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Entropy Production for Quantum Markov Semigroups

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Abstract: An invariant state of a quantum Markov semigroup is an equilibrium state if it satisfies a quantum detailed balance condition. In this paper, we introduce a notion of entropy production for faithful normal invariant states of a quantum Markov semigroup on $\mathcal{B}(\mathsf{h})$ as a numerical index measuring "how far" they are from equilibrium. The entropy production rate is defined as the derivative of the relative entropy of the one-step forward and backward evolution, in analogy with the classical probabilistic concept. We prove an explicit trace formula expressing the entropy production rate in terms of the completely positive part of the generator of a norm continuous quantum Markov semigroup, showing that it turns out to be zero if and only if a standard quantum detailed balance condition holds.

1. Introduction

This paper proposes a novel perspective on non equilibrium dissipative evolution of open quantum systems within the Markovian approach. In this context, equilibrium states are invariant states characterised by a quantum detailed balance condition (see [3,5,13,23,25,31]), a natural property generalising classical detailed balance. However, a concept that distinguishes, among non equilibrium states, those that on one hand have a rich non trivial structure and, on the other hand, are sufficiently simple to allow a detailed study, is still missing.

Entropy production has been proposed in several papers [8,9,12,21,24,27] as an index of deviation from detailed balance related with a rate of entropy variation. In [15] we proposed a definition of entropy production rate for faithful normal invariant states of quantum Markov semigroups analogous to those introduced for classical Markov semigroups in models for interacting particles.

The entropy production is defined in [15] as the relative entropy of the one-step forward and backward two-point states at time t (Definition 3 here) obtained from a maximally entangled state deformed by means of the given invariant state (see (11)).

Since it is a function vanishing at $t = 0$, the entropy production rate is its right derivative at $t = 0$.

In this paper, we prove an explicit trace formula for the entropy production in terms of the completely positive part of the generator of a norm continuous quantum Markov semigroup (Theorem 5). Our formula shows that non zero entropy production is closely related with the violation of quantum detailed balance conditions and singles out states with finite entropy production as a rich class of simple non equilibrium invariant states. Moreover, it provides an operator analogue (Theorem 8a) of a necessary condition for finiteness of classical entropy production in terms of transition intensities, namely $\gamma_{jk} > 0$ if and only $\gamma_{kj} > 0$.

The plan of the paper is as follows. In Sect. 2 quantum detailed balance conditions are reviewed and the key result on the structure of generators is recalled. The forward and backward two-point are introduced in Sect. 3, starting from quantum detailed balance conditions, and their densities are computed. Entropy production is defined in Sect. 4 and the explicit formula is proved in Sect. 5. Three examples illustrating how entropy production indicates deviation from detailed balance are presented in Sect. 7.

Finally, we discuss some features of our results and possible directions for further investigation.

2. Quantum Detailed Balance Conditions

Let $\mathcal{A}$ be a von Neumann algebra with a faithful normal state ω and identity $\mathbb{1}$. A quantum Markov semigroup (QMS) on $\mathcal{A}$ is a weakly*-continuous semigroup $\mathcal{T} = (\mathcal{T}_t)_{t\geq 0}$ of normal, unital, completely positive maps on $\mathcal{A}$. The predual semigroup on $\mathcal{A}_*$ will be denoted by $\mathcal{T}_* = (\mathcal{T}_{*t})_{t\geq 0}$.

The state ω is invariant if $\omega(\mathcal{T}_t(a)) = \omega(a)$ for all $a \in \mathcal{A}$ and $t \geq 0$. A number of conditions called *quantum detailed balance* (QDB) conditions have been proposed in the literature to distinguish, among invariant states, those enjoying reversibility properties.

The first one, to the best of our knowledge, appeared in the work of Agarwal [3] in 1973. Later extended and studied in detail by Majewski [25], it involves a reversing operation $\Theta : \mathcal{A} \to \mathcal{A}$, namely a linear $*$-map ($\Theta(a^*) = \Theta(a)^*$ for all $a \in \mathcal{A}$), that is also an antihomomorphism ($\Theta(ab) = \Theta(b)\Theta(a)$) and satisfies $\Theta^2 = I$, where I denotes the identity map on $\mathcal{A}$. A QMS satisfies the Agarwal-Majewski QDB condition if $\omega(a\mathcal{T}_t(b)) = \omega(\Theta(b)\mathcal{T}_t(\Theta(a)))$, for all $a, b \in \mathcal{A}$. If the state ω is invariant under the reversing operation, i.e. $\omega(\Theta(a)) = \omega(a)$ for all $a \in \mathcal{A}$, as we shall assume throughout the paper, this condition can be written in the equivalent form $\omega(a\mathcal{T}_t(b)) = \omega((\Theta \circ \mathcal{T}_t \circ \Theta)(a)b)$ for all $a, b \in \mathcal{A}$. Therefore the Agarwal-Majewski QDB condition means that maps $\mathcal{T}_t$ admit dual maps coinciding with $\Theta \circ \mathcal{T}_t \circ \Theta$ for all $t \geq 0$; in particular dual maps must be positive since Θ is obviously positivity preserving. The map Θ often appears in the physical literature (see e.g. Talkner [31] and the references therein) as a parity map; a self-adjoint a is an even (resp. odd) observable if $\Theta(a) = a$ (resp. $\Theta(a) = -a$).

When $\mathcal{A} = \mathcal{B}(\mathsf{h})$, the von Neumann algebra of all bounded operators on a complex separable Hilbert space h, as it is often the case for open quantum systems, the typical Θ is given by $\Theta(a) = \theta a^* \theta$ where θ is the conjugation with respect to a fixed orthonormal basis $(e_n)_{n\geq 0}$ of h acting as

$$\theta\left(\sum_{n\geq 0} u_n e_n\right) = \sum_{n\geq 0} \bar{u}_n e_n. \tag{1}$$

The operator θ, however, can be any antiunitary ($\langle \theta v, \theta u\rangle = \langle u, v\rangle$ for all $u, v \in \mathsf{h}$) such that $\theta^2 = \mathbb{1}$. Moreover, from $\omega(\theta a^*\theta) = \omega(a)$, letting ρ denote the density of ω and denoting by $\mathrm{tr}\,(\cdot)$ the trace on h, the linear operator $\theta\rho\theta$ being self-adjoint by $\langle v, \theta\rho\theta u\rangle = \langle \rho\theta u, \theta v\rangle = \langle \theta u, \rho\theta v\rangle = \langle \theta\rho\theta v, u\rangle$, we have

$$\mathrm{tr}\,(\rho a) = \mathrm{tr}\,\left(\rho\theta a^*\theta\right) = \sum_n \left\langle e_n, \rho\theta a^*\theta e_n\right\rangle = \sum_n \left\langle \theta\rho\theta a^*(\theta e_n), (\theta e_n)\right\rangle = \mathrm{tr}\,(\theta\rho\theta a)$$

for all $a \in \mathcal{A}$, thus $\rho = \theta\rho\theta$, i.e. θ commutes with ρ. This assumption is reasonable because ρ is often a function of energy which is an even observable, therefore it applies throughout the paper.

The best known QDB notion, however, is due to Alicki [5,6] and Kossakowski et al. [23]. According to these authors, the QDB holds if there exists a dual QMS $\widetilde{\mathcal{T}} = \left(\widetilde{\mathcal{T}}_t\right)_{t\ge 0}$ on $\mathcal{A}$ such that $\omega\left(a\mathcal{T}_t(b)\right) = \omega\left(\widetilde{\mathcal{T}}_t(a)b\right)$ and the difference of generators $\mathcal{L}$ and $\widetilde{\mathcal{L}}$ is a derivation.

Both the above QDB conditions depend in a crucial way from the bilinear form $(a, b) \to \omega(ab)$. Indeed, when they hold true, all positive maps $\mathcal{T}_t$ admit *positive* dual maps; as a consequence, all the maps $\mathcal{T}_t$ must commute with the modular group $(\sigma_t^{\omega})_{t\in\mathbb{R}}$ associated with the pair $(\mathcal{A}, \omega)$ (see [23] Prop. 2.1, [26] Prop. 5). This algebraic restriction is unnecessary if we consider the bilinear form $(a, b) \to \omega\left(\sigma_{\mathrm{i}/2}(a)b\right)$ introduced by Petz [29] in the study of Accardi-Cecchini conditional expectations. In this way, as noted by Goldstein and Lindsay (see [11,19]), one can define dual QMS, also when maps $\mathcal{T}_t$ do not commute with the modular group. Dual QMS defined in this way are called KMS-duals in contrast with GNS-duals defined via the bilinear form $(a, b) \to \omega\,(ab)$.

QDB conditions arising when we consider KMS-duals instead of GNS-duals are called *standard* (see e.g. [13,17]); we could not find them in the literature, but it seems that they belong to the folklore of the subject. In particular, they were considered by R. Alicki and A. Majewski (private communication).

Definition 1. Let $\mathcal{T}$ be a QMS with a dual QMS $\mathcal{T}'$ satisfying $\omega\left(\sigma_{\mathrm{i}/2}(a)\mathcal{T}_t(b)\right) = \omega\left(\sigma_{\mathrm{i}/2}\left(\mathcal{T}_t'(a)\right)b\right)$ for all $a, b \in \mathcal{A}$, $t \ge 0$. The semigroup $\mathcal{T}$ satisfies:

1. the standard quantum detailed balance condition with respect to the reversing operation Θ (SQBD-Θ) if $\mathcal{T}_t' = \Theta \circ \mathcal{T}_t \circ \Theta$ for all $t \ge 0$,
2. the standard quantum detailed balance condition (SQDB) if the difference of generators $\mathcal{L} - \mathcal{L}'$ of $\mathcal{T}$ and $\mathcal{T}'$ is a densely defined derivation.

It is worth noticing here that the above *standard* QDB conditions coincide with the Agarwal-Majewski and Alicki-Gorini-Kossakowski-Frigerio-Verri respectively when the QMS $\mathcal{T}$ commutes with the modular group $(\sigma_t)_{t\in\mathbb{R}}$ associated with the pair $(\mathcal{A}, \omega)$ (see, e.g., [11,26] and [16,17] for $\mathcal{A} = \mathcal{B}(\mathsf{h})$).

In the present paper we concentrate on QMS on $\mathcal{B}(\mathsf{h})$ which are the most frequent for open quantum systems. All states will be assumed to be normal and identified with their densities. In particular, $\omega(x) = \mathrm{tr}\,(\rho\, x)$, $\sigma_t(x) = \rho^{\mathrm{i}t} x \rho^{-\mathrm{i}t}$ and the KMS duality reads

$$\mathrm{tr}\left(\rho^{1/2}\, a\, \rho^{1/2}\, \mathcal{T}_t(b)\right) = \mathrm{tr}\left(\rho^{1/2}\, \mathcal{T}_t'(a)\, \rho^{1/2} b\right). \tag{2}$$

The map Θ will be the reversing operation $\Theta(x) = \theta x^*\theta$ where θ is the antiunitary conjugation (1) with respect to some basis and the $\mathcal{T}$-invariant state ρ *will be assumed to commute with* θ. A Gram-Schmidt process shows that it is always possible to find such an orthonormal basis $(e_j)_{j\geq 1}$ of h of eigenvectors of ρ that are also θ-invariant (see Proposition 7 here).

