}(H)} \epsilon_m P_m \quad (50)$$

and denote B_+ the set of its strictly positive Bohr frequencies (i.e. the set of strictly positive eigenvalues of $e^{itH}(\cdot)e^{-itH}$):

$$B_+ := \{\omega = \epsilon_r - \epsilon_{r'} > 0 : \epsilon_r, \epsilon_{r'} \in \text{Spec}(H)\} = \text{Spec}_+(u_t) \quad (51)$$

Definition 6. A Markov generator \mathcal{L} on $\mathcal{B}(\mathcal{H})$ is said to be of stochastic limit type with respect to the Hamiltonian (50) if it has the form:

$$\begin{aligned} \mathcal{L}(x) = & i[\Delta, x] - \\ & \sum_{\omega \in B_+} \left(\Gamma_{-, \omega} \left(\frac{1}{2} \{D_\omega^\dagger D_\omega, x\} - D_\omega^\dagger x D_\omega \right) + \Gamma_{+, \omega} \left(\frac{1}{2} \{D_\omega D_\omega^\dagger, x\} - D_\omega x D_\omega^\dagger \right) \right) \end{aligned} \quad (52)$$

where, in the notations of Appendix I below (section (11)), for each $\omega \in B_+$:

$$\Gamma_{\pm, \omega} \in \mathbb{R}_+ \quad (53)$$

$$\Delta = \Delta^* \in \{H\}' \quad (54)$$

$$D_\omega \in E_\omega(\mathcal{B}(\mathcal{H})) \quad (55)$$

The numerical coefficients (53) have a special structure given by the stochastic limit and described in Appendix II below.

7.1 Canonical form of Markov generators of stochastic limit type

Introducing the set

$$\hat{B}_+ := \{\omega \in B_+ : \text{either } \Gamma_{-, \omega} \neq 0 \text{ or } \Gamma_{+, \omega} \neq 0\} \quad (56)$$

it is convenient to write the generator (52) in the form

$$\mathcal{L}(x) = i[\Delta, x] - \sum_{\omega \in \hat{B}_+} \mathcal{L}_\omega(x) \quad (57)$$

with

$$\mathcal{L}_\omega(x) = \sum_{\omega \in B_+} \left(\Gamma_{-, \omega} \left(\frac{1}{2} \{D_\omega^\dagger D_\omega, x\} - D_\omega^\dagger x D_\omega \right) + \Gamma_{+, \omega} \left(\frac{1}{2} \{D_\omega D_\omega^\dagger, x\} - D_\omega x D_\omega^\dagger \right) \right) \quad (58)$$

Remark. Notice that, while B_+ depends only on H , \hat{B}_+ depends also on \mathcal{L} . For $\omega \in \hat{B}_+$, the operators D_ω in (57) have the form

$$\begin{aligned} D_\omega &:= E_\omega(D) = \sum_{\{(\varepsilon_m, \varepsilon_n) \in B_+(\omega)\}} P_{\varepsilon_m} D P_{\varepsilon_n} \\ &= \sum_{\{(\varepsilon_m, \varepsilon_n) \in B_+(\omega, D)\}} P_{\varepsilon_m} D P_{\varepsilon_n} = \sum_{\{(\varepsilon_m, \varepsilon_n) \in B_+(\omega, D)\}} D_{(\varepsilon_m, \varepsilon_n)} \end{aligned} \quad (59)$$

where by definition

$$B_+(\omega) := \{(\varepsilon_m, \varepsilon_n) \in (\text{Spec}(H))^2 : \varepsilon_n - \varepsilon_m = \omega\} \quad (60)$$

$$B_+(\omega, D) := \{(\varepsilon_m, \varepsilon_n) \in B_+(\omega) : P_{\varepsilon_m} D P_{\varepsilon_n} \neq 0\}$$

and for some $D \in \mathcal{B}(\mathcal{H})$, denoting $\forall (\varepsilon_m, \varepsilon_n) \in B_+(\omega)$:

$$D_{(\varepsilon_m, \varepsilon_n)} := P_{\varepsilon_m} D P_{\varepsilon_n} \quad (61)$$

Recall that (see Appendix I) for any x :

$$E_\omega(x) := \sum_{\{(\varepsilon_m, \varepsilon_n) \in B_+(\omega)\}} P_{\varepsilon_m} x P_{\varepsilon_n} \quad (62)$$

Now for each $\omega \in \hat{B}_+$ consider the generator (see (52))

$$\begin{aligned} \mathcal{L}_\omega(x) &:= \Gamma_{-, \omega} \left(\frac{1}{2} \{D_\omega^\dagger D_\omega, x\} - D_\omega^\dagger x D_\omega \right) + \Gamma_{+, \omega} \left(\frac{1}{2} \{D_\omega D_\omega^\dagger, x\} - D_\omega x D_\omega^\dagger \right) = \\ &= \frac{1}{2} \Gamma_{-, \omega} \{D_\omega^\dagger D_\omega, x\} + \frac{1}{2} \Gamma_{+, \omega} \{D_\omega D_\omega^\dagger, x\} - (\Gamma_{-, \omega} D_\omega^\dagger x D_\omega + \Gamma_{+, \omega} D_\omega x D_\omega^\dagger) \end{aligned} \quad (63)$$

Using (55), for each $x \in \mathcal{B}(\mathcal{H})$ one finds

$$\begin{aligned} &\Gamma_{-, \omega} D_\omega^\dagger x D_\omega + \Gamma_{+, \omega} D_\omega x D_\omega^\dagger = \\ &= \sum_{\{(\varepsilon_m, \varepsilon_n) \in B_+(\omega, D)\}} \sum_{\{(\varepsilon_M, \varepsilon_N) \in B_+(\omega, D)\}} \left(\Gamma_{-, \omega} D_{(\varepsilon_m, \varepsilon_n)}^\dagger x D_{(\varepsilon_M, \varepsilon_N)} + \Gamma_{+, \omega} D_{(\varepsilon_m, \varepsilon_n)} x D_{(\varepsilon_M, \varepsilon_N)}^\dagger \right) \\ &= \sum_{\{((\varepsilon_m, \varepsilon_n), (\varepsilon_M, \varepsilon_N)) \in B_+(\omega, D)^2\}} \left(\Gamma_{-, \omega} D_{(\varepsilon_m, \varepsilon_n)}^\dagger x D_{(\varepsilon_M, \varepsilon_N)} + \Gamma_{+, \omega} D_{(\varepsilon_m, \varepsilon_n)} x D_{(\varepsilon_M, \varepsilon_N)}^\dagger \right) \end{aligned} \quad (64)$$

With these notations

$$\begin{aligned} \mathcal{L}_\omega(x) &= \sum_{\{((\varepsilon_m, \varepsilon_n), (\varepsilon_M, \varepsilon_N)) \in B_+(\omega, D)^2\}} \frac{1}{2} \Gamma_{-, \omega} \{D_{(\varepsilon_m, \varepsilon_n)}^\dagger D_{(\varepsilon_M, \varepsilon_N)}, x\} \\ &\quad + \frac{1}{2} \Gamma_{+, \omega} \{D_{(\varepsilon_m, \varepsilon_n)} D_{(\varepsilon_M, \varepsilon_N)}^\dagger, x\} \\ &\quad - \left(\Gamma_{-, \omega} D_{(\varepsilon_m, \varepsilon_n)}^\dagger x D_{(\varepsilon_M, \varepsilon_N)} + \Gamma_{+, \omega} D_{(\varepsilon_m, \varepsilon_n)} x D_{(\varepsilon_M, \varepsilon_N)}^\dagger \right) \end{aligned} \quad (65)$$

Lemma 4.

$$(\varepsilon, \varepsilon'), (\varepsilon, \varepsilon'') \in B_+(\omega) \Rightarrow \varepsilon' = \varepsilon'' \quad (66)$$

$$(\varepsilon', \varepsilon), (\varepsilon'', \varepsilon) \in B_+(\omega) \Rightarrow \varepsilon' = \varepsilon'' \quad (67)$$

$$(\varepsilon, \varepsilon') \neq (\varepsilon'', \varepsilon''') \in B_+(\omega) \Rightarrow \varepsilon \neq \varepsilon'' \quad \text{and} \quad \varepsilon' \neq \varepsilon''' \quad (68)$$

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Proof. (66) follows from:

$$\varepsilon' - \varepsilon = \omega = \varepsilon'' - \varepsilon \Rightarrow 0 = (\varepsilon' - \varepsilon) - (\varepsilon'' - \varepsilon) = \varepsilon' - \varepsilon''$$

(67) follows from:

$$\varepsilon - \varepsilon' = \omega = \varepsilon - \varepsilon'' \Rightarrow 0 = (\varepsilon - \varepsilon') - (\varepsilon - \varepsilon'') = \varepsilon'' - \varepsilon'$$

Finally (67) implies that, if $\varepsilon = \varepsilon''$, then one must have also $\varepsilon' = \varepsilon'''$ against the assumption. Similarly (66) implies that, if $\varepsilon' = \varepsilon'''$, then one must have also $\varepsilon = \varepsilon''$ against the assumption. Thus (68) follows. In view of the following result, Lemma 4 is of crucial importance for the thesis of the present paper.

Lemma 5. For any $\omega \in \hat{B}_+$ and for any $(\varepsilon_m, \varepsilon_n)$ and $(\varepsilon_M, \varepsilon_N)$ in $\hat{B}_+(\omega)$ one has:

$$D_{(\varepsilon_m, \varepsilon_n)}^+ D_{(\varepsilon_M, \varepsilon_N)} \in \{H\}' \quad (69)$$

Proof. We know, from (61), that

$$D_{(\varepsilon_m, \varepsilon_n)} := P_{\varepsilon_m} D P_{\varepsilon_n} \quad ; \quad D_{(\varepsilon_m, \varepsilon_n)}^+ = P_{\varepsilon_n} D^+ P_{\varepsilon_m}$$

Therefore, if $(\varepsilon_m, \varepsilon_n) = (\varepsilon_M, \varepsilon_N)$, then

$$D_{(\varepsilon_m, \varepsilon_n)}^+ D_{(\varepsilon_m, \varepsilon_n)} = P_{\varepsilon_n} D^+ P_{\varepsilon_m} P_{\varepsilon_m} D P_{\varepsilon_n} = P_{\varepsilon_n} D^+ P_{\varepsilon_m} D P_{\varepsilon_n} \in \{H\}'$$

while, if $(\varepsilon_m, \varepsilon_n) \neq (\varepsilon_M, \varepsilon_N)$, then

$$D_{(\varepsilon_m, \varepsilon_n)}^+ D_{(\varepsilon_M, \varepsilon_N)} = P_{\varepsilon_n} D^+ P_{\varepsilon_m} P_{\varepsilon_M} D P_{\varepsilon_N}$$

From (68) we know that

$$(\varepsilon_m, \varepsilon_n) \neq (\varepsilon_M, \varepsilon_N) \in B_+(\omega) \Rightarrow \varepsilon_m \neq \varepsilon_M \quad \text{and} \quad \varepsilon_n \neq \varepsilon_N$$

Therefore, if $(\varepsilon_m, \varepsilon_n) \neq (\varepsilon_M, \varepsilon_N)$, then

$$D_{(\varepsilon_m, \varepsilon_n)}^+ D_{(\varepsilon_M, \varepsilon_N)} = 0$$

in both cases (69) holds.

Lemma 6. Suppose that $h' \in \{H\}'$ and ρ is a function of H . Then the linear map $x \mapsto \{x, h'\}$ is self-adjoint with respect to the ρ -scalar product.

Proof.

$$\begin{aligned} \text{Tr}(\rho\{h', x\}y) &= \text{Tr}(\rho h' xy) + \text{Tr}(\rho x h' y) = \text{Tr}(\rho x y h') + \text{Tr}(\rho x h' y) \\ &= \text{Tr}(\rho x y h') + \text{Tr}(\rho x h' y) = \text{Tr}(\rho x \{y, h'\}) \end{aligned}$$

Corollary 3. For any $\omega \in \hat{B}_+$ and for any $(\varepsilon_m, \varepsilon_n)$ and $(\varepsilon_M, \varepsilon_N)$ in $\hat{B}_+(\omega)$, if ρ is a function of H , then the linear operators

$$x \mapsto \{x, D_{(\varepsilon_m, \varepsilon_n)}^+ D_{(\varepsilon_M, \varepsilon_N)}\} \quad ; \quad x \mapsto \{x, D_{(\varepsilon_m, \varepsilon_n)} D_{(\varepsilon_M, \varepsilon_N)}^+\}$$

are ρ -self-adjoint.