First we recall the well-known result ([28] Theorem 30.16).

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

(i) $\mathrm{tr}(\rho L_\ell) = 0$ *for all* $\ell \geq 1$,
(ii) $\sum_{\ell\geq 1} L_\ell^* L_\ell$ *is a strongly convergent sum,*
(iii) *if* $(c_\ell)_{\ell\geq 0}$ *is a square-summable sequence of complex scalars and* $c_0 \mathbb{1} + \sum_{\ell\geq 1} c_\ell L_\ell = 0$ *then* $c_\ell = 0$ *for all* $\ell \geq 0$,
(iv) *the following representation of* $\mathcal{L}$ *holds*

$$\mathcal{L}(x) = \mathrm{i}[H, x] - \frac{1}{2}\sum_{\ell\geq 1}\left(L_\ell^* L_\ell x - 2L_\ell^* x L_\ell + x L_\ell^* L_\ell\right) \tag{3}$$

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

$$H' = H + c, \qquad L'_\ell = \sum_j u_{\ell j} L_j.$$

Formula (3) with operators L_ℓ satisfying (ii) and H self-adjoint gives a GKSL (Gorini-Kossakowski-Sudarshan-Lindblad) representation of $\mathcal{L}$. A GKSL representation of $\mathcal{L}$ by means of operators L_ℓ, H satisfying also conditions (i) and (iii) will be called *special*.

As an immediate consequence of uniqueness (up to a scalar) of the Hamiltonian H, the decomposition of $\mathcal{L}$ as the sum of the derivation $\mathrm{i}[H, \cdot]$ and a dissipative part $\mathcal{L}_0 = \mathcal{L} - \mathrm{i}[H, \cdot\,]$ determined by special GKSL representations of $\mathcal{L}$ is unique. Moreover, since $(u_{\ell j})$ is unitary, we have

$$\sum_{\ell\geq 1}\left(L'_\ell\right)^* L'_\ell = \sum_{\ell,k,j\geq 1} \bar{u}_{\ell k} u_{\ell j} L_k^* L_j = \sum_{k,j\geq 1}\left(\sum_{\ell\geq 1} \bar{u}_{\ell k} u_{\ell j}\right) L_k^* L_j = \sum_{k\geq 1} L_k^* L_k.$$

Therefore, putting $G = -\frac{1}{2}\sum_{\ell\geq 1} L_\ell^* L_\ell - iH$, we can write $\mathcal{L}$ in the form

$$\mathcal{L}(x) = G^* x + \sum_{\ell\geq 1} L_\ell^* x L_\ell + xG \tag{4}$$

where G is uniquely determined by $\mathcal{L}$ up to a purely imaginary multiple of the identity operator.

The unitary matrix $(u_{\ell j})_{\ell j}$ can obviously be realised as a unitary operator on a Hilbert space k, called the *multiplicity space* with Hilbertian dimension equal to the length of the sequence $(L_\ell)_{\ell\geq 1}$ which is also uniquely determined by $\mathcal{L}$ by the minimality condition (iii).

In [17] (Theorems 5, 8 and Remark 4) we proved the following characterisations of QMS satisfying a standard QDB condition.

Theorem 2. *A QMS $\mathcal{T}$ satisfies the SQDB if and only if for any special GKSL representation of the generator $\mathcal{L}$ by means of operators G, L_ℓ there exists a unitary $(u_{m\ell})_{m\ell}$ on* k *which is also symmetric (i.e. $u_{m\ell} = u_{\ell m}$ for all m, ℓ) such that, for all $k \geq 1$,*

$$\rho^{1/2} L_k^* = \sum_\ell u_{k\ell} L_\ell \rho^{1/2}. \tag{5}$$

Theorem 3. *A QMS $\mathcal{T}$ satisfies the SQBD-Θ condition if and only if for any special GKSL representation of $\mathcal{L}$ by means of operators G, L_ℓ, there exists a self-adjoint unitary $(u_{kj})_{kj}$ on* k *such that:*

1. $\rho^{1/2}\theta G^*\theta = G\rho^{1/2}$,
2. $\rho^{1/2}\theta L_k^*\theta = \sum_j u_{kj} L_j \rho^{1/2}$ *for all* $k \geq 1$.

The SQBD-Θ condition is more restrictive than the SQDB condition because it involves also the identity $\rho^{1/2}\theta G^*\theta = G\rho^{1/2}$ (see Example 7.3). However, this does not happen if $\theta G^*\theta = G$ and ρ commutes with G. This is a reasonable physical assumption satisfied by many QMS as, for instance, those arising from the stochastic limit (e.g. [2,13]).

The following result shows that, condition 2 alone, only implies that the difference $\mathcal{L}' - \Theta \circ \mathcal{L} \circ \Theta$ is a derivation (as in Alicki et al. QDB conditions) and clarifies differences between Theorems 2 and 3.

Theorem 4. *Let $\mathcal{T}$ be a QMS with generator $\mathcal{L}$ in a special GKSL form by means of operators G, L_ℓ. Assume that $\rho^{1/2}\theta L_k^*\theta = \sum_j u_{kj} L_j \rho^{1/2}$, for all $k \geq 1$, for a self-adjoint unitary $(u_{kj})_{kj}$ on* k*. Then*

$$\mathcal{L}'(x) - (\Theta \circ \mathcal{L} \circ \Theta)(x) = \mathrm{i}\,[K, x] \tag{6}$$

with K self-adjoint commuting with ρ.

Proof. Let $\mathcal{T}'$ be the dual QMS of $\mathcal{T}$ as in (2). Since

$$\mathcal{L}'(x) = \rho^{-1/2} \mathcal{L}_* \left(\rho^{1/2} x \rho^{1/2}\right) \rho^{-1/2},$$

comparing special GKSL of $\mathcal{L}$ and $\mathcal{L}'$ (as in [17] Theorem 4), given a special GKSL representation of $\mathcal{L}$ we can find a special GKSL representation of $\mathcal{L}'$ by means of G', L'_ℓ such that

$$G' = \rho^{1/2} G^* \rho^{-1/2}, \qquad L'_\ell = \rho^{1/2} L_\ell^* \rho^{-1/2}. \tag{7}$$

By condition (2.) of Theorem 3 and unitarity of $(u_{\ell k})_{\ell k}$ we have

$$\begin{aligned} \sum_\ell L_\ell'^* x L'_\ell &= \sum_\ell \rho^{-1/2} L_\ell \rho^{1/2} x \rho^{1/2} L_\ell^* \rho^{-1/2} \\ &= \sum_{\ell, j, k} \bar{u}_{\ell j} u_{\ell k} \theta L_k^* \theta x \theta L_j \theta \\ &= \sum_k \theta L_k^* \theta x \theta L_k \theta. \end{aligned}$$

It follows that $\mathcal{L}'$ admits the special GKSL representation

$$\mathcal{L}'(x) = G'^* x + \sum_\ell \theta L_\ell^* \theta x \theta L_\ell \theta + x G' \tag{8}$$

by means of G' and the operators $\theta L_k \theta$.

We now check that $G' - \theta G\theta$ is anti-selfadjoint. Clearly, by the first identity (7), it suffices to check that $\rho^{1/2}\left(G' - \theta G\theta\right)\rho^{1/2} = \rho G^* - \rho^{1/2}\theta G\theta\rho^{1/2}$ is anti-selfadjoint. The state ρ is an invariant state for $\mathcal{T}_*$, thus $\mathcal{L}_*(\rho) = 0$. The duality (2) with $b = \mathbb{1}$ shows that ρ is also invariant for $\mathcal{T}'_*$, then $\mathcal{L}'_*(\rho) = 0$, and we find from (8)

$$\rho G^* + G\rho = \theta\mathcal{L}'_*(\rho)\theta - \sum_{\ell} L_\ell \rho L_\ell^* = \rho\theta G'^*\theta + \theta G'\theta\rho.$$

Taking into account the identity $G'\rho = \rho^{1/2}G^*\rho^{1/2}$ we find that

$$\rho G^* + G\rho = \rho^{1/2}\theta G\theta\rho^{1/2} + \rho^{1/2}\theta G^*\theta\rho^{1/2},$$

namely

$$\rho G^* - \rho^{1/2}\theta G\theta\rho^{1/2} = \rho^{1/2}\theta G^*\theta\rho^{1/2} - G\rho = -\left(\rho G^* - \rho^{1/2}\theta G\theta\rho^{1/2}\right)^*.$$

It follows that $\mathcal{L}' - (\Theta \circ \mathcal{L} \circ \Theta) = \mathrm{i}[K, \cdot]$ with K selfadjoint commuting with ρ since $\mathcal{L}_*(\rho) = \mathcal{L}'_*(\rho) = 0$. □

The SQDB condition without reversing operation (Definition 1) might be paralleled with reversing operation, requiring (6), however, we could not find this QDB condition in the literature.

3. Forward and Backward Two-Point States

We now introduce the *two-point forward and backward states*.

Definition 2. The forward two-point state is the normal state on $\mathcal{B}(\mathsf{h}) \otimes \mathcal{B}(\mathsf{h})$ given by

$$\overrightarrow{\Omega}_t\,(a \otimes b) = \mathrm{tr}\left(\rho^{1/2}\theta a^*\theta\rho^{1/2}\mathcal{T}_t(b)\right), \qquad a, b \in \mathcal{B}(\mathsf{h}); \tag{9}$$

the *backward two-point state* is the normal state on on $\mathcal{B}(\mathsf{h}) \otimes \mathcal{B}(\mathsf{h})$ given by

$$\overleftarrow{\Omega}_t\,(a \otimes b) = \mathrm{tr}\left(\rho^{1/2}\theta\mathcal{T}_t(a^*)\theta\rho^{1/2}b\right), \qquad a, b \in \mathcal{B}(\mathsf{h}). \tag{10}$$

It is clear that both $\overrightarrow{\Omega}_t$ and $\overleftarrow{\Omega}_t$ are normalised linear functionals on $\mathcal{B}(\mathsf{h}) \otimes \mathcal{B}(\mathsf{h})$ since $\theta(za)^*\theta = \theta\bar{z}a^*\theta = z\theta a^*\theta$, for all $z \in \mathbb{C}$ and all $a \in \mathcal{B}(\mathsf{h})$. They are positive and normal by the following proposition also giving their densities.

Proposition 1. *Let $\rho = \sum_j \rho_j \left|e_j\right\rangle\!\left\langle e_j\right|$ be a spectral decomposition of ρ. The density of states $\overrightarrow{\Omega}_0 = \overleftarrow{\Omega}_0$ is the rank one projection*

$$D = |r\rangle\,\langle r|\,, \qquad r = \sum_j \rho_j^{1/2}\theta e_j \otimes e_j \tag{11}$$

The densities of the forward and backward states are respectively

$$\overrightarrow{D}_t = (I \otimes \mathcal{T}_{*t})(D), \qquad \overleftarrow{D}_t = (\mathcal{T}_{*t} \otimes I)(D). \tag{12}$$

Proof. For all $a, b \in \mathcal{B}(\mathsf{h})$ we have

$$\begin{aligned}\langle r, (a\otimes b)r\rangle &= \sum_{j,k}\left(\rho_j\rho_k\right)^{1/2}\left\langle\theta e_j\otimes e_j, (a\otimes b)\theta e_k\otimes e_k\right\rangle\\ &= \sum_{j,k}\left(\rho_j\rho_k\right)^{1/2}\left\langle\theta e_j, a\theta e_k\right\rangle\left\langle e_j, be_k\right\rangle\\ &= \sum_{j,k}\left(\rho_j\rho_k\right)^{1/2}\left\langle\theta a\theta e_k, e_j\right\rangle\left\langle e_j, be_k\right\rangle\\ &= \sum_{k}\rho_k^{1/2}\left\langle\theta a\theta e_k, \rho^{1/2}be_k\right\rangle\\ &= \sum_{k}\left\langle\theta a\theta\rho^{1/2}e_k, \rho^{1/2}be_k\right\rangle\\ &= \operatorname{tr}\left(\rho^{1/2}\theta a^*\theta\rho^{1/2}b\right).\end{aligned}$$

Formulae (12) follow immediately from

$$\overrightarrow{\Omega}_t(a\otimes b) = \overrightarrow{\Omega}_0(a\otimes\mathcal{T}_t(b)), \qquad \overleftarrow{\Omega}_t(a\otimes b) = \overleftarrow{\Omega}_0(\mathcal{T}_t(a)\otimes b).$$

□

The entropy production will be defined in the next section by means of the relative entropy of the forward and backward two-point states.

Remark 1. Note that, when $\mathsf{h} = \mathbb{C}^d$ and $\theta e_j = e_j$ for all j, we have

$$|r\rangle\langle r| = \left(\rho^{1/2}\otimes\mathbb{1}\right)\left(\sum_{j,k=1}^{d}\left|e_j\otimes e_j\right\rangle\langle e_k\otimes e_k|\right)\left(\rho^{1/2}\otimes\mathbb{1}\right)$$

(and the same formula replacing $\rho^{1/2}\otimes\mathbb{1}$ by $\mathbb{1}\otimes\rho^{1/2}$). Therefore $|r\rangle\langle r|$ may be viewed as a ρ deformation of a maximally entangled state and $\overrightarrow{D}_t$, $\overleftarrow{D}_t$ are the image of $I\otimes\mathcal{T}_{*t}$, $\mathcal{T}_{*t}\otimes I$ under the Choi-Jamiołkowski isomorphism.

Remark 2. Operators $\theta x^*\theta$ can be thought of as elements of the *opposite* algebra $\mathcal{B}(\mathsf{h})^{\mathrm{o}}$ of $\mathcal{B}(\mathsf{h})$. Indeed, recall that $\mathcal{B}(\mathsf{h})^{\mathrm{o}}$ is in one-to-one correspondence with $\mathcal{B}(\mathsf{h})$ as a set via the trivial identification $x \to x^{\mathrm{o}}$, has the same vector space structure, involution and norm but the product $\circledcirc$ is given by $x^{\mathrm{o}}\circledcirc y^{\mathrm{o}} = (yx)^{\mathrm{o}}$. Therefore, the linear map $\Theta : \mathcal{B}(\mathsf{h}) \to \mathcal{B}(\mathsf{h})^{\mathrm{o}}$ defined by $x \to \theta x^*\theta$ is a *-isomorphism of $\mathcal{B}(\mathsf{h})$ onto $\mathcal{B}(\mathsf{h})^{\mathrm{o}}$ since

$$\Theta(x)\circledcirc\Theta(y) = \theta x^*\theta\circledcirc\theta y^*\theta = \theta y^*\theta\theta x^*\theta = \theta(xy)^*\theta = \Theta(xy).$$

Clearly $\Theta\otimes I : \mathcal{B}(\mathsf{h})\otimes\mathcal{B}(\mathsf{h}) \to \mathcal{B}(\mathsf{h})^{\mathrm{o}}\otimes\mathcal{B}(\mathsf{h})$ is a *-isomorphism. This remark is useful for defining entropy production as an index measuring deviation from standard detailed balance *without* time reversal in a similar way. One can define the state $\overrightarrow{\Omega}'_0 = \overleftarrow{\Omega}'_0$ on $\mathcal{B}(\mathsf{h})^{\mathrm{o}}\otimes\mathcal{B}(\mathsf{h})$ by

$$\overrightarrow{\Omega}'_0(x\otimes y) = \operatorname{tr}\left(\rho^{1/2}x\rho^{1/2}y\right)$$

Note that element Z of $\mathcal{B}(\mathsf{h})^{\mathrm{o}} \otimes \mathcal{B}(\mathsf{h})$ is "positive" if and only if $(\Theta \otimes I)(Z)$ is positive in $\mathcal{B}(\mathsf{h}) \otimes \mathcal{B}(\mathsf{h})$ because $\Theta \otimes I$ is a *-isomorphism and $(\Theta \otimes I)^2$ is the identity map.

We can define the entropy production again considering the relative entropy of $\overrightarrow{D}_t$ and $\overleftarrow{D}_t$ but now viewed as densities of states on $\mathcal{B}(\mathsf{h})^{\mathrm{o}} \otimes \mathcal{B}(\mathsf{h})$.

We finish this section with a couple of useful properties of r.

Proposition 2. *The vector r is cyclic and separating for subalgebras $\mathbb{1} \otimes \mathcal{B}(\mathsf{h})$ and $\mathcal{B}(\mathsf{h}) \otimes \mathbb{1}$.*

Proof. Let $X \in \mathcal{B}(\mathsf{h})$ and let $\rho = \sum_j \rho_j \left|e_j\right\rangle\!\left\langle e_j\right|$ be a spectral decomposition of ρ. Then $(\mathbb{1} \otimes X)r = 0$ if and only if $\sum_j \rho_j^{1/2}\, \theta e_j \otimes (X e_j) = 0$, i.e. $X e_j = 0$ for all j since $\rho_j > 0$ and vectors θe_j are linearly independent. It follows that $X = 0$.

The same argument shows that r is also separating for $\mathcal{B}(\mathsf{h}) \otimes \mathbb{1}$. Therefore it is cyclic for $\mathbb{1} \otimes \mathcal{B}(\mathsf{h})$ and $\mathcal{B}(\mathsf{h}) \otimes \mathbb{1}$ because these subalgebras of $\mathcal{B}(\mathsf{h}) \otimes \mathcal{B}(\mathsf{h})$ are mutual commutants. □

Proposition 3. *An operator $X \in \mathcal{B}(\mathsf{h})$ satisfies* $\mathrm{tr}\,(\rho X) = 0$ *if and only if $(\mathbb{1} \otimes X)r$ and $(X \otimes \mathbb{1})r$ are orthogonal to r in $\mathsf{h} \otimes \mathsf{h}$.*

Proof. Immediate from $\langle r, (\mathbb{1} \otimes X)r\rangle = \langle r, (X \otimes \mathbb{1})r\rangle = \mathrm{tr}\,(\rho X)$. □

4. Entropy Production for a QMS

In the sequel $\mathrm{Tr}\,(\cdot)$ denotes the trace on $\mathsf{h} \otimes \mathsf{h}$.

The *relative entropy* of $\overrightarrow{\Omega}_t$ with respect to $\overleftarrow{\Omega}_t$ is given by

$$S\left(\overrightarrow{\Omega}_t, \overleftarrow{\Omega}_t\right) = \mathrm{Tr}\left(\overrightarrow{D}_t \left(\log \overrightarrow{D}_t - \log \overleftarrow{D}_t\right)\right),$$

if the support of $\overrightarrow{\Omega}_t$ is included in that of $\overleftarrow{\Omega}_t$ and $+\infty$ otherwise.

Definition 3. The *entropy production rate* of a QMS $\mathcal{T}$ and invariant state ρ is defined by

$$\mathbf{ep}(\mathcal{T}, \rho) = \limsup_{t \to 0^+} \frac{S\left(\overrightarrow{\Omega}_t, \overleftarrow{\Omega}_t\right)}{t} \tag{13}$$

Remark 3. The entropy production rate (entropy production for short) $\mathbf{ep}(\mathcal{T}, \rho)$ is clearly non-negative. It coincides with the right derivative of $S\left(\overrightarrow{\Omega}_t, \overleftarrow{\Omega}_t\right)$ at $t = 0$, if the limit exists, since $S\left(\overrightarrow{\Omega}_0, \overleftarrow{\Omega}_0\right) = 0$. Moreover, $\mathbf{ep}(\mathcal{T}, \rho)$ vanishes if the SQBD-Θ (or the SQDB viewing $\overrightarrow{\Omega}_t$ and $\overleftarrow{\Omega}_t$ as states on $\mathcal{B}(\mathsf{h})^{\mathrm{o}} \otimes \mathcal{B}(\mathsf{h})$) holds.

Under the assumptions of Theorem 5, the entropy production formula (16) we are going to prove, shows that, if $\mathbf{ep}(\mathcal{T}, \rho) = 0$, then the SQDB condition holds as well as the SQBD-Θ condition if $\theta G^* \theta = G$ and $\rho\theta = \theta\rho$. A counterexample in Sect. 7.3 shows that SQBD-Θ may fail without these commutation assumptions even if $\mathbf{ep}(\mathcal{T}, \rho)$ is zero.

Our definition gives a true non-commutative analogue of entropy production for classical Markov semigroups [12]. We refer to [15] subsection 2.2 for a detailed discussion.

Besides this, we have chosen the quantum relative entropy because it is a natural measure of distinguishability between the two quantum states $\overrightarrow{\Omega}_t$, $\overleftarrow{\Omega}_t$. Moreover, it has been extensively used in the physical literature in the study of non-equilibrium (see e.g. [8,9,21,24] and the references therein). Deviation from detailed balance can be measured also by some distance of the above quantum states. In [4] a distance extending the classical Wasserstein distance to a non-commutative algebra was used instead of quantum relative entropy.