Proof. Since

$$D_{(\varepsilon_m, \varepsilon_n)}^+ D_{(\varepsilon_M, \varepsilon_N)} \in \{H\}' \quad (70)$$

the thesis is an immediate consequence of Lemma 6.

Corollary 3 implies that the anticommutator part of the generator (65) is ρ -self-adjoint for any state ρ which is a function of H . Let us consider the completely positive part of (65), i.e.

$$\Psi(x) := \left(\Gamma_{-, \omega} D_{(\varepsilon_m, \varepsilon_n)}^+ x D_{(\varepsilon_M, \varepsilon_N)} + \Gamma_{+, \omega} D_{(\varepsilon_m, \varepsilon_n)} x D_{(\varepsilon_M, \varepsilon_N)}^+ \right)$$

$$\begin{aligned}
\mathrm{Tr}(\rho D_{(\varepsilon_m, \varepsilon_n)} x D_{(\varepsilon_M, \varepsilon_N)}^\dagger y) &= \mathrm{Tr}(\rho D_{(\varepsilon_m, \varepsilon_n)} x D_{(\varepsilon_M, \varepsilon_N)}^\dagger \rho^{-1} \rho y) \\
&= \rho_m \rho_n^{-1} \rho_M \rho_N^{-1} \mathrm{Tr}(D_{(\varepsilon_m, \varepsilon_n)} \rho x \rho^{-1} D_{(\varepsilon_M, \varepsilon_N)}^\dagger \rho y) \\
&= \rho_m \rho_n^{-1} \mathrm{Tr}(\rho x D_{(\varepsilon_M, \varepsilon_N)}^\dagger y D_{(\varepsilon_m, \varepsilon_n)})
\end{aligned}$$

Therefore

$$\left(D_{(\varepsilon_m, \varepsilon_n)} \cdot D_{(\varepsilon_M, \varepsilon_N)}^\dagger \right)_\rho^* = \rho_m \rho_n^{-1} \left(D_{(\varepsilon_M, \varepsilon_N)}^\dagger \cdot D_{(\varepsilon_m, \varepsilon_n)} \right)$$

where $(X)_\rho^*$ denotes the ρ -adjoint of X

Similarly

$$\begin{aligned}
\mathrm{Tr}(\rho D_{(\varepsilon_m, \varepsilon_n)}^\dagger x D_{(\varepsilon_M, \varepsilon_N)} y) &= \mathrm{Tr}(\rho D_{(\varepsilon_m, \varepsilon_n)}^\dagger x D_{(\varepsilon_M, \varepsilon_N)} \rho^{-1} \rho y) \\
&= \rho_m^{-1} \rho_n \rho_M^{-1} \rho_N \mathrm{Tr}(D_{(\varepsilon_m, \varepsilon_n)}^\dagger \rho x \rho^{-1} D_{(\varepsilon_M, \varepsilon_N)} \rho y) \\
&= \rho_m^{-1} \rho_n \mathrm{Tr}(D_{(\varepsilon_m, \varepsilon_n)}^\dagger \rho x D_{(\varepsilon_M, \varepsilon_N)} y) \\
&= \rho_m^{-1} \rho_n \mathrm{Tr}(\rho x D_{(\varepsilon_M, \varepsilon_N)} y D_{(\varepsilon_m, \varepsilon_n)}^\dagger)
\end{aligned}$$

Therefore

$$\left(D_{(\varepsilon_m, \varepsilon_n)}^\dagger \cdot D_{(\varepsilon_M, \varepsilon_N)} \right)_\rho^* = \rho_m^{-1} \rho_n \left(D_{(\varepsilon_M, \varepsilon_N)} \cdot D_{(\varepsilon_m, \varepsilon_n)}^\dagger \right)$$

In conclusion, the ρ -adjoint of $\Psi(\cdot)$ is

$$(\Psi)_\rho^*(\cdot) = \rho_m^{-1} \rho_n \Gamma_{-, \omega} \left(D_{(\varepsilon_M, \varepsilon_N)} \cdot D_{(\varepsilon_m, \varepsilon_n)}^\dagger \right) + \rho_m \rho_n^{-1} \Gamma_{+, \omega} \left(D_{(\varepsilon_M, \varepsilon_N)}^\dagger \cdot D_{(\varepsilon_m, \varepsilon_n)} \right)$$

and we conclude that the adjoint of \mathcal{L}_ω is:

$$\begin{aligned}
&(\mathcal{L}_\omega)_\rho^* \\
&= \sum_{\{((\varepsilon_m, \varepsilon_n), (\varepsilon_M, \varepsilon_N)) \in B_+(\omega, D)^2\}} \left\{ \frac{1}{2} \Gamma_{-, \omega} \{ D_{(\varepsilon_m, \varepsilon_n)}^\dagger D_{(\varepsilon_M, \varepsilon_N)}, x \} + \frac{1}{2} \Gamma_{+, \omega} \{ D_{(\varepsilon_m, \varepsilon_n)} D_{(\varepsilon_M, \varepsilon_N)}^\dagger, x \} \right. \\
&\quad \left. - \left(\rho_m^{-1} \rho_n \Gamma_{-, \omega} \left(D_{(\varepsilon_M, \varepsilon_N)} \cdot D_{(\varepsilon_m, \varepsilon_n)}^\dagger \right) + \rho_m \rho_n^{-1} \Gamma_{+, \omega} \left(D_{(\varepsilon_M, \varepsilon_N)}^\dagger \cdot D_{(\varepsilon_m, \varepsilon_n)} \right) \right) \right\} \\
&= \sum_{\{((\varepsilon_m, \varepsilon_n), (\varepsilon_M, \varepsilon_N)) \in B_+(\omega, D)^2\}} \left\{ \frac{1}{2} \Gamma_{-, \omega} \{ D_{(\varepsilon_m, \varepsilon_n)}^\dagger D_{(\varepsilon_M, \varepsilon_N)}, x \} + \frac{1}{2} \Gamma_{+, \omega} \{ D_{(\varepsilon_m, \varepsilon_n)} D_{(\varepsilon_M, \varepsilon_N)}^\dagger, x \} \right. \\
&\quad \left. - \left(\Gamma_{-, \omega} \left(D_{(\varepsilon_M, \varepsilon_N)} \cdot D_{(\varepsilon_m, \varepsilon_n)}^\dagger \right) + \Gamma_{+, \omega} \left(D_{(\varepsilon_M, \varepsilon_N)}^\dagger \cdot D_{(\varepsilon_m, \varepsilon_n)} \right) \right) \right\} \\
&\quad - \sum_{\{((\varepsilon_m, \varepsilon_n), (\varepsilon_M, \varepsilon_N)) \in B_+(\omega, D)^2\}} \left\{ \left((\rho_m^{-1} \rho_n - 1) \Gamma_{-, \omega} \left(D_{(\varepsilon_M, \varepsilon_N)} \cdot D_{(\varepsilon_m, \varepsilon_n)}^\dagger \right) + (\rho_m \rho_n^{-1} - 1) \Gamma_{+, \omega} \left(D_{(\varepsilon_M, \varepsilon_N)}^\dagger \cdot D_{(\varepsilon_m, \varepsilon_n)} \right) \right) \right\}
\end{aligned}$$

Thus, introducing the ω -current operator

$$\begin{aligned}
\Pi_{\omega, \rho} := & - \sum_{\{((\varepsilon_m, \varepsilon_n), (\varepsilon_M, \varepsilon_N)) \in B_+(\omega, D)^2\}} \\
& \left\{ \left((\rho_m^{-1} \rho_n - 1) \Gamma_{-, \omega} \left(D_{(\varepsilon_M, \varepsilon_N)} \cdot D_{(\varepsilon_m, \varepsilon_n)}^\dagger \right) + (\rho_m \rho_n^{-1} - 1) \Gamma_{+, \omega} \left(D_{(\varepsilon_M, \varepsilon_N)}^\dagger \cdot D_{(\varepsilon_m, \varepsilon_n)} \right) \right) \right\}
\end{aligned}$$

one obtains

$$(\mathcal{L}_\omega)_\rho^* = \mathcal{L}_\omega + \Pi_{\omega, \rho}$$

In conclusion the ρ -adjoint of the generator (57) has the form

$$(\mathcal{L})_\rho^* = -i[\Delta, \cdot] - \sum_{\omega \in B_+} \{ \mathcal{L}_\omega + \Pi_{\omega, \rho} \}$$

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7.2 Markov generators of stochastic limit type satisfy a weighted detailed balance condition

Since the set $\{(\epsilon_m, \epsilon_n) \in B_+(\omega, D)\}$ is at most countable we can fix an identification of this set with the set of numbers:

$$\{(\epsilon_m, \epsilon_n) \in B_+(\omega, D)\} \equiv \hat{I}_{\omega, D} := \{0, \dots, |B_+(\omega, D)| - 1\} \subseteq \mathbb{N} \tag{71}$$

With this identification the generator (63) can be written in the form

$$\begin{aligned} \mathcal{L}_\omega(x) = & \sum_{\{(j,k) \in I_{\omega, D}^2\}} \frac{1}{2} \Gamma_{-, \omega} \{D_j^\dagger D_k, x\} + \frac{1}{2} \Gamma_{+, \omega} \{D_j D_k^\dagger, x\} \\ & - \left(\Gamma_{-, \omega} D_j^\dagger x D_k + \Gamma_{+, \omega} D_j x D_k^\dagger \right) \end{aligned} \tag{72}$$

Now, for $j \in \hat{I}_{\omega, D}$, define:

$$\gamma_{2j} := \Gamma_{-, j} ; \gamma_{2j+1} := \Gamma_{+, j} ; L_{2j} := \gamma_{2j}^{1/2} D_j ; L_{2j+1} := \gamma_{2j+1}^{1/2} D_j^* \tag{73}$$

Notice that, with this notation, the new index k varies in the set

$$I_{\omega, D} = \{0, 1, \dots, 2|B_+(\omega)| - 1\} \tag{74}$$

Moreover one has:

$$L_{2j}^+ := \Gamma_{-, \omega}^{1/2} D_j^* = \gamma_{2j}^{1/2} \gamma_{2j+1}^{-1/2} L_{2j+1} ; L_{2j+1}^+ := \Gamma_{+, \omega}^{1/2} D_j = \gamma_{2j+1}^{1/2} \gamma_{2j}^{-1/2} L_{2j} \tag{75}$$

With these notations (72) becomes:

$$\begin{aligned} \mathcal{L}_\omega(x) = & \sum_{\{(j,k) \in I_{\omega, D}^2\}} \left(\frac{1}{2} \{L_{2j} L_{2k+1}, x\} + \frac{1}{2} \{L_{2j+1} L_{2k}, x\} - (L_{2j} x L_{2k+1} + L_{2j} x L_{2k}) \right) \end{aligned} \tag{76}$$

The definition (71) of the set $\hat{I}_{\omega, D}$ shows that each index j in the set (86) defines exactly one pair $(\epsilon_m, \epsilon_n) \in B_+(\omega, D)$ of eigenvalues of H . Conversely, any such a pair is naturally associated, through (73), to two indices $2j$ and $2j + 1$ of the $\hat{I}_{\omega, D}$ given by (74).

Definition 7. An index $j \in I_{\omega, D}$ with the property just described is said to correspond to the ordered pair (ϵ_m, ϵ_n) of eigenvalues of H .