Proposition 4. *Let $\overrightarrow{D}_t$ and $\overleftarrow{D}_t$ be the densities of the forward and backward two-point states as in (12). The following are equivalent:*

(a) $\overrightarrow{D}_t = \overleftarrow{D}_t$, *for all $t \geq 0$,*
(b) $(I \otimes \mathcal{L}_*)(D) = (\mathcal{L}_* \otimes I)(D)$.

Proof. Clearly (a) implies (b) by differentiation at time $t = 0$.

Conversely, if (b) holds, since $I \otimes \mathcal{L}_*$ and $\mathcal{L}_* \otimes I$ commute, we have

$$(I \otimes \mathcal{L}_*)^2(D) = (I \otimes \mathcal{L}_*)(\mathcal{L}_* \otimes I)(D) = (\mathcal{L}_* \otimes I)(I \otimes \mathcal{L}_*)(D) = (\mathcal{L}_* \otimes I)^2(D).$$

Thus, by induction, we find $(I \otimes \mathcal{L}_*)^n(D) = (\mathcal{L}_* \otimes I)^n(D)$, for all $n \geq 1$, so that

$$\overrightarrow{D}_t = \sum_{n\geq 0} \frac{t^n}{n!}(I \otimes \mathcal{L}_*)^n(D) = \sum_{n\geq 0} \frac{t^n}{n!}(\mathcal{L}_* \otimes I)^n(D) = \overleftarrow{D}_t,$$

for all $t \geq 0$ and (a) is proved. □

The following proposition shows, in particular, that the relative entropy of the forward and backward two-point state is symmetric.

Proposition 5. *The relative entropy of $\overrightarrow{\Omega}_t$ with respect to $\overleftarrow{\Omega}_t$ satisfies*

$$S\left(\overrightarrow{\Omega}_t, \overleftarrow{\Omega}_t\right) = \frac{1}{2}\mathrm{Tr}\left(\left(\overrightarrow{D}_t - \overleftarrow{D}_t\right)\left(\log \overrightarrow{D}_t - \log \overleftarrow{D}_t\right)\right). \tag{14}$$

In particular, if $S\left(\overrightarrow{\Omega}_t, \overleftarrow{\Omega}_t\right)$ is finite, then the densities $\overrightarrow{D}_t$, $\overleftarrow{D}_t$ have the same support.

Proof. Let F be the unitary flip operator on $\mathsf{h} \otimes \mathsf{h}$ defined by $Fe_j \otimes e_k = e_k \otimes e_j$. Noting that $F\overrightarrow{D}_t F = \overleftarrow{D}_t$ and then $F \log\left(\overrightarrow{D}_t\right) F = \log\left(\overleftarrow{D}_t\right)$, we have

$$\begin{aligned} S\left(\overrightarrow{\Omega}_t, \overleftarrow{\Omega}_t\right) &= \mathrm{Tr}\left(F\overrightarrow{D}_t\left(\log \overrightarrow{D}_t - \log \overleftarrow{D}_t\right)F\right) \\ &= \mathrm{Tr}\left(-\overleftarrow{D}_t\left(\log \overrightarrow{D}_t - \log \overleftarrow{D}_t\right)\right) \end{aligned}$$

Therefore

$$2S\left(\overrightarrow{\Omega}_t, \overleftarrow{\Omega}_t\right) = \mathrm{Tr}\left(\overrightarrow{D}_t\left(\log \overrightarrow{D}_t - \log \overleftarrow{D}_t\right)\right) + \mathrm{Tr}\left(-\overleftarrow{D}_t\left(\log \overrightarrow{D}_t - \log \overleftarrow{D}_t\right)\right)$$

and (14) follows.

If $S\left(\overrightarrow{\Omega}_t, \overleftarrow{\Omega}_t\right)$ is finite, then the support $\mathrm{supp}(\overrightarrow{D}_t)$ of $\overrightarrow{D}_t$ is contained in the support $\mathrm{supp}(\overleftarrow{D}_t)$ of $\overleftarrow{D}_t$. By the identity $F\overrightarrow{D}_t F = \overleftarrow{D}_t$, we have then

$$\mathrm{supp}(\overleftarrow{D}_t) = F\,\mathrm{supp}(\overrightarrow{D}_t)F \subseteq F\,\mathrm{supp}(\overleftarrow{D}_t)F = \mathrm{supp}(\overrightarrow{D}_t),$$

and the proof is complete. □

Proposition 5 shows that the first step towards the computation of the entropy production is to check if $\overrightarrow{D}_t$ and $\overleftarrow{D}_t$ have the same support for t in a right neighbourhood of 0. This is a somewhat technical point (as in the classical case [12]) if both $\overrightarrow{D}_t$ and $\overleftarrow{D}_t$ do not have full support. In Sect. 6 we develop a simple method for solving this problem.

5. Entropy Production Formula

In this section we establish our entropy production formula under the following assumption on supports of the forward and backward state.

(**FBS**) *Supports of* $\overrightarrow{D}_t$ *and* $\overleftarrow{D}_t$ *coincide and are finite dimensional.*

By the definition of relative entropy and Proposition 5, this condition is necessary and sufficient for the relative entropy $S(\overrightarrow{D}_t, \overleftarrow{D}_t)$ to be finite for $t > 0$ when h is finite dimensional. In this case, if (**FBS**) does not hold, then $S(\overrightarrow{D}_t, \overleftarrow{D}_t) = +\infty$ for all $t > 0$ and $S(\overrightarrow{D}_0, \overleftarrow{D}_0) = 0$ and the entropy production rate (13) obviously is infinite. This difficulty does not arise for the classical entropy production rate as defined in [12]. Indeed, if the invariant state ρ is faithful, then the initial density $\overrightarrow{D}_0 = \overleftarrow{D}_0$ is also, and the forward and backward state are faithful for $t \geq 0$. This assumption is too restrictive in our non-commutative framework because the initial densities, here, are pure.

If h is infinite dimensional, condition (**FBS**) ensures that the relative entropy $S(\overrightarrow{D}_t, \overleftarrow{D}_t)$ is finite for all $t > 0$, a preliminary step in the attempt to compute its right derivative at $t = 0$. Indeed, in this case, even if the supports of $\overrightarrow{D}_t$ and $\overleftarrow{D}_t$ coincide, but are not finite dimensional, it is not clear whether the relative entropy is finite and, apparently, another condition is needed to ensure finiteness of $S(\overrightarrow{D}_t, \overleftarrow{D}_t)$ for t in a right neighbourhood of 0.

Finite dimensionality turns out to be extremely useful for the application of results in perturbation theory because supports of $\overrightarrow{D}_t$ and $\overleftarrow{D}_t$ may vary with t even if they coincide and are finite dimensional. A simple example arises when we consider a semigroup $(\mathcal{T}_t)_{t\geq 0}$ of automorphisms of $\mathcal{B}(\mathsf{h})$ with $L_\ell = 0$ for all ℓ and a non-zero self-adjoint operator H. Any faithful density ρ commuting with H provides a faithful invariant state.

Let $\overrightarrow{\Phi}_*$ and $\overleftarrow{\Phi}_*$ be the linear maps on trace class operators on $\mathsf{h} \otimes \mathsf{h}$

$$\overrightarrow{\Phi}_*(X) = \sum_\ell (\mathbb{1} \otimes L_\ell)\, X \left(\mathbb{1} \otimes L_\ell^*\right), \qquad \overleftarrow{\Phi}_*(X) = \sum_\ell (L_\ell \otimes \mathbb{1})\, X \left(L_\ell^* \otimes \mathbb{1}\right) \quad (15)$$

where L_ℓ are the operators of a special GKSL representation of $\mathcal{L}$. Recall that, by Proposition 3, $(\mathbb{1} \otimes L_\ell)\, r$ and $(L_\ell \otimes \mathbb{1})\, r$ are orthogonal to r.

Theorem 5. *Let $\mathcal{T}$ be a norm continuous QMS on $\mathcal{B}(\mathsf{h})$ with a faithful, normal invariant state ρ. Under the assumption* (**FBS**) *the entropy production is*

$$\mathbf{ep}(\mathcal{T}, \rho) = \frac{1}{2}\mathrm{Tr}\left(\left(\overrightarrow{\Phi}_*(D) - \overleftarrow{\Phi}_*(D)\right)\left(\log\left(\overrightarrow{\Phi}_*(D)\right) - \log\left(\overleftarrow{\Phi}_*(D)\right)\right)\right). \quad (16)$$

The rest of this section is devoted to proving (16).

Let S_t denote this common finite dimensional ($k+1$ dimensional, say) support of $\overrightarrow{D}_t$ and $\overleftarrow{D}_t$. Since $\overleftarrow{D}_t = F\overrightarrow{D}_t F$, for all t, we can write spectral decompositions

$$\overrightarrow{D}_t = \sum_{\ell=0}^{k} \lambda_\ell(t)\,\overrightarrow{E}_\ell(t), \qquad \overleftarrow{D}_t = \sum_{\ell=0}^{k} \lambda_\ell(t)\,\overleftarrow{E}_\ell(t), \tag{17}$$

where $\lambda_\ell(t)$ are common eigenvalues and all spectral projections satisfy

$$\overleftarrow{E}_\ell(t) = F\,\overrightarrow{E}_\ell(t)\,F$$

for all $t \geq 0$. Moreover, since S_t is $(k+1)$-dimensional for all $t > 0$, we have $\lambda_\ell(t) > 0$ for all $t > 0$ and $\ell = 0, 1, \ldots, k$.

It is well known that, by deep results in finite-dimensional perturbation theory, Rellich's theorem and its consequences (see e.g. Kato[22], Theorem 6.1 p. 120, Reed and Simon[30] Theorems XII.3 p. 4, XII.4 p. 8 and concluding remark), that we can choose

$$t \to \lambda_\ell(t), \qquad t \to \overrightarrow{E}_\ell(t)$$

as single-valued analytic functions of t for t in a neighbourhood of 0. Moreover, noting that both $\overrightarrow{D}_t$ and $\overleftarrow{D}_t$ converge in trace norm to D as t tends to 0 and 1 is a simple eigenvalue of D, we can suppose, relabeling indexes if necessary, that

$$\lim_{t\to 0} \lambda_0(t) = 1, \qquad \lim_{t\to 0} \overrightarrow{E}_0(t) = \lim_{t\to 0} \overleftarrow{E}_0(t) = D. \tag{18}$$

The difference $\log\left(\overrightarrow{D}_t\right) - \log\left(\overleftarrow{D}_t\right)$ is a bounded operator on S_t and we can define it as 0 on the orthogonal complement of S_t. Moreover, denoting $\log\left(\overrightarrow{D}_t\right)|_{S_t}$ and $\log\left(\overleftarrow{D}_t\right)|_{S_t}$ restrictions to S_t, we can prove the following

Lemma 1. *There exists constants $c > 0$, $t_+ > 0$ and $m \in \mathbb{N}$ such that*

$$\left\|\log\left(\overrightarrow{D}_t\right)|_{S_t}\right\| \leq c - m\log(t), \qquad \left\|\log\left(\overleftarrow{D}_t\right)|_{S_t}\right\| \leq c - m\log(t)$$

for all $t \in]0, t_+]$.

Proof. Recall that functions $t \to \lambda_\ell(t)$ are analytic and strictly positive in a right neighbourhood of 0. For each ℓ, let m_ℓ be the order of the first non-zero (hence strictly positive) derivative of $t \to \lambda_\ell(t)$ at $t = 0$. There exists $\varepsilon_\ell \in]0, 1[$ and $t_\ell > 0$ such that $\lambda_\ell(t) \geq \varepsilon_\ell t^{m_\ell}$ for all $t \in]0, t_\ell]$. Putting

$$\varepsilon = \min_{0\leq\ell\leq k} \varepsilon_\ell, \qquad m = \max_{0\leq\ell\leq k} m_\ell, \qquad t_+ = \min_{0\leq\ell\leq k} t_\ell$$

we find then the inequality $\lambda_\ell(t) \geq \varepsilon_\ell t^{m_\ell} \geq \varepsilon\, t^m$ for all ℓ and $t \in]0, t_+]$. Therefore we have

$$\overrightarrow{D}_t\big|_{S_t} \geq \varepsilon t^m \mathbb{1}_{S_t}$$

where $\mathbb{1}_{S_t}$ is the orthogonal projection onto S_t, and the norm estimate follows.

The proof for $\overleftarrow{D}_t$ is identical. □

We now start computing the limit of

$$t^{-1}\mathrm{Tr}\left(\left(\overrightarrow{D}_t - \overleftarrow{D}_t\right)\left(\log \overrightarrow{D}_t - \log \overleftarrow{D}_t\right)\right) \tag{19}$$

for $t \to 0^+$. As a first step note that

$$\lim_{t\to 0^+} t^{-1}\left(\overrightarrow{D}_t - \overleftarrow{D}_t\right) = (I\otimes \mathcal{L}_*)(D) - (\mathcal{L}_*\otimes I)(D)$$

in trace norm. Moreover, denoting $\|\cdot\|_1$ the trace norm

$$\left\| t^{-1}\left(\overrightarrow{D}_t - \overleftarrow{D}_t\right) - ((I\otimes \mathcal{L}_*)(D) - (\mathcal{L}_*\otimes I)(D))\right\|_1$$

is infinitesimal of order at most t for t tending to 0, therefore the modulus of the difference of (19) and

$$\mathrm{Tr}\left(((I\otimes \mathcal{L}_*)(D) - (\mathcal{L}_*\otimes I)(D))\left(\log \overrightarrow{D}_t - \log \overleftarrow{D}_t\right)\right), \tag{20}$$

by Lemma 1 is not bigger than a constant times $(c - m\log(t))t$ and goes to 0 for t tending to 0^+.

It suffices then to compute the limit of (20) for t tending to 0^+.

We first analyse the behaviour of the 0-th term of (17).

Lemma 2. *The following limits hold:*

$$\lim_{t\to 0^+} t^{-1}\left(\lambda_0(t)\overrightarrow{E}_0(t) - D\right) = |(\mathbb{1}\otimes G)r\rangle\langle r| + |r\rangle\langle(\mathbb{1}\otimes G)r| \tag{21}$$

$$\lim_{t\to 0^+} t^{-1}\left(\lambda_0(t)\overleftarrow{E}_0(t) - D\right) = |(G\otimes \mathbb{1})r\rangle\langle r| + |r\rangle\langle(G\otimes \mathbb{1})r| \tag{22}$$

Proof. The proof is the same for $\overrightarrow{E}_0(t)$ and $\overleftarrow{E}_0(t)$, therefore we consider $\overrightarrow{E}_0(t)$ dropping the arrows and writing $\mathcal{L}_*(D)$ instead of $(I\otimes\mathcal{L}_*)(D)$ for notational convenience.

Let $t_0 > 0$ be sufficiently small such that D_t has only the simple eigenvalue $\lambda_0(t)$ in $[3/4, 1]$ and all other eigenvalues in $[0, 1/4]$ for all $t\in[0, t_0[$. By well known formulae (see e.g. [22] Ch. I) for spectral projections, for t small enough we have

$$E_0(t) = \frac{1}{2\pi \mathrm{i}}\int_C (\zeta - D_t)^{-1}\,d\zeta, \qquad D = \frac{1}{2\pi \mathrm{i}}\int_C \zeta\,(\zeta - D)^{-1}\,d\zeta,$$

$$\lambda_0(t)E_0(t) = \frac{1}{2\pi \mathrm{i}}\int_C \zeta\,(\zeta - D_t)^{-1}\,d\zeta$$

where C is the circle $\{z\in\mathbb{C} \mid |z-1| = 1/2\}$. Therefore we can write

$$\frac{\lambda_0(t)E_0(t) - D}{t} = \frac{1}{2\pi \mathrm{i}}\int_C \frac{(\zeta - D_t)^{-1} - (\zeta - D)^{-1}}{t}\,\zeta\,d\zeta \tag{23}$$

Note that, for all $t\in]0, t_0[$

$$t^{-1}\left((\zeta - D_t)^{-1} - (\zeta - D)^{-1}\right) = t^{-1}(\zeta - D_t)^{-1}(D_t - D)(\zeta - D)^{-1}$$

implying the norm estimate

$$t^{-1}\left\|(\zeta-D_t)^{-1}-(\zeta-D)^{-1}\right\|_1 \le \left\|t^{-1}(D_t-D)\right\|_1 \cdot \left\|(\zeta-D_t)^{-1}\right\| \cdot \left\|(\zeta-D)^{-1}\right\|.$$

Now, since the operators $(\zeta-D_t)^{-1}$ and $(\zeta-D)^{-1}$ are normal with discrete spectrum, contained in the union of the intervals $[0, 1/4]$ and $[3/4, 1]$ of the real axis, their norm is smaller than

$$\sup_{\zeta\in C,\, x\in[0,1/4]\cup[3/4,1]} |\zeta-x|^{-1} \le 4.$$

Moreover

$$\left\|\frac{D_t-D}{t}\right\|_1 = \frac{1}{t}\left\|\int_0^t \mathcal{T}_{*s}(\mathcal{L}_*(D))ds\right\|_1 \le \frac{1}{t}\int_0^t \|\mathcal{L}_*(D)\|_1\, ds = \|\mathcal{L}_*(D)\|_1\,,$$

thus we have

$$t^{-1}\left\|(\zeta-D_t)^{-1}-(\zeta-D)^{-1}\right\| \le 16\,\|\mathcal{L}_*(D)\|_1\,.$$

The integrand of (23) converges to $\zeta\,(\zeta-D)^{-1}\,\mathcal{L}_*(D)\,(\zeta-D)^{-1}$ for t going to 0 thus, by the dominated convergence theorem, we find

$$\lim_{t\to 0^+}\frac{\lambda_0(t)E_0(t)-D}{t} = \frac{1}{2\pi\mathrm{i}}\int_C \zeta\,(\zeta-D)^{-1}\,\mathcal{L}_*(D)\,(\zeta-D)^{-1}\,d\zeta. \qquad (24)$$

The proof of Lemma 2 ends computing the right-hand side. First note that

$$\frac{1}{2\pi\mathrm{i}}\int_C \zeta\left\langle r, (\zeta-D)^{-1}\,\mathcal{L}_*(D)\,(\zeta-D)^{-1}\,r\right\rangle d\zeta = \frac{1}{2\pi\mathrm{i}}\int_C \langle r, \mathcal{L}_*(D)r\rangle\,\frac{\zeta\, d\zeta}{(\zeta-1)^2}$$

with $\langle r, \mathcal{L}_*(D)r\rangle = 2\Re\langle r, Gr\rangle$ and

$$\frac{1}{2\pi\mathrm{i}}\int_C \frac{\zeta\,d\zeta}{(\zeta-1)^2} = \frac{1}{2\pi\mathrm{i}}\int_C \frac{(\zeta-1)\,d\zeta}{(\zeta-1)^2} + \frac{1}{2\pi\mathrm{i}}\int_C \frac{d\zeta}{(\zeta-1)^2} = \frac{1}{2\pi\mathrm{i}}\int_C \frac{d\zeta}{\zeta-1} = 1$$

so that

$$\lim_{t\to 0^+}\frac{1}{2\pi\mathrm{i}}\int_C \left\langle r, (\zeta-D)^{-1}\,\mathcal{L}_*(D)\,(\zeta-D)^{-1}\,r\right\rangle d\zeta = 2\Re\langle r, Gr\rangle. \qquad (25)$$

Second, for all vector v orthogonal to r we have

$$\begin{aligned}\frac{1}{2\pi\mathrm{i}}\int_C \zeta\left\langle r, (\zeta-D)^{-1}\,\mathcal{L}_*(D)\,(\zeta-D)^{-1}\,v\right\rangle d\zeta &= \frac{1}{2\pi\mathrm{i}}\int_C \langle r, \mathcal{L}_*(D)v\rangle\,\frac{d\zeta}{\zeta-1}\\ &= \langle r, \mathcal{L}_*(D)v\rangle = \langle Gr, v\rangle\end{aligned}$$

since r is orthogonal to all $(\mathbb{1}\otimes L_\ell)r$ and $(L_\ell\otimes\mathbb{1})r$, and, in a similar way,

$$\frac{1}{2\pi\mathrm{i}}\int_C \left\langle v, (\zeta-D)^{-1}\,\mathcal{L}_*(D)\,(\zeta-D)^{-1}\,r\right\rangle d\zeta = \langle v, Gr\rangle\,.$$

Third, for all v, u orthogonal to r

$$\frac{1}{2\pi\mathrm{i}}\int_C \left\langle v, (\zeta-D)^{-1}\,\mathcal{L}_*(D)\,(\zeta-D)^{-1}\,u\right\rangle d\zeta = \frac{1}{2\pi\mathrm{i}}\int_C \langle v, \mathcal{L}_*(D)u\rangle\,\frac{d\zeta}{\zeta} = 0$$

because $\zeta\to\zeta^{-1}$ is holomorphic on the half plane containing C.

This completes the proof. □

Lemma 3. *The following limits hold:*

$$\lim_{t\to 0^+}\sum_{\ell=1}^{k} t^{-1}\lambda_\ell(t)\overrightarrow{E}_\ell(t) = \overrightarrow{\Phi}_*(D), \qquad \lim_{t\to 0^+}\sum_{\ell=1}^{k} t^{-1}\lambda_\ell(t)\overleftarrow{E}_\ell(t) = \overleftarrow{\Phi}_*(D)$$

Moreover there exists a special GKSL representation of $\mathcal{L}$ such that $\lambda'_\ell(0) = \left\|\overrightarrow{L}_\ell r\right\|^2 = \left\|\overleftarrow{L}_\ell r\right\|^2$ for $\ell = 1, \ldots, d$ and

$$\lim_{t\to 0^+}\overrightarrow{E}_\ell(t) = \frac{\left|\overrightarrow{L}_\ell r\right\rangle\left\langle\overrightarrow{L}_\ell r\right|}{\left\|\overrightarrow{L}_\ell r\right\|^2}, \qquad \lim_{t\to 0^+}\overleftarrow{E}_\ell(t) = \frac{\left|\overleftarrow{L}_\ell r\right\rangle\left\langle\overleftarrow{L}_\ell r\right|}{\left\|\overleftarrow{L}_\ell r\right\|^2}$$

for all $\ell = 1, \ldots, d$.