Theorem 9. For each $\omega \in \hat{B}_+$ (see (56)) the expression (76) of the Markov generator of stochastic limit type \mathcal{L}_ω , associated with a discrete spectrum Hamiltonian H

$$H = \sum_{\epsilon_k \in \text{Spec}(H)} \epsilon_k P_k \tag{77}$$

and with a faithful invariant state of the form

$$\rho = \sum_{\epsilon_k \in \text{Spec}(H)} \rho_k P_k \in \{H\}'' \tag{78}$$

(i.e. which is a function of H) is a privileged decomposition with eigenvalues (λ_j) defined as follows: if the index $j \in I$ corresponds to the ordered pair (ϵ_m, ϵ_n) in the sense of Definition (7), then:

$$\lambda_j := \begin{cases} \rho_n \rho_m^{-1} , & \text{if } j \text{ is even} \\ \rho_n^{-1} \rho_m , & \text{if } j \text{ is odd} \end{cases} \tag{79}$$

Moreover the Markov generator \mathcal{L}_ω , in the expression (76), satisfies a weighted detailed balance condition in which $\tilde{L}_k = q_k^{\frac{1}{2}} L_k''$, where $L_k'' = \sum_j u_{kj} L_j$ with $u \equiv (u_{k,j})_{k,j \in I}$ the unitary (permutation) operator whose elements are defined by

$$u_{k,j} := \begin{cases} \delta_{k+1,j} , & \text{if } k \text{ is even} \\ \delta_{k-1,j} , & \text{if } k \text{ is odd} \end{cases} \quad (80)$$

and, in the notation, (73), (79), the sequence of weights $q \equiv (q_k)$ is given by:

$$q_k := \begin{cases} \lambda_k^{-1} \gamma_k \gamma_{k+1}^{-1} , & \text{if } k \text{ is even} \\ \lambda_k^{-1} \gamma_k^{-1} \gamma_{k+1} , & \text{if } k \text{ is odd} \end{cases} \quad (81)$$

Remark. Notice that the eigenvalues of the privileged decomposition do not depend on $(\varepsilon_m, \varepsilon_n) \equiv \omega \in \hat{B}_+$.

Proof. One can easily see that the representation (76) is special. For $j \equiv (\varepsilon_m, \varepsilon_n)$ even one has, using (61)

$$\rho L_{2j} = \gamma_{2j}^{\frac{1}{2}} \rho D_{(\varepsilon_m, \varepsilon_n)} = \gamma_{2j}^{\frac{1}{2}} \rho P_{\varepsilon_m} D P_{\varepsilon_n} = \gamma_{2j}^{\frac{1}{2}} \rho_m \rho_n^{-1} P_{\varepsilon_m} D P_{\varepsilon_n} \rho = \lambda_j L_{2j} \rho \quad (82)$$

where the (λ_j) are defined as in (79).

$$\begin{aligned} \rho L_{2j+1} &= \gamma_{2j+1}^{\frac{1}{2}} \rho D_j^* = \gamma_{2j+1}^{\frac{1}{2}} \rho (D_{(\varepsilon_m, \varepsilon_n)})^* = \gamma_{2j+1}^{\frac{1}{2}} \rho P_{\varepsilon_n} D^* P_{\varepsilon_m} \\ &= \rho_n \rho_m^{-1} \gamma_{2j+1}^{\frac{1}{2}} P_{\varepsilon_n} D^* P_{\varepsilon_m} \rho = \rho_n \rho_m^{-1} \gamma_{2j+1}^{\frac{1}{2}} D_{(\varepsilon_m, \varepsilon_n)}^* \rho \\ &= \rho_n \rho_m^{-1} \gamma_{2j+1}^{\frac{1}{2}} D_j^* \rho = \rho_n \rho_m^{-1} L_{2j+1} \rho \end{aligned} \quad (83)$$

This implies that the representation (76) of \mathcal{L}_ω is privileged with eigenvalues (λ_j) given by (79).

Finally, let us verify that condition (ii) in Theorem 8 holds.

From (75) we see that for every $j \in \hat{I}_{\omega, D}$ we have

$$L_j^* = \begin{cases} \gamma_j^{\frac{1}{2}} \gamma_{j+1}^{-\frac{1}{2}} L_{j+1} & , \text{ if } j \text{ is even} \\ \gamma_j^{\frac{1}{2}} \gamma_{j-1}^{-\frac{1}{2}} L_{j-1} & , \text{ if } j \text{ is odd} \end{cases}$$

Hence defining for $2j, 2j+1 \in \hat{I}_{\omega, D}$

$$q_{2j} := \lambda_{2k}^{-1} \gamma_{2j} \gamma_{2j+1}^{-1} \quad ; \quad q_{2j+1} := \lambda_{2k+1}^{-1} \gamma_{2j}^{-1} \gamma_{2j+1}$$

and, using (80) to define the unitary operator $u \equiv (u_{k,j})_{k,j \in I}$, one obtains the relation:

$$\tilde{L}_k = \lambda_k^{-\frac{1}{2}} L_k^* = q_k^{\frac{1}{2}} L_k'' \quad (84)$$

with $L_k'' = \sum_j u_{kj} L_j$. This finishes the proof.

Theorem 10. Let \mathcal{L} be a generator of stochastic limit type with respect to an Hamiltonian H of the form (77). Suppose that, the representation (57) of \mathcal{L} :

$$\Delta \in \{H\}' \quad (85)$$

and that $\rho \in \{H\}''$ is a faithful \mathcal{L} -invariant state of the form (78). Then the representation (76) of \mathcal{L} is a privileged representation with eigenvalues (λ_j) defined by (79) and \mathcal{L} satisfies a weighted detailed balance condition with respect to ρ , which can be explicitly described.

Proof. We know that, for each $\omega \in \hat{B}_+$, the representation (76) is a privileged decomposition of \mathcal{L}_ω with eigenvalues (λ_j) and that \mathcal{L}_ω satisfies a weighted detailed balance condition with respect to ρ , given explicitly by Theorem 9. Moreover, under assumption (85) one has

$$([i\Delta, \cdot])_\rho^* = -[i\Delta, \cdot]$$

From this the thesis immediately follows.

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7.3 Generic Markov generators of stochastic limit type satisfy a weighted detailed balance condition

The simplest class of Markov generators on $\mathcal{B}(\mathcal{H})$, of stochastic limit type with respect to a discrete spectrum Hamiltonian H is obtained when the Hamiltonian H is *generic* in the sense of [6], i.e.

Definition 8. A Markov generator (6), of stochastic limit type with respect to a discrete spectrum Hamiltonian H is called *generic* if:

- (i) H has a simple spectrum
- (ii) for any $\omega \in B_+$, there exists a unique ordered pair (ϵ_m, ϵ_n) of eigenvalues of H such that

$$\epsilon_m - \epsilon_n = \omega > 0$$

(this is equivalent to say that the strictly positive eigenvalues of $e^{itH}(\cdot)e^{-itH}$ are simple).

In the present subsection we shall prove that this special class of generators satisfy a weighted detailed balance condition. It is convenient, for simplicity of notations, to rewrite the Markov generator (52) exploiting the genericity assumption and simplifying the set of indices, so to make the multiplicity space clear. To this goal we denote

$$\hat{B}_+ := \{\omega_j \in B_+ : \text{either } \Gamma_{-, \omega} \neq 0 \text{ or } \Gamma_{+, \omega} \neq 0\}$$

Since the set \hat{B}_+ is at most countable, we can write

$$\hat{B}_+ = \{\omega_j : 0 \leq j \leq |\hat{B}_+|\} \subseteq \mathbb{N} \quad (86)$$

hence denoting

$$\Gamma_{\pm, j} = \Gamma_{\pm, \omega_j} \quad \text{and} \quad D_j = D_{\omega_j}$$

the generator (52) can be written in the form

$$\begin{aligned} \mathcal{L}(x) = & i[\Delta, x] - \\ & \sum_{j \in \hat{B}_+} \left(\Gamma_{-, j} \left(\frac{1}{2} \{D_j^\dagger D_j, x\} - D_j^\dagger x D_j \right) + \Gamma_{+, j} \left(\frac{1}{2} \{D_j D_j^\dagger, x\} - D_j x D_j^\dagger \right) \right) \end{aligned} \quad (87)$$

Defining, for each $j \in \hat{B}_+$:

$$\gamma_{2j} := \Gamma_{-, j} ; \quad \gamma_{2j+1} := \Gamma_{+, j} ; \quad L_{2j} := \gamma_{2j}^{\frac{1}{2}} D_j ; \quad L_{2j+1} := \gamma_{2j+1}^{\frac{1}{2}} D_j^* \quad (88)$$

we have that

$$j \in \{0 \leq j \leq 2|\hat{B}_+| - 1\} =: I \quad (89)$$

finally write the generator (52) in the form

$$\mathcal{L}(x) = \Phi(x) + G^* x + xG \quad (90)$$

where

$$\Phi(x) = \sum_{j \in I} L_j^* x L_j \quad ; \quad G = -\frac{1}{2} \Phi(I) - i\Delta$$

Recalling the definition of the operators D_j (see Appendix I), if the index $j \in I$ corresponds to the ordered pair (ϵ_m, ϵ_n) of eigenvalues of H , then we can write:

$$\begin{aligned} L_{2j} &= \gamma_j^{\frac{1}{2}} D_j = \gamma_j^{\frac{1}{2}} E_j(D) = \gamma_j^{\frac{1}{2}} \langle \epsilon_n | D | \epsilon_m \rangle | \epsilon_n \rangle \langle \epsilon_m | \\ L_{2j+1} &= \gamma_{j+1}^{\frac{1}{2}} D_{j+1} = \gamma_{j+1}^{\frac{1}{2}} E_j(D)^* = \gamma_{j+1}^{\frac{1}{2}} \overline{\langle \epsilon_n | D | \epsilon_m \rangle} | \epsilon_m \rangle \langle \epsilon_n | \end{aligned} \quad (91)$$

since by genericity $\epsilon_n \neq \epsilon_m$, one has:

$$\text{tr}(\rho L_j) = \gamma_j^{\frac{1}{2}} \langle \epsilon_n | D | \epsilon_m \rangle \text{tr}(\rho | \epsilon_n \rangle \langle \epsilon_m |) \sum_k \rho_k \text{tr}(| \epsilon_k \rangle \langle \epsilon_k | | \epsilon_n \rangle \langle \epsilon_m |)$$

$$= \gamma_j^{\frac{1}{2}} \langle \epsilon_n | D | \epsilon_m \rangle \text{tr}(|\epsilon_n\rangle\langle\epsilon_m|) = 0 \tag{92}$$

It follows that, if $0 = c_0 + \sum_j c_j L_j$ then

$$0 = \text{tr} \left((c_0 + \sum_j c_j L_j)^* (c_0 + \sum_{j'} c_{j'} L_{j'}) \right) = \sum_j |c_j|^2$$

and therefore $c_j = 0$ for all $j \geq 0$. Therefore the set $\{1, (L_k)_{k \in I}\}$ is linearly independent, hence I is the multiplicity space of \mathcal{L} .

Theorem 11. *The expression (90) of a Markov generator \mathcal{L} , of stochastic limit type associated with a generic Hamiltonian H and with a faithful invariant state of the form*

$$\rho = \sum_{\epsilon_k \in \text{Spec}(H)} \rho_k |\epsilon_k\rangle\langle\epsilon_k| \in \{H\}' \equiv \{H\}'' \tag{93}$$

is a privileged decomposition with eigenvalues (λ_j) defined as follows: if the index $j \in I$ corresponds to the ordered pair (ϵ_m, ϵ_n) , then:

$$\lambda_j := \begin{cases} \rho_n \rho_m^{-1}, & \text{if } j \text{ is even} \\ \rho_n^{-1} \rho_m, & \text{if } j \text{ is odd} \end{cases} \tag{94}$$

Moreover the Markov generator \mathcal{L} , in the expression (90), satisfies a weighted detailed balance condition in which $\tilde{L}_k = q_k^{\frac{1}{2}} L_k''$ where $L_k'' = \sum_j u_{kj} L_j$ with $u \equiv (u_{k,j})_{k,j \in I}$ the unitary (permutation) operator whose elements are defined by

$$u_{k,j} := \begin{cases} \delta_{k+1,j}, & \text{if } k \text{ is even} \\ \delta_{k-1,j}, & \text{if } k \text{ is odd} \end{cases} \tag{95}$$

and the sequence of weights $q \equiv (q_k)$ is given by (94) and, in the notation (88):

$$q_k := \begin{cases} \lambda_k^{-1} \gamma_k \gamma_{k+1}^{-1}, & \text{if } k \text{ is even} \\ \lambda_k^{-1} \gamma_k^{-1} \gamma_{k+1}, & \text{if } k \text{ is odd} \end{cases} \tag{96}$$

Proof. For j even one has, if the (λ_j) are defined as in (94):

$$\begin{aligned} \rho L_j &= \gamma_j^{\frac{1}{2}} \langle \epsilon_n | D | \epsilon_m \rangle \rho | \epsilon_n \rangle \langle \epsilon_m | = \gamma_j^{\frac{1}{2}} \rho_n \rho_m^{-1} \langle \epsilon_n | D | \epsilon_m \rangle | \epsilon_n \rangle \langle \epsilon_m | \rho = \lambda_j L_j \rho \\ \rho L_{j+1} &= \gamma_{j+1}^{\frac{1}{2}} \overline{\langle \epsilon_n | D | \epsilon_m \rangle} \rho | \epsilon_m \rangle \langle \epsilon_n | = \gamma_{j+1}^{\frac{1}{2}} \overline{\langle \epsilon_n | D | \epsilon_m \rangle} \rho_m \rho_n^{-1} | \epsilon_m \rangle \langle \epsilon_n | \rho = \lambda_{j+1} L_{j+1} \rho \end{aligned}$$

This implies that the representation of \mathcal{L} by means of operators $(L_j)_j$ and Δ is privileged with eigenvalues (λ_j) given by (94).