Proof. The first identities follow immediately from Lemma 2 writing

$$\sum_{\ell=1}^{k} t^{-1}\lambda_\ell(t)\overrightarrow{E}_\ell(t) = t^{-1}\left(\overrightarrow{D}_t - D\right) - t^{-1}\left(\overrightarrow{E}_0(t) - D\right)$$

and recalling that $t^{-1}\left(\overrightarrow{D}_t - D\right)$ converges to $(I \otimes \mathcal{L}_*)(D)$. Moreover, note that the $d \times d$ matrix C with $c_{jk} = \left\langle\overrightarrow{L}_j r, \overrightarrow{L}_k r\right\rangle = \mathrm{tr}\left(\rho L_j^* L_k\right) = \left\langle\overleftarrow{L}_j r, \overleftarrow{L}_k r\right\rangle$ is self-adjoint. Let $U = (u_{jk})_{1\le j,k\le d}$ be a $d \times d$ unitary matrix such that U^*CU is diagonal and consider the new special GKSL representation of $\mathcal{L}$ obtained replacing the operators L_ℓ by $\sum_h u_{h\ell} L_h$. Now we have

$$\left\langle\overrightarrow{L}_j r, \overrightarrow{L}_k r\right\rangle = \left\langle\overleftarrow{L}_j r, \overleftarrow{L}_k r\right\rangle = \sum_{1\le h,m\le d} \bar{u}_{hj} c_{hm} u_{mk} = (U^*CU)_{jk}$$

and vectors $\overrightarrow{L}_j r$, $\overrightarrow{L}_k r$ are ortogonal.

For all j with $1 \le j \le d$, denote v_j the normalised vector $\overrightarrow{L}_j r / \left\|\overrightarrow{L}_j r\right\|^2$, orthogonal to r. Clearly we have

$$\begin{aligned}
\lim_{t\to 0^+}\sum_{\ell=1}^{k} t^{-1}\lambda_\ell(t)\left\langle v_j, \overrightarrow{E}_\ell(t) v_k\right\rangle &= \sum_{\ell=1}^{k}\lambda'_\ell(0)\left\langle v_j, \overrightarrow{E}_\ell(0) v_k\right\rangle \\
&= \left\langle v_j, \overrightarrow{\Phi}_*(D) v_k\right\rangle \\
&= \sum_{\ell=1}^{d}\left\langle v_j, \left|\overrightarrow{L}_\ell r\right\rangle\left\langle\overrightarrow{L}_\ell r\right| v_k\right\rangle
\end{aligned}$$

for all j, k. Therefore $\lambda'_\ell(0) = 0$ for all $\ell = d+1, \ldots, k$, $\lambda'_\ell(0) = \left\|\overrightarrow{L}_\ell r\right\|^2$ for all $\ell = 1, \ldots, d$ and $E_\ell(t)$ converges to the orthogonal projection onto v_ℓ for all $\ell = 1, \ldots, d$. □

Lemma 4. *The following limits hold:*

$$\lim_{t\to 0^+} \mathrm{Tr}\left(|(\mathbb{1}\otimes G)r\rangle\langle r|\left(\log \overrightarrow{D}_t - \log \overleftarrow{D}_t\right)\right) = 0$$
$$\lim_{t\to 0^+} \mathrm{Tr}\left(|r\rangle\langle(\mathbb{1}\otimes G)r|\left(\log \overrightarrow{D}_t - \log \overleftarrow{D}_t\right)\right) = 0$$
$$\lim_{t\to 0^+} \mathrm{Tr}\left(|(G\otimes \mathbb{1})r\rangle\langle r|\left(\log \overrightarrow{D}_t - \log \overleftarrow{D}_t\right)\right) = 0$$
$$\lim_{t\to 0^+} \mathrm{Tr}\left(|r\rangle\langle(G\otimes \mathbb{1})r|\left(\log \overrightarrow{D}_t - \log \overleftarrow{D}_t\right)\right) = 0$$

Proof. Clearly

$$\mathrm{Tr}\left(|(\mathbb{1}\otimes G)r\rangle\langle r|\left(\log \overrightarrow{D}_t - \log \overleftarrow{D}_t\right)\right) = \left\langle\left(\log \overrightarrow{D}_t - \log \overleftarrow{D}_t\right) r, (\mathbb{1}\otimes G)r\right\rangle.$$

Writing $\left(\log \overrightarrow{D}_t - \log \overleftarrow{D}_t\right) r$ as

$$\log(\lambda_0(t))\left(\overrightarrow{E}_0(t)r - \overleftarrow{E}_0(t)r\right) + \sum_{\ell=1}^{k} \log(\lambda_\ell(t))\left(\overrightarrow{E}_\ell(t)r - \overleftarrow{E}_\ell(t)r\right)$$

we start noting that, for $t \to 0^+$, the first term vanishes because $\lambda_0(t)$ converges to 1. The other terms also vanish because $\overrightarrow{E}_\ell(t)r$ and $\overleftarrow{E}_\ell(t)r$ converge to 0 for all $\ell \geq 1$ by (18) and are infinitesimal in norm of order t or higher by analyticity. Therefore, since $\lambda_\ell(t)$ goes to 0 polynomially, as t^{m_ℓ} with $m_\ell \geq 1$, say, we have

$$\left\|\log(\lambda_\ell(t))\overrightarrow{E}_\ell(t)r\right\| \leq c\,t\,|\log(\lambda_\ell(t))|, \qquad \left\|\log(\lambda_\ell(t))\overleftarrow{E}_\ell(t)r\right\| \leq c\,t\,|\log(\lambda_\ell(t))|$$

for some constant c and t small enough. This proves the first identity.

The other follow by repeating the above argument. □

Proof. (of Theorem 5) The above Lemma 4 and (20) show that it suffices to compute the limit for $t \to 0^+$ of

$$\mathrm{Tr}\left(\left(\overrightarrow{\Phi}_*(D) - \overleftarrow{\Phi}_*(D)\right)\left(\log \overrightarrow{D}_t - \log \overleftarrow{D}_t\right)\right), \tag{26}$$

Note that, since supports of $\overrightarrow{D}_t$ and $\overleftarrow{D}_t$ are equal, we have

$$\sum_{\ell=0}^{k} \overrightarrow{E}_\ell(t) = \sum_{\ell=0}^{k} \overleftarrow{E}_\ell(t)$$

therefore

$$\sum_{\ell=0}^{k} \mathrm{Tr}\left(\left(\overrightarrow{\Phi}_*(D) - \overleftarrow{\Phi}_*(D)\right)\log(t)\left(\overrightarrow{E}_\ell(t) - \overleftarrow{E}_\ell(t)\right)\right) = 0.$$

Subtracting this from (26), we can write (26) as

$$\sum_{\ell=0}^{k} \mathrm{Tr}\left(\left(\overrightarrow{\Phi}_*(D) - \overleftarrow{\Phi}_*(D)\right)\log\left(\frac{\lambda_\ell(t)}{t}\right)\left(\overrightarrow{E}_\ell(t) - \overleftarrow{E}_\ell(t)\right)\right).$$

Now, the term with $\ell = 0$ vanishes for t going to 0 since the logarithm diverges as $\log(t)$ but

$$\mathrm{Tr}\left(\left(\overrightarrow{\Phi}_*(D) - \overleftarrow{\Phi}_*(D)\right)\left(\overrightarrow{E}_0(t) - \overleftarrow{E}_0(t)\right)\right)$$

goes to 0 (both $\overrightarrow{E}_0(t) - \overleftarrow{E}_0(t)$ converge to D, a one-dimensional projection orthogonal to the support of $\overrightarrow{\Phi}_*(D)$ and $\overleftarrow{\Phi}_*(D)$) and the order of infinitesimal is at least t by analyticity.

By Lemma 3, $\log(\lambda_\ell(t)/t)$ converges to $\log\left\|\overrightarrow{L}_\ell r\right\|^2 = \log\left\|\overrightarrow{L}_\ell r\right\|^2$ and each $\overrightarrow{E}_\ell(t)$ (resp. $\overleftarrow{E}_\ell(t)$) also converges to a spectral projection of $\overrightarrow{\Phi}_*(D)$ (resp. $\overleftarrow{\Phi}_*(D)$). This completes the proof of Theorem 5. □

6. Supports of Forward and Backward States

In this section we prove a couple of characterisations of the support projection of a pure state evolving under the action of a QMS that turn out to be helpful for determining the supports of forward and backward densities.

Theorem 6. *Let $(\mathcal{T}_t)_{t\geq 0}$ be a norm continuous QMS on $\mathcal{B}(\mathsf{h})$ with generator $\mathcal{L}$ as in (3) and let $P_t = \mathrm{e}^{tG}$. For all unit vector $u \in \mathsf{h}$ and all $t \geq 0$, the support projection of the state $\mathcal{T}_{*t}(|u\rangle\langle u|)$ is the closed linear span of $P_t u$ and vectors*

$$P_{s_1} L_{\ell_1} P_{s_2-s_1} L_{\ell_2} P_{s_3-s_2} \ldots P_{s_n-s_{n-1}} L_{\ell_n} P_{t-s_n} u \tag{27}$$

for all $n \geq 1$, $0 \leq s_1 \leq s_2 \leq \cdots \leq s_n \leq t$ and $\ell_1, \ldots, \ell_n \geq 1$.

Proof. For all $t > 0$, differentiating with respect to s we have

$$\frac{d}{ds}\mathcal{T}_{*s}\left(P_{t-s}\,|u\rangle\langle u|\,P_{t-s}^*\right) = \sum_{\ell\geq 1}\mathcal{T}_{*s}\left(|P_{t-s}L_\ell u\rangle\langle P_{t-s}L_\ell u|\right).$$

Integrating on $[0, t]$ we find

$$\mathcal{T}_{*t}\left(|u\rangle\langle u|\right) = |P_t u\rangle\langle P_t u| + \sum_{\ell\geq 1}\int_0^t \mathcal{T}_{*s}\left(|L_\ell P_{t-s}u\rangle\langle L_\ell P_{t-s}u|\right)\mathrm{d}s.$$

Iterating yields

$$\begin{aligned}\mathcal{T}_{*t}\left(|u\rangle\langle u|\right) &= |P_t u\rangle\langle P_t u| \\ &+ \sum_{n\geq 1}\sum_{\ell_1,\ldots\ell_n\geq 1}\int_0^t \mathrm{d}s_n \ldots \int_0^{s_2}\mathrm{d}s_1\,\left|u_{t,s_n,\ldots,s_1,\ell_1,\ldots,\ell_n}\right\rangle\!\left\langle u_{t,s_n,\ldots,s_1,\ell_1,\ldots,\ell_n}\right|\end{aligned} \tag{28}$$

where $u_{t,s_n,\ldots,s_1,\ell_1,\ldots,\ell_n}$ is the vector given by (27).

Any $v \in \mathsf{h}$, orthogonal to the support of the state $\mathcal{T}_{*t}(|u\rangle\langle u|)$ satisfies $\langle v, \mathcal{T}_{*t}(|u\rangle\langle u|)\,v\rangle = 0$. Therefore, since all the terms in (28) are positive operators, it turns out that v must be orthogonal to all vectors $P_t u$ and all the iterated integrals

$$\int_0^t \mathrm{d}s_n \ldots \int_0^{s_2}\mathrm{d}s_1\,\left|\left\langle v, P_{s_1}L_{\ell_1}P_{s_2-s_1}L_{\ell_2}P_{s_3-s_2}\ldots P_{s_n-s_{n-1}}L_{\ell_n}P_{t-s_n}u\right\rangle\right|^2$$

vanish. It follows then, from the time continuity of the integrands, that v must be orthogonal also to all the vectors of the form (27) and the proof is complete. □

We now give another characterisation of the support of $\mathcal{T}_{*t}(|u\rangle\langle u|)$ in terms of P_t, non-commutative polynomials in L_ℓ and their multiple commutators with G. Denote $\delta_G^0(L_\ell) = L_\ell,\ \delta_G(L_\ell) = [G, L_\ell],\ \delta_G^2(L_\ell) = [G,[G,L_\ell]], ...$

Theorem 7. *Let $(\mathcal{T}_t)_{t\geq 0}$ be a norm continuous QMS on $\mathcal{B}(\mathsf{h})$ with generator $\mathcal{L}$ as in (3) and let $P_t = \mathrm{e}^{tG}$. For all unit vector $u \in \mathsf{h}$ and all $t > 0$, the support projection of the state $\mathcal{T}_{*t}(|u\rangle\langle u|)$ is the linear manifold $P_t\,\mathcal{S}(u)$ where $\mathcal{S}(u)$ is the closure of linear span of u and*

$$\delta_G^{m_1}(L_{\ell_1})\delta_G^{m_2}(L_{\ell_2})\cdots\delta_G^{m_n}(L_{\ell_n})u \tag{29}$$

for all $n \geq 1$, $m_1,\ldots,m_n \geq 0$ and $\ell_1,\ldots,\ell_n \geq 1$.

Proof. Let v be a vector orthogonal to the suport of $\mathcal{T}_{*t}(|u\rangle\langle u|)$. Differentiating

$$\left\langle v,\, P_{s_1}L_{\ell_1}P_{s_2-s_1}L_{\ell_2}P_{s_3-s_2}\ldots P_{s_n-s_{n-1}}L_{\ell_n}P_{t-s_n}u\right\rangle = 0$$

m_k times with respect to s_k for all k, we find that v is also orthogonal to $P_t\,\mathcal{S}(u)$.

Conversely, if $v \in \mathsf{h}$ is orthogonal to $P_t\,\mathcal{S}(u)$, then the analytic function

$$(s_1,\ldots,s_n) \to \left\langle v,\, P_{s_1}L_{\ell_1}P_{s_2-s_1}L_{\ell_2}P_{s_3-s_2}\ldots P_{s_n-s_{n-1}}L_{\ell_n}P_{t-s_n}u\right\rangle,$$

as well as its extension to $\mathbb{C}^n$

$$(z_1,\ldots,z_n) \to \left\langle v,\, P_{z_1}L_{\ell_1}P_{z_2-z_1}L_{\ell_2}P_{z_3-z_2}\ldots P_{z_n-z_{n-1}}L_{\ell_n}P_{t-z_n}u\right\rangle,$$

has all partial derivatives at $z_1 = \cdots = z_n = t$ equal to 0. Thus it is identically equal to 0 and v is orthogonal to the support of $\mathcal{T}_{*t}(|u\rangle\langle u|)$. □

Corollary 1. *Let $(\mathcal{T}_t)_{t\geq 0}$ be a norm continuous QMS on $\mathcal{B}(\mathsf{h})$ with generator $\mathcal{L}$ as in (3) and let $P_t = \mathrm{e}^{tG}$. For all unit vector $u \in \mathsf{h}$ the support projection of the state $\mathcal{T}_{*t}(|u\rangle\langle u|)$ is independent of t, for $t > 0$, if and only if the linear manifold $\mathcal{S}(u)$ is G-invariant.*

Proof. For all $u \in \mathsf{h}$, $S(u)$ is L_ℓ-invariant for all $\ell \geq 1$ because $\delta_G^0(L_\ell) = L_\ell$. If it is also G-invariant, then it is also P_t-invariant for all $t \geq 0$ since $P_t = \sum_{n\geq 0} t^n G^n/n!$ and supports of states $\mathcal{T}_{*t}(|u\rangle\langle u|)$ coincide with $S(u)$ for all $t > 0$ by Theorem 7.

Conversely, if the support projection of $\mathcal{T}_{*t}(|u\rangle\langle u|)$ is independent of t, then $P_t\mathcal{S}(u) = \mathcal{S}(u)$ for all $t \geq 0$, by continuity of P_t at $t = 0$. Differentiating at $t = 0$ we find then $G\mathcal{S}(u) \subseteq \mathcal{S}(u)$. □

The above results have been recently extended by Hachicha [20] to non pure states proving a quantum analogue of the classical Lévy–Austin–Ornstein theorem.

Theorem 8. *Let $\mathcal{T}$ be a QMS with generator $\mathcal{L}$ as in Theorem 1 and suppose that $\rho^{1/2}\theta G^*\theta = G\rho^{1/2}$. The following conditions are equivalent:*

(a) *the closed linear spans of $\left\{L_\ell\rho^{1/2} \mid \ell \geq 1\right\}$ and $\left\{\rho^{1/2}\theta L_\ell^*\theta \mid \ell \geq 1\right\}$ in the Hilbert space of Hilbert-Schmidt operators on h coincide,*

(b) *the forward and backward states $\overrightarrow{D}_t$ and $\overleftarrow{D}_t$ have the same support.*

Proof. Putting $\overrightarrow{\mathcal{T}}_t = I \otimes \mathcal{T}_t$ and $\overleftarrow{\mathcal{T}}_t = \mathcal{T}_t \otimes I$, we define the forward and backward QMS $\overrightarrow{\mathcal{T}}$ and $\overleftarrow{\mathcal{T}}$ on $\mathcal{B}(\mathsf{h}) \otimes \mathcal{B}(\mathsf{h})$. Their generators can be written in a special GKSL representation, with respect to the faithful normal invariant state $\rho \otimes \rho$ by means of operators $\overrightarrow{G} = \mathbb{1} \otimes G$, $\overrightarrow{L}_\ell = \mathbb{1} \otimes L_\ell$ and $\overleftarrow{G} = G \otimes \mathbb{1}$, $\overleftarrow{L}_\ell = L_\ell \otimes \mathbb{1}$. Denote $(\overrightarrow{P}_t)_{t\geq 0}$ and $(\overleftarrow{P}_t)_{t\geq 0}$ the semigroups on $\mathsf{h} \otimes \mathsf{h}$ generated by $\overrightarrow{G}$ and $\overleftarrow{G}$ respectively.

By Theorem 6, it suffices to show that condition (a) holds if and only if the closed linear spans in $\mathsf{h} \otimes \mathsf{h}$ of the sets

$$\overrightarrow{P}_t r, \quad \overrightarrow{P}_{s_1} \overrightarrow{L}_{\ell_1} \overrightarrow{P}_{s_2-s_1} \overrightarrow{L}_{\ell_2} \overrightarrow{P}_{s_3-s_2} \dots \overrightarrow{P}_{s_n-s_{n-1}} \overrightarrow{L}_{\ell_n} \overrightarrow{P}_{t-s_n} r \tag{30}$$

$$\overleftarrow{P}_t r, \quad \overleftarrow{P}_{s_1} \overleftarrow{L}_{\ell_1} \overleftarrow{P}_{s_2-s_1} \overleftarrow{L}_{\ell_2} \overleftarrow{P}_{s_3-s_2} \dots \overleftarrow{P}_{s_n-s_{n-1}} \overleftarrow{L}_{\ell_n} \overleftarrow{P}_{t-s_n} r \tag{31}$$

for all $n \geq 1$, $0 \leq s_1 \leq s_2 \leq \cdots \leq s_n \leq t$ and $\ell_1, \dots, \ell_n \geq 1$ coincide.

Let $w = \sum_{\alpha,\beta} w_{\beta\alpha} e_\alpha \otimes e_\beta$ be a vector in $\mathsf{h} \otimes \mathsf{h}$. Note that $\|w\|^2 = \sum_{\alpha,\beta} |w_{\beta\alpha}|^2$, therefore the matrix $(w_{\beta\alpha})_{\alpha,\beta\geq 1}$ defines a Hilbert-Schmidt operator W on h with $w_{\beta\alpha} = \langle e_\alpha, W e_\beta \rangle$. The vector w is orthogonal to $(X \otimes \mathbb{1})r$ if and only if

$$0 = \sum_{j,\alpha,\beta} \rho_j^{1/2} \langle (X \otimes \mathbb{1}) e_j \otimes e_j, e_\alpha \otimes e_\beta \rangle w_{\beta\alpha} = \sum_{j,\alpha} \rho_j^{1/2} \langle X e_j, e_\alpha \rangle \langle e_j, W e_\alpha \rangle$$

i.e.

$$\begin{aligned} 0 &= \sum_{j,\alpha} \rho_j^{1/2} \langle e_\alpha, \theta X \theta e_j \rangle \langle e_j, W e_\alpha \rangle \\ &= \sum_{j,\alpha} \left\langle \rho^{1/2} \theta X^* \theta e_\alpha, e_j \right\rangle \langle e_j, W e_\alpha \rangle \\ &= \mathrm{tr} \left(\left(\rho^{1/2} \theta X^* \theta \right)^* W \right) \end{aligned}$$

namely $\rho^{1/2}\theta X^* \theta$ is orthogonal to W in Hilbert-Schmidt operators on h. In a similar way, a straightforward computation shows that w is orthogonal to $(\mathbb{1} \otimes X)r$ if and only if $X\rho^{1/2}$ is orthogonal to W in Hilbert-Schmidt operators on h.