Finally, let us verify that condition (ii) in Theorem 8 holds.

From (91) we see that for every $j \in I$ we have

$$L_j^* = \begin{cases} \gamma_j^{\frac{1}{2}} \gamma_{j+1}^{-\frac{1}{2}} L_{j+1} & , \text{ if } j \text{ is even} \\ \gamma_j^{\frac{1}{2}} \gamma_{j-1}^{-\frac{1}{2}} L_{j-1} & , \text{ if } j \text{ is odd} \end{cases}$$

Hence denoting for $2j, 2j + 1 \in I$

$$q_{2j} := \lambda_{2j}^{-1} \gamma_{2j} \gamma_{2j+1}^{-1} \quad ; \quad q_{2j+1} := \lambda_{2j+1}^{-1} \gamma_{2j}^{-1} \gamma_{2j+1}$$

and, using (95) to define the unitary operator $u \equiv (u_{k,j})_{k,j \in I}$, one obtains the relation:

$$\tilde{L}_k = \lambda_k^{-1} L_k^* = q_k^{\frac{1}{2}} L_k'' \tag{97}$$

This finishes the proof.

Remark. Notice that, if the index $k \in I$ corresponds to the ordered pair (ϵ_m, ϵ_n) in the sense of Definition 7, then the identity (96) implies that, for generic Markov generators of stochastic limit type, one has:

$$q_k = \lambda_k^{-1} \gamma_k \gamma_{k+1}^{-1} = \lambda_k^{-1} \Gamma_{-, \epsilon_m - \epsilon_n} (\Gamma_{+, \epsilon_m - \epsilon_n})^{-1} =: \lambda_k^{-1} q_{mn} q_{nm}^{-1} \tag{98}$$

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Combining this with (94) and (88), we see that in this case the current operator Π_ρ in the weighted detailed balance condition (i) of Theorem 8, takes the form

$$\begin{aligned} \Pi_\rho(x) &= \sum_{j,l} \left(\sum_k (q_k - 1) \bar{u}_{kj} u_{kl} \right) L_j^* x L_l \\ &= \sum_{k \geq 0} \left((q_{2k} - 1) L_{2k+1}^* x L_{2k+1} + (q_{2k+1} - 1) L_{2k}^* x L_{2k} \right) \\ &= \sum_{\{(m,n): \epsilon_m - \epsilon_n > 0\}} \left(\left(\frac{\rho_m q_{mn}}{\rho_n q_{nm}} - 1 \right) q_{nm} D_{mn}^* x D_{mn} + \left(\frac{\rho_n q_{nm}}{\rho_m q_{mn}} - 1 \right) q_{mn} D_{nm}^* x D_{nm} \right) \\ &= \sum_{\{(m,n): \epsilon_m - \epsilon_n > 0\}} \left(J_{mn} \rho_n^{-1} D_{mn}^* x D_{mn} + J_{nm} \rho_m^{-1} D_{nm}^* x D_{nm} \right) \end{aligned} \quad (99)$$

where

$$J_{mn} = \rho_m q_{mn} - \rho_n q_{nm}, \quad J_{nm} = -J_{mn} \quad (100)$$

In [2] it was proved that the quantities J_{mn} have a natural interpretation as (**micro**)–**currents** of quanta from the level ϵ_m to the level ϵ_n . This is the operator Π arising in the *dynamical detailed balance* of Accardi-Imafuku in [2]. The case of all currents equal zero, corresponds with the notion of quantum detailed balance in the sense of (49). But in section (9), we will show that even relatively simple physical situations can give rise to generic Markov generators with non-zero currents.

8 Cycle description of Markov generators

It is known that generic Markov generators with respect to an Hamiltonian H are associated with H in the sense of Definition 3 and that their invariant states coincide with the invariant state of the classical Markov chain induced by their restriction on $\{H\}' = \{H\}''$. This allows to reduce the problem of describing the invariant states of these generators to a problem on classical Markov chains.

In this section we discuss the connections between the notion of weighted detailed balance of Markov generators and the cycle decomposition of such generators due to Kalpazidou and Qian [20], [25]. These connections will be used in the following sections to analyze the properties of some non equilibrium states arising from concrete physical models.

We shall consider the case of generators of the form (52) with finite dimensional state space:

$$\mathcal{H} = \mathbb{C}^d$$

and H generic. Clearly in our assumptions $\text{Spect}(H_S)$ finite. Under these assumptions the following two propositions are an immediate consequence of Kalpazidou's cyclic decomposition for the currents (100) $J_{mn} = \rho_m q_{mn} - \rho_n q_{nm}$, see [20], and Theorems 2.1.2 and 2.2.10 in [25].

Proposition 2. *Assume that:*

- H is generic,
- $S = \text{Spect}(H)$ is finite
- the diagonal restriction of the QMS generated by a Markov generator of the form (52) is a finite classical Markov chain irreducible, recurrent and stationary with faithful invariant state (measure) ρ .

Then

$$\begin{aligned} \mathcal{L}(x) - \mathcal{L}_\rho^*(x) &= 2i[\Delta, x] - \\ &= \sum_{\{(m,n): \epsilon_m > \epsilon_n\}} \sum_{c \in \mathcal{C}_\infty} (w_c - w_{c_-}) J_c(m, n) \left(\rho_m^{-1} D_{mn}^* x D_{mn} - \rho_n^{-1} D_{mn} x D_{mn}^* \right) = \\ &= 2i[K, x] - \sum_{c \in \mathcal{C}_\infty} (w_c - w_{c_-}) \sum_{\{(m,n): \epsilon_m > \epsilon_n\}} J_c(m, n) \left(\rho_m^{-1} D_{mn}^* x D_{mn} - \rho_n^{-1} D_{mn} x D_{mn}^* \right) \end{aligned} \quad (101)$$

Where in Kalpazidou–Qian's notations, w_c are the cycle skipping rates of the classical Markov chain, \mathcal{C}_∞ is the set of cycles and $J_c(m, n)$ is the passage function for the cycle c , i.e., $J_c(m, n) = 1$ if the edge (m, n) belongs to the cycle c and zero otherwise. Notice that only those edges (m, n) that belong to a cycle give a non-trivial contribution.

Theorem 12. *The following are equivalent:*

- (i) *The adjoint generator \mathcal{L}_ρ^* satisfies quantum detailed balance condition (49),*
- (ii) *The associated classical Markov chain is reversible,*
- (iii) *The classical Markov chain is in detailed balance,*
- (iv) *The classical (or diagonal restriction) generator $Q = (q_{i,j})_{i,j \in S}$ satisfies Kolmogorov's reversibility condition:*

$$q_{\epsilon_0, \epsilon_1} q_{\epsilon_1, \epsilon_2} \cdots q_{\epsilon_{s-1}, \epsilon_s} = q_{\epsilon_s, \epsilon_{s-1}} \cdots q_{\epsilon_2, \epsilon_1} q_{\epsilon_1, \epsilon_0} \quad (102)$$

for any finite collection (cycle) $\{\epsilon_0, \dots, \epsilon_s\}$ of different elements of S , $s \geq 2$ and $\epsilon_0 = \epsilon_s$.

- (v) $w_c = w_{c^-}$, $\forall c \in \mathcal{C}_\infty$,
- (vi) *The classical entropy production rate e_p in the sense of Qian (Definition 2.2.3 of Qian's book), equals zero.*

8.1 Invariant states with constant micro-currents

Theorem 13. *Assume H is generic, $S = \text{Spect}(H)$ is finite and the diagonal restriction of a GKSL generator \mathcal{L} of the form (52) is the generator of an irreducible, recurrent and stationary classical Markov chain with a faithful invariant state (measure) ρ . Then \mathcal{L} satisfies a WDB condition (45)-(46) with a current operator Π of the form (99)-(100) with constant currents up to the sign.*

Proof. Under the above assumptions, in the notation (100) and given the explicit form (99) of the current operator Π_ρ , equation $\Pi_{\rho^*}(\rho) = 0$ takes the form

$$\sum_{\{(m,n): \epsilon_m > \epsilon_n\}} \left(\frac{J_{mn}}{\rho_m} D_{mn} \rho D_{mn}^* + \frac{J_{nm}}{\rho_n} D_{mn}^* \rho D_{mn} \right) = 0 \quad (103)$$

Equivalently, given the form (93) of ρ and the fact that $D_{mn} := |\epsilon_n\rangle\langle\epsilon_m|$:

$$\sum_{\{(m,n): \epsilon_m > \epsilon_n\}} J_{nm} \left(|\epsilon_m\rangle\langle\epsilon_m| - |\epsilon_n\rangle\langle\epsilon_n| \right) = 0 \quad (104)$$

Notice that the above equation (104) is equivalent to a system of homogeneous d linear equations for the currents J_{mn} given by (100). Indeed, (104) yields the system

$$J_{01} + J_{02} + J_{03} + \cdots + J_{0d} = 0 \quad (105)$$

$$J_{10} + J_{12} + J_{13} + \cdots + J_{1d} = 0 \quad (106)$$

$$J_{20} + J_{21} + J_{23} + \cdots + J_{2d} = 0 \quad (107)$$

$$\vdots \quad (108)$$

$$J_{d0} + J_{d1} + J_{d2} + \cdots + J_{d(d-1)} = 0 \quad , \quad (109)$$

that together with the linear equations $J_{mn} = -J_{nm}$ determine all currents.

Due to the above Theorem, Kolmogorov's reversibility condition holds if and only if $J_{mn} = 0$ for all m, n and the GKSL generator satisfies a detailed balance condition.

Now assume that Kolmogorov's reversibility condition does not hold, i.e., there exists a non-empty set of cycles

$$\mathcal{C} = \{c = \{\epsilon_0, \dots, \epsilon_s\} : \epsilon_j \in S, s \geq 2, \text{ with } \epsilon_0 = \epsilon_s, \text{ such that}$$

$$q_{\epsilon_0, \epsilon_1} q_{\epsilon_1, \epsilon_2} \cdots q_{\epsilon_{s-1}, \epsilon_s} \neq q_{\epsilon_s, \epsilon_{s-1}} \cdots q_{\epsilon_2, \epsilon_1} q_{\epsilon_1, \epsilon_0}\} \quad (110)$$

For generators of the form (52) one has that $q_{ij} > 0$ if and only if $q_{ji} > 0$, therefore all factors in the above product are positive and consequently the corresponding currents $J_{\epsilon_j \epsilon_{j+1}}$ are non-zero whenever the oriented edge $(\epsilon_j, \epsilon_{j+1})$, $0 \leq j \leq s$, belongs to a cycle in \mathcal{C} . With this subset \mathcal{C} of cycles corresponds an oriented graph with vertices (or nodes) in the elements of S and oriented edges

$$E_{\mathcal{C}} = \{(\epsilon_j, \epsilon_{j+1}) : \epsilon_j \in c, 0 \leq j \leq s, \text{ some } c \in \mathcal{C}\}$$

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The incidence matrix of this graph coincides with the matrix of system (105), where all currents equal zero with the exception of those corresponding with edges of the graph. Now we apply the well known fact that the null space of the incidence matrix coincides with the cycle space of a graph, see for instance [12], to obtain a non-trivial solution of (105) given by $J_{mn} = \eta(\epsilon_m, \epsilon_n) J_{\epsilon_0 \epsilon_1}$ with $\eta(\epsilon_m, \epsilon_n) = 0$ if the edge (ϵ_m, ϵ_n) does not belong to some cycle $c \in \mathcal{C}$ and $\eta(\epsilon_m, \epsilon_n) = \pm 1$ otherwise, the sign depending on whether J_{mn} has the same direction as $J_{\epsilon_0 \epsilon_1}$ or the opposite direction, according to the cycle orientation. Since the classical Markov chain is irreducible, one can reach any final level ϵ_f starting from any initial level ϵ_i , i.e., the graph is connected. This implies that every cycle has at least one edge or node in common with some other cycle in the set \mathcal{C} . Hence, if two cycles have a common edge, since the current associated with this common edge is the same, the values of currents in both cycles coincide up to the sign. If the cycles have a node but not an edge in common, then we can consider the cycle formed by concatenation. This finishes the proof.

9 Example: A non-equilibrium steady state for a quantum spin chain

Following the approach in the above section, see also [2], let us consider a quantum chain consisting of two spin interacting with two boson fields in equilibrium at different temperatures so that the global system is in non-equilibrium. The Hamiltonian of the spin chain is defined by means of

$$H = \lambda_1 \sigma_1^z + \lambda_2 \sigma_2^z + (1 + \gamma) \sigma_1^x \sigma_2^x + (1 - \gamma) \sigma_1^y \sigma_2^y \quad (111)$$

where λ_1, λ_2 and $\gamma \neq 0$ are real numbers, $\sigma^x, \sigma^y, \sigma^z$ are Pauli matrices and we set σ_1^z for $\sigma^z \otimes I$. For $\lambda_1 \lambda_2 < 1 - \gamma^2$ the spectral representation of the above Hamiltonian is given by

$$H = \sum_{l=0}^3 \epsilon_l |\epsilon_l\rangle \langle \epsilon_l| \quad (112)$$

where

$$\begin{aligned} \epsilon_0 &= -\sqrt{(\lambda_1 - \lambda_2)^2 + 4}, & \epsilon_1 &= -\sqrt{(\lambda_1 + \lambda_2)^2 + 4\gamma^2} \\ \epsilon_2 &= -\epsilon_1 & ; & \quad \epsilon_3 = -\epsilon_0 \end{aligned}$$

and with respect to the basis

$$e_- \otimes e_+, e_- \otimes e_-, e_+ \otimes e_+, e_+ \otimes e_-$$

where e_{\pm} are unit vectors in \mathbb{C}^2 such that $\sigma^x e_{\pm} = e_{\mp}$ and $\sigma^y e_{\pm} = \pm i e_{\mp}$, the coordinates of $(|\epsilon_j\rangle)_{0 \leq j \leq 3}$ are given by

$$\begin{aligned} |\epsilon_0\rangle &= c_0^{-\frac{1}{2}} \left(0, 2, (\lambda_1 - \lambda_2) - \sqrt{(\lambda_1 - \lambda_2)^2 + 4}, 0 \right) \\ |\epsilon_1\rangle &= c_1^{-\frac{1}{2}} \left(2\gamma, 0, 0, (\lambda_1 + \lambda_2) - \sqrt{(\lambda_1 + \lambda_2)^2 + 4\gamma^2} \right) \\ |\epsilon_2\rangle &= c_2^{-\frac{1}{2}} \left(2\gamma, 0, 0, (\lambda_1 + \lambda_2) + \sqrt{(\lambda_1 + \lambda_2)^2 + 4\gamma^2} \right) \\ |\epsilon_3\rangle &= c_3^{-\frac{1}{2}} \left(0, 2, (\lambda_1 - \lambda_2) + \sqrt{(\lambda_1 - \lambda_2)^2 + 4}, 0 \right) \end{aligned}$$

with

$$\begin{aligned} c_0 &= c_0(\lambda_1, \lambda_2) = 4 + \left((\lambda_1 - \lambda_2) - \sqrt{(\lambda_1 - \lambda_2)^2 + 4} \right)^2 \\ c_1 &= c_1(\lambda_1, \lambda_2) = 4\gamma^2 + \left((\lambda_1 + \lambda_2) - \sqrt{(\lambda_1 + \lambda_2)^2 + 4\gamma^2} \right)^2 \\ c_2 &= c_2(\lambda_1, \lambda_2) = 4\gamma^2 + \left((\lambda_1 + \lambda_2) + \sqrt{(\lambda_1 + \lambda_2)^2 + 4\gamma^2} \right)^2 \\ c_3 &= c_3(\lambda_1, \lambda_2) = 4 + \left((\lambda_1 - \lambda_2) + \sqrt{(\lambda_1 - \lambda_2)^2 + 4} \right)^2 \end{aligned} \quad (113)$$

Notice that $\epsilon_0 < \epsilon_1 < \epsilon_2 < \epsilon_3$ and the set of Bohr frequencies is given explicitly

$$F = \{\omega = \epsilon_r - \epsilon_{r'} : \epsilon_r, \epsilon_{r'} \in \text{Spec}(H)\} = \{\omega_{10}, \omega_{20}, \omega_{30}, \omega_{21}\} \quad (114)$$

with

$$\begin{aligned} \omega_{10} &= \epsilon_1 - \epsilon_0, \omega_{20} = \epsilon_2 - \epsilon_0, \omega_{30} = \epsilon_3 - \epsilon_0, \omega_{21} = \epsilon_2 - \epsilon_1 \\ \omega_{31} &= \epsilon_3 - \epsilon_1 = \omega_{20} \\ \omega_{32} &= \epsilon_3 - \epsilon_2 = \omega_{10} \end{aligned}$$

Hence we are in the case of a non-generic Hamiltonian. For simplicity we will write simply

$$\omega_1 = \omega_{10}, \omega_2 = \omega_{20}, \omega_3 = \omega_{30}, \omega_4 = \omega_{21}, \omega_5 = \omega_{31} \text{ and } \omega_6 = \omega_{32}$$

The interaction of the spin chain with the two non-equilibrium boson fields is described by the Hamiltonian

$$H = H_0 + \lambda \sum_{j=1,2} H_{I_j} \quad (115)$$

where λ is a coupling constant,

$$\begin{aligned} H_0 &= H + H_B \\ H_B &= \sum_j \int \omega_j(k) a_{j,k}^\dagger a_{j,k} \\ [a_{j,k}, a_{j',k'}^\dagger] &= \delta_{jj'} \delta(k - k'), \\ H_{I_j} &= \int dk \left(g_j(k) D_j a_{j,k}^\dagger + g_j^*(k) D_j^\dagger a_{j,k} \right) \end{aligned}$$

where $D_j = \sigma_j^-$,

$$\sigma^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad (116)$$

$a_{j,k}$ and $a_{j,k}^\dagger$ are the annihilation and creation operators of the j -th field ($j = 1, 2$) and $g_j(k)$ is a form factor.

The initial state of each field is a Gibbs state at constant temperature β_j^{-1} and chemical potential μ_j with respect to the free Hamiltonian (in this example we assume $\mu_j = 0$, $j = 1, 2$), i.e., the mean zero gauge invariant Gaussian state with correlations

$$\langle a_{j,k}^\dagger a_{j',k'} \rangle = \delta_{jj'} N(k; \beta_j) \delta(k - k') \quad ; \quad N(k; \beta_j) = \frac{1}{e^{\beta_j \omega_j(k)} - 1} \quad (117)$$

The Schrödinger equation in the interaction picture is

$$\frac{d}{dt} U_t^{(\lambda)} = -i\lambda H_I(t) U_t^{(\lambda)}, \quad U_t^{(\lambda)} = e^{itH} e^{-itH_0} \quad (118)$$

where

$$\begin{aligned} H_I(t) &= \sum_{j=1,2} e^{itH_0} H_{I_j} e^{-itH_0} \\ &= \sum_{j=1,2} \sum_{\omega \in F} \sum_{l,m} \int dk \\ &\quad \left(g_{j;l,m}(k) E_\omega(l, m) a_{j,k}^\dagger e^{i(\omega_j(k) - \omega)t} + g_{j;l,m}^*(k) E_\omega^\dagger(l, m) a_{j,k} e^{-i(\omega_j(k) - \omega)t} \right) \end{aligned} \quad (119)$$

with

$$\begin{aligned} g_{j;l,m}(k) &= g_j(k) \langle \epsilon_l, D_j \epsilon_m \rangle \\ E_\omega(l, m) &= \sum_{\epsilon_r \in F_\omega} \langle \epsilon_r - \omega | \epsilon_l \rangle \langle \epsilon_m | \epsilon_r \rangle | \epsilon_r - \omega \rangle \langle \epsilon_r |, \omega = \epsilon_m - \epsilon_l, \epsilon_m > \epsilon_l \end{aligned} \quad (120)$$

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$$F_\omega = \{\epsilon_{r'} \in \text{Spec}(H) : \epsilon_{r'} - \omega \in \text{Spec}(H)\}$$

The spectrum of H is not degenerate but,

$$F_{\omega_1} = \{\epsilon_1, \epsilon_3\} = F_{\omega_6} \quad ; \quad F_{\omega_2} = \{\epsilon_2, \epsilon_3\} = F_{\omega_5}$$

Hence the state $\rho_{H,\beta} = (\rho_0, \dots, \rho_n)$, $\rho_n = e^{-\beta(\epsilon_n)\epsilon_n}$ with $\beta(\epsilon_n) = \epsilon_n^{-1} \log \rho_n$ is non-generic. After some simple computations we get

$$E_{\omega_{10}} = E_{\omega_{10}}(0, 1) = |\epsilon_0\rangle\langle\epsilon_1|$$

$$E_{\omega_{32}} = E_{\omega_{10}}(2, 3) = |\epsilon_2\rangle\langle\epsilon_3|$$

$$E_{\omega_{20}} = E_{\omega_{20}}(0, 2) = |\epsilon_0\rangle\langle\epsilon_2|$$

$$E_{\omega_{31}} = E_{\omega_{20}}(1, 3) = |\epsilon_1\rangle\langle\epsilon_3|$$

This shows that the contribution due to the two frequencies that do not satisfy condition (152) equals the contribution of the same frequencies in the generic case. Therefore the generator of this semigroup belongs to the generic class defined in section (7.3).

The master equation for the reduced dynamics of the spin chain is given by

$$\frac{d\rho(t)}{dt} = \mathcal{L}_*(\rho(t)), \quad (121)$$

With Δ , $\gamma_{\pm,j,\omega}$ given by (163), and (164), respectively. Taking

$$g_j(k) = e^{-\frac{1}{2}|k|^2} \quad (122)$$

$j = 1, 2$ using (164) and (120), after some computation we get for $\lambda_1\lambda_2 < 1 - \gamma^2$ and $d = 3$

$$q_{10} = \Gamma_{-, \epsilon_1 - \epsilon_0} = 4\pi^2 \frac{(c_1 - 4\gamma^2)}{c_0 c_1} \omega_1 e^{-\omega_1} \left(4 \frac{e^{\beta_1 \omega_1}}{e^{\beta_1 \omega_1} - 1} + (c_0 - 4)^2 \frac{e^{\beta_2 \omega_1}}{e^{\beta_2 \omega_1} - 1} \right) \quad (123)$$

$$q_{01} = 4\pi^2 \frac{(c_1 - 4\gamma^2)}{c_0 c_1} \omega_1 e^{-\omega_1} \left(\frac{4}{e^{\beta_1 \omega_1} - 1} + \frac{(c_0 - 4)^2}{e^{\beta_2 \omega_1} - 1} \right)$$

$$q_{20} = 8\pi^2 \frac{(c_2 - 4\gamma^2)^2}{c_0 c_2} \omega_2 e^{-\omega_2} \left(4 \frac{e^{\beta_1 \omega_2}}{e^{\beta_1 \omega_2} - 1} + (c_0 - 4)^2 \frac{e^{\beta_2 \omega_2}}{e^{\beta_2 \omega_2} - 1} \right)$$

$$q_{02} = 8\pi^2 \frac{(c_2 - 4\gamma^2)^2}{c_0 c_2} \omega_2 e^{-\omega_2} \left(\frac{4}{e^{\beta_1 \omega_2} - 1} + \frac{(c_0 - 4)^2}{e^{\beta_2 \omega_2} - 1} \right)$$

$$q_{31} = 8\pi^2 \frac{4\gamma^2}{c_1 c_3} \omega_2 e^{-\omega_2} \left((c_3 - 4)^2 \frac{e^{\beta_1 \omega_2}}{e^{\beta_1 \omega_2} - 1} + 4 \frac{e^{\beta_2 \omega_2}}{e^{\beta_2 \omega_2} - 1} \right)$$

$$q_{13} = 8\pi^2 \frac{4\gamma^2}{c_1 c_3} \omega_2 e^{-\omega_2} \left(\frac{(c_3 - 4)^2}{e^{\beta_1 \omega_2} - 1} + \frac{4}{e^{\beta_2 \omega_2} - 1} \right)$$

$$q_{32} = 8\pi^2 \frac{1}{c_2 c_3} \omega_1 e^{-\omega_1} \left((c_3 - 4)^2 \frac{e^{\beta_1 \omega_1}}{e^{\beta_1 \omega_1} - 1} + 16\gamma^2 \frac{e^{\beta_2 \omega_1}}{e^{\beta_2 \omega_1} - 1} \right)$$

$$q_{23} = 8\pi^2 \frac{1}{c_2 c_3} \omega_1 e^{-\omega_1} \left(\frac{(c_3 - 4)^2}{e^{\beta_1 \omega_1} - 1} + \frac{16\gamma^2}{e^{\beta_2 \omega_1} - 1} \right)$$

And all remaining q'_{ij} s equal zero.

Moreover, the restriction of the pre-dual generator to the diagonal sub-algebra, is the generator of a classical Markov chain whose Q -matrix is given by

$$Q = \begin{pmatrix} -(q_{01} + q_{02}) & q_{01} & q_{02} & 0 \\ q_{10} & -(q_{10} + q_{13}) & 0 & q_{13} \\ q_{20} & 0 & -(q_{20} + q_{23}) & q_{23} \\ 0 & q_{31} & q_{32} & -(q_{31} + q_{32}) \end{pmatrix} \quad (124)$$

One can easily see that the classical Markov chain with the above Q -matrix is irreducible, i.e., for every ϵ_j, ϵ_k , there exists $n \geq 1$ and $\epsilon_1, \dots, \epsilon_n$ such that $q_{\epsilon_j \epsilon_1}, q_{\epsilon_1 \epsilon_2}, \dots, q_{\epsilon_n \epsilon_k} > 0$. In other words, starting from any ϵ_j it is possible to reach any ϵ_k with positive probability. Moreover it has an invariant measure, that we identify with the generalized Gibbs state ρ . The explicit form of ρ is given below in equation (129).

The Markov generator \mathcal{L} has the form (52). Hence it is a weighted detailed balance generator. There exists the minimal QMS generated by \mathcal{L} and we denote by \mathcal{T}_{*t} the pre-dual semigroup.

To identify the cycles that does not satisfy Kolmogorov's reversibility condition, one can use formula (2.9) in Theorem 2.1.2 of [25], to evaluate the cycle skipping rates in terms of the matrix elements of Q . It follows that for all cycles we have $w_c = w_{c_-}$ with the exception of the cycle

$$c = (0, 2, 3, 1)$$

It follows from the above Theorem 12 that Kolmogorov's reversibility condition does not hold for this cycle. Moreover we can prove the following.

Proposition 3. *Kolmogorov's reversibility condition holds for the cycle $(0, 2, 3, 1)$, i.e.,*

$$q_{02}q_{23}q_{31}q_{10} = q_{01}q_{13}q_{32}q_{20},$$

for all values of ω_1, ω_2 ; if and only if the boson fields are at the same temperature, $\beta_1^{-1} = \beta_2^{-1}$.

Proof. A simple computation using (123) shows that

$$q_{02}q_{23}q_{31}q_{10} = q_{01}q_{13}q_{32}q_{20}$$

for all ω_1, ω_2 , if and only if

$$\frac{f(\omega_2)}{h(\omega_2)} = \frac{f(\omega_1)}{g(\omega_1)}, \quad (125)$$

for all ω_1, ω_2 . Where

$$\begin{aligned} f(\omega) &= \frac{4(e^{\beta_2\omega} - 1) + (c_0 - 4)^2 e^{(\beta_2 - \beta_1)\omega} (e^{\beta_1\omega} - 1)}{4(e^{\beta_2\omega} - 1) + (c_0 - 4)^2 (e^{\beta_1\omega} - 1)} \\ g(\omega) &= \frac{(c_3 - 4)^2 (e^{\beta_2\omega} - 1) + 16\gamma^2 e^{(\beta_2 - \beta_1)\omega} (e^{\beta_1\omega} - 1)}{(c_3 - 4)^2 (e^{\beta_2\omega} - 1) + 16\gamma^2 (e^{\beta_1\omega} - 1)} \\ h(\omega) &= \frac{(c_3 - 4)^2 (e^{\beta_2\omega} - 1) + 4e^{(\beta_2 - \beta_1)\omega} (e^{\beta_1\omega} - 1)}{(c_3 - 4)^2 (e^{\beta_2\omega} - 1) + 4(e^{\beta_1\omega} - 1)} \end{aligned} \quad (126)$$

If $\beta_1 = \beta_2$, then $f(\omega) = g(\omega) = h(\omega) = 1$ and (125) clearly holds for all ω_1, ω_2 .

Conversely, if $\beta_1 \neq \beta_2$, let us say $\beta_2 > \beta_1$, then when $\lambda_1, \lambda_2 \rightarrow 0$ and $\gamma \rightarrow 1$ we have $\omega_1 \rightarrow 0$ and $\omega_2 \rightarrow 4$ therefore $\frac{f(\omega_1)}{g(\omega_1)} \rightarrow 1$, but $\frac{f(\omega_2)}{h(\omega_2)}$ approaches the value

$$1 + (e^{4(\beta_2 - \beta_1)} - 1) \left(\frac{\frac{e^{4\beta_1} - 1}{e^{4\beta_2} - 1}}{4 + 16 \frac{e^{4\beta_1} - 1}{e^{4\beta_2} - 1}} \right) > 1.$$

Therefore (125) does not hold for all ω_1, ω_2 . This finishes the proof.

Corollary 4. *If $\beta_1^{-1} \neq \beta_2^{-1}$ then the GKSL generator of the QMS associated with the above spin chain, satisfies a weighted detailed balance condition with constant currents $J = J_{10}$ up to the sign.*

Proof. If $\beta_1^{-1} \neq \beta_2^{-1}$, then Kolmogorov's reversibility condition is violated for the cycle $(0, 2, 3, 1)$ i.e.,

$$q_{02}q_{23}q_{31}q_{10} \neq q_{01}q_{13}q_{32}q_{20}. \quad (127)$$

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Then, associated with this cycle is the solution of system (105): $J_{20} = -J_{10}$, $J_{30} = J_{10}$, $J_{21} = -J_{10}$ and all remaining J_{mn} 's equal zero. This proves the corollary.

The invariant state ρ is a solution of the linear system,

$$C\rho = \mathbf{j}, \quad (128)$$

with $\mathbf{j} = J_{10}(1, -1, 1, -1)$ and

$$C = \begin{pmatrix} -q_{01} & q_{10} & 0 & 0 \\ -q_{02} & 0 & q_{20} & 0 \\ 0 & -q_{13} & 0 & q_{31} \\ 0 & 0 & -q_{23} & q_{32} \end{pmatrix}$$

Direct computations show that the unique solution of (128) has the explicit form $\tilde{\rho} = (\rho_0, \rho_1, \rho_2, \rho_3)$, with

$$\begin{aligned} \rho_0 &= \frac{(q_{13}q_{20}q_{32} + q_{10}(q_{23}q_{31} + q_{20}(q_{31} + q_{32})))J_{10}}{\text{Det}(C)} \\ \rho_1 &= \frac{(q_{02}q_{23}q_{31} + q_{01}(q_{23}q_{31} + q_{20}(q_{31} + q_{32})))J_{10}}{\text{Det}(C)} \\ \rho_2 &= \frac{(q_{01}q_{13}q_{32} + q_{02}(q_{13}q_{32} + q_{10}(q_{31} + q_{32})))J_{10}}{\text{Det}(C)} \\ \rho_3 &= \frac{(q_{02}(q_{10} + q_{13})q_{23} + q_{01}q_{13}(q_{20} + q_{23}))J_{10}}{\text{Det}(C)} \end{aligned} \quad (129)$$

Where

$$\text{Det}(C) = q_{02}q_{23}q_{31}q_{10} - q_{01}q_{13}q_{32}q_{20}.$$

The value of the current J_{10} is obtained in terms of the q'_{ij} 's from the normalization condition $\text{tr}(\tilde{\rho}) = 1$. It is well known that, if an irreducible Markov chain has an invariant measure, then this is unique and has a positive mass at every site of the state space. Moreover it was proven in Proposition 5.2 of [10], that if the classical restriction of a generic QMS $(\mathcal{T}_t)_{t \geq 0}$ is irreducible and has an invariant measure ρ , then this state is the unique \mathcal{T}_t -invariant state and

$$\lim_{t \rightarrow \infty} \mathcal{T}_{*t}(\sigma) = \rho, \quad (130)$$

in the trace norm for every initial normal state σ . Hence, as a consequence of the above result, the QMS associated with our quantum spin chain has a unique non-equilibrium (or dynamical equilibrium) invariant state ρ given up to normalization by (129) if and only if the boson fields are at different temperatures, i.e., $\beta_1^{-1} = \beta_2^{-1}$; and it is ergodic, in the sense that any initial normal state is driven by the QMS towards the dynamical equilibrium steady state ρ .

10 Cycle dynamics and entropy production

Our analysis of the cycle decomposition of a GKSL generator satisfying a weighted detailed balance reveals that, in a non-equilibrium stationary state of the small system coupled to the environment, there exists a dynamics associated with the set \mathcal{C} of cycles violating Kolmogorov's reversibility condition.

The first important question is to give a physical meaning to the current operator $\Pi_{\rho_{H,\beta}}$ in current decomposition (99). First of all notice that this is a CCP map, i.e., a quantum object. One can compute explicitly $\Pi_{\rho_{H,\beta}}$ in the case of the spin chain of Example 1 above. In this case $\Pi_{\rho_{H,\beta}}$ is not identically zero, it has a non-trivial contribution coming from the cycle $(0, 2, 3, 1)$. Moreover, denoting by $\Pi_{\rho_{H,\beta},*}$ its predual, one can show that $\Pi_{\rho_{H,\beta},*}(\rho_{H,\beta})$ is the diagonal matrix

$$\begin{pmatrix} w_{(0231)} - w_{(1320)} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -w_{(0231)} + w_{(1320)} \end{pmatrix} \quad (131)$$

A naive interpretation of this quantity is the following: $\Pi_{\rho_{H,\beta}}(\rho_{H,\beta})$ represents the net current (or flow of energy) between the fields through the small system, i.e., the spin chain. Indeed, at level ϵ_0 , the spin chain is taken a quantity $w_{(0231)} - w_{(1320)}$ of energy from environment at temperature $\beta_1^{-1} > \beta_2^{-1}$ and the same quantity is transfer to environment at temperature β_2^{-1} at level ϵ_3 . The quantity $w_{(0231)} - w_{(1320)}$ can be computed explicitly in terms of the matrix elements q_{mn} of the classical generator Q , i.e., in terms of the temperatures $\beta_1^{-1}, \beta_2^{-1}$. See equation (2.9) in Theorem 2.1.1, page 49 of Qian's book [25]. For an irreducible and stationary continuous time Markov chain, the notion of entropy production was defined by the Qian's and collaborators, see Chapter 2 in [25], in terms of the relative entropy of the probabilities of the Markov chain and its time reversed. This entropy production rate has a simple expression in terms of the cycle skipping rates w_c of cycles in \mathcal{C} , indeed,

$$e_p = \frac{1}{2} \sum_{c \in \mathcal{C}_\infty} (w_c - w_{c^-}) \log\left(\frac{w_c}{w_{c^-}}\right) \quad (132)$$

Therefore using again formula (2.9) in Theorem 2.1.2 of [25], to evaluate the cycle skipping rates in terms of the matrix elements of Q , one can evaluate the entropy production in both examples of the above section. Indeed, for the spin chain in Example 1, a direct computation show that

$$\begin{aligned} e_p &= (w_{(0231)} - w_{(0132)}) \log \frac{w_{(0231)}}{w_{(0132)}} \\ &= - \frac{q_{02}q_{23}q_{31}q_{10} - q_{01}q_{13}q_{32}q_{20}}{\sum_{j=0}^3 \tilde{D}(\{j\}^c)} \log \frac{q_{02}q_{23}q_{31}q_{10}}{q_{01}q_{13}q_{32}q_{20}} \end{aligned} \quad (133)$$

where

$$\begin{aligned} \tilde{D}(\{0\}^c) &= q_{13}q_{20}q_{32} + q_{10}q_{23}q_{31} + q_{10}q_{20}q_{31} + q_{10}q_{20}q_{32} \\ \tilde{D}(\{1\}^c) &= q_{02}q_{23}q_{31} + q_{01}q_{23}q_{31} + q_{01}q_{20}q_{31} + q_{01}q_{20}q_{32} \\ \tilde{D}(\{2\}^c) &= q_{01}q_{13}q_{32} + q_{02}q_{13}q_{32} + q_{02}q_{10}q_{31} + q_{02}q_{10}q_{32} \\ \tilde{D}(\{3\}^c) &= q_{02}q_{10}q_{23} + q_{02}q_{13}q_{23} + q_{01}q_{12}q_{20} + q_{01}q_{13}q_{23} \end{aligned}$$

Therefore, entropy production is non-zero since Kolmogorov's reversibility condition is violated on the cycle (0231) and consequently

$$q_{02}q_{23}q_{31}q_{10} - q_{01}q_{13}q_{32}q_{20} \neq 0$$

11 Appendix (I): Eigenoperators of $Ad(e^{itH})$

In the present Appendix we recall some useful notions from [6].

Theorem 14. (see Theorem 34 in [6]) Let $H = H^* \hat{\in} \mathcal{B}(\mathcal{H})$ be a pure point spectrum Hamiltonian

$$H = \sum_{\epsilon \in \text{spec}(H)} \epsilon P_\epsilon = \sum_m \epsilon_m P_m \quad (134)$$

Consider the associated 1-parameter automorphism group;

$$u_t(\cdot) := e^{itH}(\cdot)e^{-itH} \quad (135)$$

and the associated set of Bohr frequencies.

$$B = B_H := \{\omega = \epsilon_r - \epsilon_{r'} : \epsilon_r, \epsilon_{r'} \in \text{Spec}(H)\} = \text{Spec}(u_t) \quad (136)$$

Then one has:

$$u_t(x) = \sum_{\omega \in B} e^{-it\omega} E_\omega(x) \quad ; \quad \forall x \in \mathcal{B}(\mathcal{H}), \quad \forall t \in \mathbb{R}_+ \quad (137)$$

where, for each $\omega \in B$, the operator E_ω is defined by (62) and the operators E_ω satisfy the identities

$$E_\omega(x)^* = E_{-\omega}(x^*) \quad ; \quad \forall x \in \mathcal{B}(\mathcal{H}) \quad (138)$$

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$$E_\omega E_{\omega'} = \delta_{\omega, \omega'} E_\omega \quad (\text{mutual orthogonality}) \tag{139}$$

$$\sum_{\omega \in B} E_\omega(\cdot) = id_{\mathcal{B}(\mathcal{H})} \quad (\text{normalization}) \tag{140}$$

$$E_0(\cdot) = \sum_{\{\varepsilon_n \in \text{Spec}(H)\}} P_{\varepsilon_n}(\cdot) P_{\varepsilon_n} \tag{141}$$

is the Umegaki conditional expectation onto $\{H\}'$.

Remark. One easily verifies (see Proposition 33 of [6]) that

$$E_\omega(\mathcal{B}(\mathcal{H})) = \{x \in \mathcal{B}(\mathcal{H}) : e^{itH} x e^{-itH} = e^{-it\omega} x\} \tag{142}$$

Any element of this subspace will be called an ω -eigen-operator of $Ad(e^{itH})$. (140) is equivalent to

$$\mathcal{B}(\mathcal{H}) = \bigoplus_{\omega} E_\omega(\mathcal{B}(\mathcal{H})) \tag{143}$$

the sum being orthogonal in the sense that, if $\omega' \neq \omega$, then

$$E_{\omega'} E_\omega(x) = 0 \quad ; \quad \forall x \in \mathcal{B}(\mathcal{H})$$

The sum (143) is orthogonal also in another sense, specified by the following Lemma.

Lemma 7. If $\rho \in \{H\}'$ (in particular if $\rho \in \{H\}''$), then for any $\omega, \omega' \in B$ one has:

$$Tr(\rho E_\omega(x)^* E_{\omega'}(y)) = \delta_{\omega, \omega'} Tr(\rho E_\omega(x)^* E_\omega(y)) \quad ; \quad \forall x, y \in \mathcal{B}(\mathcal{H})$$

Proof. If $\rho \in \{H\}'$ then, using (142) and (138), we see that:

$$\begin{aligned} Tr(\rho E_\omega(x)^* E_{\omega'}(y)) &= Tr(e^{itH} \rho E_{-\omega}(x^*) E_{\omega'}(y) e^{-itH}) \\ &= Tr(\rho (e^{itH} E_{-\omega}(x^*) e^{-itH}) (e^{itH} E_{\omega'}(y) e^{-itH})) \\ &= e^{it(\omega - \omega')} Tr(\rho E_\omega(x)^* E_{\omega'}(y)) \end{aligned}$$

If $\omega - \omega' \neq 0$, this is possible only if $Tr(\rho E_\omega(x)^* E_{\omega'}(y)) = 0$.

Lemma 8. For any $\omega, \omega' \in B$ one has:

$$E_\omega(\mathcal{B}(\mathcal{H})) \cdot E_{\omega'}(\mathcal{B}(\mathcal{H})) \subseteq E_{\omega + \omega'}(\mathcal{B}(\mathcal{H})) \quad (\text{grading}) \tag{144}$$

$$E_\omega(\mathcal{B}(\mathcal{H}))^* = E_{-\omega}(\mathcal{B}(\mathcal{H})) \tag{145}$$

Proof. For any $t \in \mathbb{R}$, $\omega, \omega' \in B$ and $x, y \in \mathcal{B}(\mathcal{H})$ one has:

$$\begin{aligned} e^{itH} E_\omega(x) E_{\omega'}(y) e^{-itH} &= (e^{itH} E_\omega(x) e^{-itH}) (e^{itH} E_{\omega'}(y) e^{-itH}) \\ &= (e^{it\omega} E_\omega(x)) (e^{it\omega'} E_{\omega'}(y)) = e^{it(\omega + \omega')} E_\omega(x) E_{\omega'}(y) \end{aligned}$$

Thus $E_\omega(x) E_{\omega'}(y) \in E_{\omega + \omega'}(\mathcal{B}(\mathcal{H}))$ and this proves (144). (145) follows from (138) and the fact that $\mathcal{B}(\mathcal{H})^* = \mathcal{B}(\mathcal{H})$.

Corollary 5. For all $\omega \in B$ and any operator $A \in \{H\}' \equiv E_0(\mathcal{B}(\mathcal{H}))$, one has

$$[A, E_\omega(\mathcal{B}(\mathcal{H}))] \subseteq E_\omega(\mathcal{B}(\mathcal{H})) \tag{146}$$

$$\{A, E_\omega(\mathcal{B}(\mathcal{H}))\} \subseteq E_\omega(\mathcal{B}(\mathcal{H})) \tag{147}$$

Moreover, $\forall \omega, \omega' \in B$ and $\forall D_\omega \in E_\omega(\mathcal{B}(\mathcal{H}))$, one has:

$$D_\omega^* D_\omega, D_\omega D_\omega^* \in \{H\}' \equiv E_0(\mathcal{B}(\mathcal{H})) \tag{148}$$

$$D_\omega^* E_{\omega'}(\mathcal{B}(\mathcal{H})) D_\omega \subseteq E_{\omega'}(\mathcal{B}(\mathcal{H})) \tag{149}$$

Proof. All the identities are immediate consequences of Lemma 8.

Lemma 9. Let $F : \text{spec}(H) \rightarrow \mathbb{R}$ be a Borel function. Then $\forall y$ and $\forall m, n \in \mathbb{N}$

$$\begin{aligned} F(H)P_m y &= F(\varepsilon_m)P_m y \\ yP_n F(H) &= F(\varepsilon_n)yP_n \end{aligned}$$

in particular, if y has the form

$$y = P_m z P_n \quad ; \quad z \in \mathcal{B}(\mathcal{H}) \quad ; \quad m, n \in \mathbb{N} \quad (150)$$

Then

$$e^{\beta(H)H} y e^{-\beta(H)H} = e^{\beta(\varepsilon_m)\varepsilon_m - \varepsilon_n}\varepsilon_n y \quad (151)$$

Proof. Clear from the spectral decomposition (15) of H .

11.1 The generic case

The generic case is characterized by the condition

$$|B_\omega| = 1 \quad ; \quad \forall \omega \in B_+ \quad (152)$$

Let $\omega \in B_+$. Condition (152) is characterized by the existence of a unique pair $(\varepsilon_\omega^+, \varepsilon_\omega^-)$ such that $\varepsilon_\omega^+, \varepsilon_\omega^- \in \text{spec}(H)$ and

$$\varepsilon_\omega^- := \varepsilon_\omega^+ - \omega \in \text{spec}(H)$$

or equivalently

$$\varepsilon_\omega^+ - \varepsilon_\omega^- = \omega > 0$$

In this case the spectrum of H is non degenerate so that

$$P_\varepsilon = |\varepsilon\rangle\langle\varepsilon|$$

Therefore

$$E_0(x) = \sum_n \langle \varepsilon_n, x \varepsilon_n \rangle |\varepsilon_n\rangle\langle\varepsilon_n|$$

and, if $\omega > 0$, in the generic case

$$\begin{aligned} E_\omega &= |\varepsilon_\omega^+\rangle\langle\varepsilon_\omega^+|(\cdot)|\varepsilon_\omega^-\rangle\langle\varepsilon_\omega^-| \\ E_\omega(x) &= \langle\varepsilon_\omega^+, x \varepsilon_\omega^-\rangle |\varepsilon_\omega^+\rangle\langle\varepsilon_\omega^-| \\ E_\omega^*(x) &= E_{-\omega} = \langle\varepsilon_\omega^-, x^* \varepsilon_\omega^+\rangle |\varepsilon_\omega^-\rangle\langle\varepsilon_\omega^+| \\ E_{-\omega} &= |\varepsilon_\omega^-\rangle\langle\varepsilon_\omega^-|(\cdot)|\varepsilon_\omega^+\rangle\langle\varepsilon_\omega^+| \\ E_\omega^*(x) &= E_{-\omega}(x^*) \\ E_\omega &\rightarrow E_\omega(D) \\ E_\omega^* &\rightarrow E_{-\omega}(D^*) \end{aligned}$$

For $\omega \in B_+$ define

$$E_\omega(D) = \langle\varepsilon_\omega^+, D\varepsilon_\omega^-\rangle |\varepsilon_\omega^+\rangle\langle\varepsilon_\omega^-| =: \delta_\omega |\varepsilon_\omega^+\rangle\langle\varepsilon_\omega^-|$$

Then

$$\begin{aligned} E_\omega(D)E_\omega(D)^* &= E_\omega(D)E_{-\omega}(D^*) = \langle\varepsilon_\omega^-, D^* \varepsilon_\omega^+\rangle |\varepsilon_\omega^-\rangle\langle\varepsilon_\omega^-| \\ &= \overline{\langle\varepsilon_\omega^+, D\varepsilon_\omega^-\rangle} |\varepsilon_\omega^-\rangle\langle\varepsilon_\omega^-| =: \bar{\delta}_\omega |\varepsilon_\omega^-\rangle\langle\varepsilon_\omega^-| \\ E_\omega(D)E_\omega(D)^* &= E_\omega(D)E_{-\omega}(D^*) = |\delta_\omega|^2 |\varepsilon_\omega^+\rangle\langle\varepsilon_\omega^+| =: q_\omega P_{\varepsilon_\omega^+} \\ E_\omega(D)^*E_\omega(D) &= E_{-\omega}(D^*)E_\omega(D) = |\delta_\omega|^2 P_{\varepsilon_\omega^-} = q_\omega P_{\varepsilon_\omega^-} \\ E_\omega(D)^*x E_\omega(D) &= E_{-\omega}(D^*)x E_\omega(D) = q_\omega \langle\varepsilon_\omega^+, x \varepsilon_\omega^+\rangle P_{\varepsilon_\omega^-} \end{aligned}$$

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$$E_\omega(D)x E_\omega(D)^* = E_\omega(D)x E_{-\omega}(D^*) = q_\omega \langle \varepsilon_\omega^-, \lambda \varepsilon_\omega \rangle P_{\varepsilon_\omega^\pm}$$

$$\Delta|\varepsilon\rangle = i\hat{d}_\varepsilon|\varepsilon\rangle \quad ; \quad d_\omega := \hat{d}_{\varepsilon_\omega^+} - \hat{d}_{\varepsilon_\omega^-}$$

$$\begin{aligned} & \mathcal{L}(|\varepsilon_\omega^+\rangle\langle\varepsilon_\omega^-|) \\ &= id_\omega |\varepsilon_\omega^+\rangle\langle\varepsilon_\omega^-| + \Gamma_{\omega,-} \left(-\frac{1}{2} q_\omega |\varepsilon_\omega^+\rangle\langle\varepsilon_\omega^-| \right) + \Gamma_{\omega,+} \left(-\frac{1}{2} q_\omega |\varepsilon_\omega^+\rangle\langle\varepsilon_\omega^-| \right) \\ &= \left[-\left(\frac{\Gamma_{\omega,-} + \Gamma_{\omega,+}}{2} \right) q_\omega + id_\omega \right] |\varepsilon_\omega^+\rangle\langle\varepsilon_\omega^-| \end{aligned}$$

$$\begin{aligned} \mathcal{L}(|\varepsilon_\omega^-\rangle\langle\varepsilon_\omega^+|) &= -id_\omega |\varepsilon_\omega^-\rangle\langle\varepsilon_\omega^+| - \left(\frac{\Gamma_{\omega,-} + \Gamma_{\omega,+}}{2} \right) q_\omega |\varepsilon_\omega^-\rangle\langle\varepsilon_\omega^+| \\ &= \left[-\left(\frac{\Gamma_{\omega,-} + \Gamma_{\omega,+}}{2} \right) - id_\omega \right] |\varepsilon_\omega^-\rangle\langle\varepsilon_\omega^+| \end{aligned}$$

Under our assumptions the right hand side of (41) is equal to

$$e^{\beta(\varepsilon_n)\varepsilon_m - \beta(\varepsilon_n)\varepsilon_n} Tr(\rho \mathcal{L}(y)x)$$

Let

$$\omega = \varepsilon_m - \varepsilon_n$$

Therefore the right hand side of (41) is equal to

$$e^{\beta(\varepsilon_m)\varepsilon_m - \beta(\varepsilon_n)\varepsilon_n} \left[-\frac{1}{2} (\Gamma_{\omega,-} + \Gamma_{\omega,+}) q_\omega + id_\omega \right] Tr(\rho |\varepsilon_n\rangle\langle\varepsilon_n|)$$

and, using that:

$$\rho = \sum F(\varepsilon_n) |\varepsilon_n\rangle\langle\varepsilon_n|$$

this is equal to

$$e^{\beta(\varepsilon_m)\varepsilon_m - \beta(\varepsilon_n)\varepsilon_n} F(\varepsilon_m) \left[-\frac{1}{2} (\Gamma_{\omega,-} + \Gamma_{\omega,+}) q_\omega + id_\omega \right]$$

12 Appendix (II): Stochastic limit of systems interacting with fields in a non-equilibrium state (level I)

Consider a system interacting with a boson field in momentum representation

$$[a_k, a_{k'}^\dagger] = \delta(k - k') \quad (153)$$

whose initial state is a mean zero gauge invariant Gaussian state with correlations:

$$\langle a_k^\dagger a_{k'} \rangle = N(k) \delta(k - k') \quad ; \quad N(k) = \frac{1}{e^{\beta(\omega(k))\omega(k)} - 1} \quad (154)$$

$\beta(\omega(k))$ is positive function (generalized inverse temperature) which is a natural generalization of the Gibbs factor, to which it reduces when $\beta(\omega)$ is constant:

$$\beta(\omega) = \beta \quad (155)$$

This class of (in general non equilibrium) states of the field includes many important examples, including the usual Gibbs states and the state of two equilibrium heat baths at different temperatures (and possibly different chemical potentials).

The full Hamiltonian is given by

$$H = H_0 + \lambda H_I \quad ; \quad (\lambda \text{ is a coupling constant}) \quad (156)$$

where

$$H_0 = H + H_B \quad ; \quad H := \sum_l \epsilon_l |\epsilon_l\rangle \langle \epsilon_l| \quad ; \quad H_B := \int \omega(k) a_k^\dagger a_k \quad (157)$$

$$H_I := \int dk \left(g(k) D a_k^\dagger + g^*(k) D^\dagger a_k \right) \quad (158)$$

Using the *stochastic golden rule* (see [1]) one deduces the white noise Hamiltonian equation

$$\frac{d}{dt} U_t = -i \sum_{\omega \in F} \left(D_\omega b_{t;\omega}^\dagger + D_\omega^\dagger b_{t;\omega} \right) U_t \quad (159)$$

driven by the Boson white noises

$$b_{\omega,t} = \int dk g_\omega^*(k) b_{\omega,t}(k) \quad ; \quad b_{\omega,t}(k) = \lim_{\lambda \rightarrow 0} \frac{1}{\lambda} e^{-i(\omega_j(k) - \omega)t/\lambda^2} a_k \quad (160)$$

the limit being meant in the sense of operator valued distributions.

The operators D_ω , in the white noise Hamiltonian equation (159), are defined by

$$D_\omega := E_\omega(D) \quad (161)$$

where D is the operator which enters in the interaction Hamiltonian (158) and E_ω is defined by (62). The state of the limit white noise will be of the same type as (154) but with correlations

$$\langle b_{\omega,t}^\dagger(k) b_{\omega',t'}(k') \rangle = \delta_{\omega\omega'} 2\pi \delta(t-t') \delta(k-k') \delta(\omega(k) - \omega) N(k)$$

$$\langle b_{\omega,t}(k) b_{\omega',t'}^\dagger(k') \rangle = \delta_{\omega\omega'} 2\pi \delta(t-t') \delta(k-k') \delta(\omega(k) - \omega) (N(k) + 1)$$

From this, using a standard procedure of the stochastic limit approach (causal normal order of the white noise Hamiltonian equation) one deduces the master equation for a system density operator:

$$\begin{aligned} \frac{d}{dt} \rho(t) = & -i[\Delta, \rho(t)] - \sum_{\omega \in F} \Gamma_{-, \omega} \left(\frac{1}{2} \{ D_\omega^\dagger D_\omega, \rho(t) \} - D_\omega \rho(t) D_\omega^\dagger \right) \\ & - \sum_{\omega \in F} \Gamma_{+, \omega} \left(\frac{1}{2} \{ D_\omega D_\omega^\dagger, \rho(t) \} - D_\omega^\dagger \rho(t) D_\omega \right) \end{aligned} \quad (162)$$

where the operators D_ω are as above and:

$$\Delta = i \sum_{\omega \in F} (\text{Im}(\gamma_{-\omega}) D_\omega^\dagger D_\omega - \text{Im}(\gamma_{+\omega}) D_\omega D_\omega^\dagger) \quad (163)$$

$$\Gamma_{\mp, \omega} = 2\text{Re} \gamma_{\mp, \omega} \geq 0 \quad \text{for } \omega > 0 \quad (164)$$

$$\Gamma_{\mp, \omega} = 0 \quad \text{for } \omega \leq 0 \quad (165)$$

$$\begin{aligned} \gamma_{-, \omega} &= \int dk |g_\omega(k)|^2 \frac{-i(N(k)+1)}{\omega - \omega(k) - i0} \\ &= \pi \int dk |g_\omega(k)|^2 \frac{e^{\beta(\omega(k))\omega(k)}}{e^{\beta(\omega(k))\omega(k)} - 1} \delta(\omega(k) - \omega) - i\text{P.P} \int dk \frac{|g_\omega(k)|^2 e^{\beta(\omega(k))\omega(k)}}{(\omega(k) - \omega)(e^{\beta(\omega(k))\omega(k)} - 1)} \\ &= \pi \frac{e^{\beta(\omega)\omega}}{e^{\beta(\omega)\omega} - 1} \int dk |g_\omega(k)|^2 \delta(\omega(k) - \omega) - i\text{P.P} \int dk \frac{|g_\omega(k)|^2 e^{\beta(\omega(k))\omega(k)}}{\omega(k) - \omega} \frac{1}{e^{\beta(\omega(k))\omega(k)} - 1} \\ &=: \pi \frac{e^{\beta(\omega)\omega}}{e^{\beta(\omega)\omega} - 1} \frac{G_\omega}{2\pi} - iG_{-, \omega} \end{aligned} \quad (166)$$

$$\begin{aligned} \gamma_{+, \omega} &= \int dk |g_\omega(k)|^2 \frac{-iN(k)}{\omega - \omega(k) - i0} \\ &= \pi \int dk |g_\omega(k)|^2 \frac{1}{e^{\beta(\omega(k))\omega(k)} - 1} \delta(\omega(k) - \omega) - i\text{P.P} \int dk \frac{|g_\omega(k)|^2}{\omega(k) - \omega} \frac{1}{e^{\beta(\omega(k))\omega(k)} - 1} \\ &= \pi \frac{1}{e^{\beta(\omega)\omega} - 1} \int dk |g_\omega(k)|^2 \delta(\omega(k) - \omega) - i\text{P.P} \int dk \frac{|g_\omega(k)|^2}{\omega(k) - \omega} \frac{1}{e^{\beta(\omega(k))\omega(k)} - 1} \\ &=: \pi \frac{1}{e^{\beta(\omega)\omega} - 1} \frac{G_\omega}{2\pi} - iG_{+, \omega} \end{aligned} \quad (167)$$

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and we have defined

$$\begin{aligned} \frac{G_\omega}{2\pi} &:= \int dk |g_\omega(k)|^2 \delta(\omega(k) - \omega) \geq 0 \\ G_{-, \omega} &:= \text{P.P} \int dk \frac{|g_\omega(k)|^2}{\omega(k) - \omega} \frac{e^{\beta(\omega(k))\omega(k)}}{e^{\beta(\omega(k))\omega(k)} - 1} \\ G_{+, \omega} &:= \text{P.P} \int dk \frac{|g_\omega(k)|^2}{\omega(k) - \omega} \frac{1}{e^{\beta(\omega(k))\omega(k)} - 1} \end{aligned}$$

Notice that both G_ω and

$$G_{-, \omega} - G_{+, \omega} = \text{P.P} \int dk \frac{|g_\omega(k)|^2}{\omega(k) - \omega} =: I_\omega$$

are independent of β . From equation (164) we then obtain, for $\omega > 0$:

$$\Gamma_{-, \omega} = 2\text{Re} \gamma_{-, \omega} = 2\pi \frac{e^{\beta(\omega)\omega}}{e^{\beta(\omega)\omega} - 1} \frac{G_\omega}{2\pi} = \frac{e^{\beta(\omega)\omega}}{e^{\beta(\omega)\omega} - 1} G_\omega \tag{168}$$

$$\Gamma_{+, \omega} = 2\text{Re} \gamma_{+, \omega} = 2\pi \frac{1}{e^{\beta(\omega)\omega} - 1} \frac{G_\omega}{2\pi} = \frac{1}{e^{\beta(\omega)\omega} - 1} G_\omega \tag{169}$$

Notice that $\Gamma_{\pm, \omega}$ are both ≥ 0 if

$$\omega > 0 \Rightarrow \beta(\omega) > 0 \tag{170}$$

With these expressions for the parameters the master equation (162) becomes:

$$\begin{aligned} \frac{d}{dt} \rho(t) &= \mathcal{L}_*(\rho(t)) = -i[\Delta, \rho(t)] \\ &- \sum_{\omega \in F} \frac{e^{\beta(\omega)\omega}}{e^{\beta(\omega)\omega} - 1} G_\omega \left(\frac{1}{2} \{D_\omega^\dagger D_\omega, \rho(t)\} - D_\omega \rho(t) D_\omega^\dagger \right) \\ &- \sum_{\omega \in F} \frac{1}{e^{\beta(\omega)\omega} - 1} G_\omega \left(\frac{1}{2} \{D_\omega D_\omega^\dagger, \rho(t)\} - D_\omega^\dagger \rho(t) D_\omega \right) \end{aligned} \tag{171}$$

Remark.

We have to check if the generator

$$\begin{aligned} \mathcal{L} &= i[\Delta, (\cdot)] \\ &- \sum_{\omega \in F} \frac{e^{\beta(\omega)\omega}}{e^{\beta(\omega)\omega} - 1} G_\omega \left(\frac{1}{2} \{D_\omega^\dagger D_\omega, (\cdot)\} - D_\omega^\dagger (\cdot) D_\omega \right) \\ &- \sum_{\omega \in F} \frac{1}{e^{\beta(\omega)\omega} - 1} G_\omega \left(\frac{1}{2} \{D_\omega D_\omega^\dagger, (\cdot)\} - D_\omega (\cdot) D_\omega^\dagger \right) \end{aligned}$$

satisfies equation (24), i.e.

$$\text{Tr}(\rho e^{\beta(H)H} \mathcal{L}(y) e^{-\beta(H)H} x) = \text{Tr}(\rho x \mathcal{L}(y)); \quad \forall x, y \in \mathcal{B}(\mathcal{H})$$

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