Since $\rho^{1/2}\theta G^* \theta = G\rho^{1/2}$, by induction we have immediately $\rho^{1/2}\theta G^{*k}\theta = G^k \rho^{1/2}$ for all $k \geq 0$ and then

$$P_t \rho^{1/2} = \sum_{k\geq 0} \frac{t^k}{k!} G^k \rho^{1/2} = \sum_{k\geq 0} \frac{t^k}{k!} \rho^{1/2} \theta G^{*k} \theta = \rho^{1/2} \theta P_t^* \theta.$$

Thus w is orthogonal to $\overrightarrow{P}_t r$ if and only if the Hilbert-Schmidt operator W is orthogonal to $P_t \rho^{1/2} = \rho^{1/2} \theta P_t^* \theta$ namely w is orthogonal to $\overleftarrow{P}_t r$. Moreover, w is orthogonal to the second vector in (30) given by

$$\left(\mathbb{1} \otimes (P_{s_1} L_{\ell_1} P_{s_2-s_1} L_{\ell_2} P_{s_3-s_2} \dots P_{s_n-s_{n-1}} L_{\ell_n} P_{t-s_n}) \right) r$$

if and only if W is orthogonal to

$$P_{s_1} L_{\ell_1} P_{s_2-s_1} L_{\ell_2} P_{s_3-s_2} \dots P_{s_n-s_{n-1}} L_{\ell_n} P_{t-s_n} \rho^{1/2}$$

namely W is orthogonal to

$$\rho^{1/2} \theta (P_{s_1} L_{\ell_1} P_{s_2-s_1} L_{\ell_2} P_{s_3-s_2} \dots P_{s_n-s_{n-1}} L_{\ell_n} P_{t-s_n})^* \theta$$

namely w is orthogonal to the second vector in (31). □

Proposition 6. *The following conditions are equivalent:*

(a) *the closures of the linear spans of* $\{L_\ell \rho^{1/2} \mid \ell \geq 1\}$ *and* $\{\rho^{1/2}\theta L_\ell^* \theta \mid \ell \geq 1\}$ *in the Hilbert space of Hilbert-Schmidt operators on* h *coincide,*

(b) *the supports of* $\overrightarrow{\Phi}_*(D)$ *and* $\overleftarrow{\Phi}_*(D)$ *coincide.*

Proof. Let $w = \sum_{\alpha,\beta} w_{\beta\alpha}\, \theta e_\alpha \otimes e_\beta$ be a vector in $\mathsf{h}\otimes\mathsf{h}$ orthogonal to r and let W be the Hilbert-Schmidt operator $\mathsf{h}\otimes\mathsf{h}$ with $w_{\beta\alpha} = \langle e_\alpha, We_\beta\rangle$. Straightforward computations yield

$$\overrightarrow{\Phi}_*(D)w = \sum_{\ell,\alpha,\beta} w_{\beta\alpha} \left\langle (\mathbb{1}\otimes L_\ell)r, \theta e_\alpha \otimes e_\beta \right\rangle (\mathbb{1}\otimes L_\ell)r,$$
$$\overleftarrow{\Phi}_*(D)w = \sum_{\ell,\alpha,\beta} w_{\beta\alpha} \left\langle (L_\ell \otimes \mathbb{1})r, \theta e_\alpha \otimes e_\beta \right\rangle (L_\ell \otimes \mathbb{1})r.$$

If $\overrightarrow{\Phi}_*(D)w = 0$, since the vector r is separating for $\mathbb{1}\otimes\mathcal{B}(\mathsf{h})$, we have

$$\sum_{\ell,\alpha,\beta} w_{\beta\alpha} \left\langle (\mathbb{1}\otimes L_\ell)r, \theta e_\alpha \otimes e_\beta \right\rangle (\mathbb{1}\otimes L_\ell) = \sum_{\ell,\alpha,\beta} w_{\beta\alpha}\rho_\alpha^{1/2} \left\langle L_\ell e_\alpha, e_\beta\right\rangle (\mathbb{1}\otimes L_\ell) = 0.$$

namely, by the linear independence of the L_ℓ,

$$0 = \sum_{\alpha,\beta} w_{\beta\alpha}\rho_\alpha^{1/2} \left\langle L_\ell e_\alpha, e_\beta\right\rangle = \sum_{\alpha,\beta} w_{\beta\alpha} \left\langle L_\ell \rho^{1/2} e_\alpha, e_\beta\right\rangle = \sum_{\alpha} \left\langle L_\ell \rho^{1/2} e_\alpha, W e_\alpha\right\rangle$$

for all $\ell \geq 1$. Therefore $\overrightarrow{\Phi}_*(D)w = 0$ if and only if $\mathrm{tr}\left((L_\ell\rho^{1/2})^* W\right) = 0$.

We can show that $\overleftarrow{\Phi}_*(D)w = 0$ if and only if $\mathrm{tr}\left((\rho^{1/2}\theta L_\ell^*\theta)^* W\right) = 0$ in the same way. It follows that $\{L_\ell\rho^{1/2} \mid \ell \geq 1\}$ and $\{\rho^{1/2}\theta L_\ell^*\theta \mid \ell \geq 1\}$ in the Hilbert space of Hilbert-Schmidt operators on h have the same orthogonal and the equivalence of (a) and (b) is clear. □

7. Examples

In this section we collect three examples illustrating our entropy production formula. The antiunitary θ will always be conjugation with respect to the chosen basis of h.

7.1. Trivial cycle on an n-level system. Consider the QMS on $\mathcal{B}(\mathbb{C}^n)$ $(n \geq 3)$ generated by

$$\mathcal{L}(x) = \lambda\, S^* x S + \mu\, S x S^* - x + \mathrm{i}[H, x]$$

where S is the unitary right shift defined on the orthonormal basis $(e_j)_{0\leq j\leq n-1}$ of $\mathbb{C}^n$ by $Se_j = e_{j+1}$ (the sum must be understood mod n), $\lambda, \mu > 0$. The Hamiltonian H is a real matrix which is diagonal in this basis.

This QMS may arise in the stochastic (weak coupling) limit of a three-level system dipole-type interacting with two reservoirs at different temperatures under the generalised rotating wave approximation. The parameters λ, μ are related to the temperatures of the reservoirs and $\lambda = \mu$ if the temperatures coincide. Its structure is clear:

1. $\rho = \mathbb{1}/n$ is a faithful invariant state, therefore the QMS commutes with the trivial modular group,
2. $d = 2$, and $L_1 = \lambda^{1/2} S$, $L_2 = \mu^{1/2} S^*$, together with $G = -\frac{1}{2}\mathbb{1} - \mathrm{i}H$ give a special GKSL representation of $\mathcal{L}$,
3. we have $\rho^{1/2}\theta G^*\theta = \rho^{1/2} G = G\rho^{1/2}$,
4. quantum detailed balance conditions are satisfied if and only if $\lambda = \mu$ since

$$\begin{bmatrix} \rho^{1/2}\theta L_1^*\theta \\ \rho^{1/2}\theta L_1^*\theta \end{bmatrix} = \begin{bmatrix} 0 & (\mu/\lambda)^{1/2} \\ (\lambda/\mu)^{1/2} & 0 \end{bmatrix} \begin{bmatrix} L_1\rho^{1/2} \\ L_2\rho^{1/2} \end{bmatrix}$$

and the above matrix is unitary if and only if $\lambda = \mu$.

A complete study of the qualitative behaviour of this QMS can be done by applying our methods in [14].

The assumption (**FBS**) is immediately checked applying Theorem 8a because the linear spans of both set of operators coincide with the Abelian algebra generated by the shift S, namely the algebra of $n \times n$ circulant matrices.

The entropy production is easily computed applying our formula (16). Indeed

$$\overrightarrow{\Phi}_*(D) = \frac{\lambda}{n}\sum_{j,k=0}^{n-1} \left|e_j \otimes e_{j+1}\right\rangle \left\langle e_k \otimes e_{k+1}\right| + \frac{\mu}{n}\sum_{j,k=0}^{n-1} \left|e_j \otimes e_{j-1}\right\rangle \left\langle e_k \otimes e_{k-1}\right|$$

$$\overleftarrow{\Phi}_*(D) = \frac{\lambda}{n}\sum_{j,k=0}^{n-1} \left|e_{j+1} \otimes e_j\right\rangle \left\langle e_{k+1} \otimes e_k\right| + \frac{\mu}{n}\sum_{j,k=0}^{n-1} \left|e_{j-1} \otimes e_j\right\rangle \left\langle e_{k-1} \otimes e_k\right|$$

where sums $j \pm 1$, $k \pm 1$ are modulo n. A quick inspection shows that, denoting ψ_+, ψ_- the unit vectors

$$\psi_+ = \frac{1}{\sqrt{n}}\sum_{j=0}^{n-1} e_j \otimes e_{j+1}, \qquad \psi_- = \frac{1}{\sqrt{n}}\sum_{j=0}^{n-1} e_j \otimes e_{j-1},$$

we have $\langle \psi_-, \psi_+\rangle = 0$ and

$$\overrightarrow{\Phi}_*(D) = \lambda \left|\psi_+\right\rangle \left\langle\psi_+\right| + \mu \left|\psi_-\right\rangle \left\langle\psi_-\right|, \qquad \overleftarrow{\Phi}_*(D) = \lambda \left|\psi_-\right\rangle \left\langle\psi_-\right| + \mu \left|\psi_+\right\rangle \left\langle\psi_+\right|.$$

It follows that

$$\overrightarrow{\Phi}_*(D) - \overleftarrow{\Phi}_*(D) = (\lambda - \mu)\left(\left|\psi_+\right\rangle \left\langle\psi_+\right| - \left|\psi_-\right\rangle \left\langle\psi_-\right|\right)$$

$$\log\left(\overrightarrow{\Phi}_*(D)\right) - \log\left(\overleftarrow{\Phi}_*(D)\right) = \log\left(\frac{\lambda}{\mu}\right)\left(\left|\psi_+\right\rangle \left\langle\psi_+\right| - \left|\psi_-\right\rangle \left\langle\psi_-\right|\right)$$

and the entropy production is

$$\frac{\lambda - \mu}{2}\log\left(\frac{\lambda}{\mu}\right).$$

Therefore, the entropy production is non zero if and only if $\lambda \neq \mu$ since there is a "current" determined by different intensities in "raising" ($e_j \to e_{j+1}$) and "lowering" ($e_k \to e_{k-1}$) transitions.

Note that this entropy production coincides with the entropy production of the classical QMS obtained by restriction to the commutative subalgebra of diagonal matrices.

A wider class of QMS like those considered in this example has been studied by Bolaños and Quezada [7] computing directly the entropy production rate.

7.2. Generic QMS. Generic QMS arise in the stochastic limit of a open discrete quantum system with generic Hamiltonian, interacting with Gaussian fields through a dipole type interaction (see [2,10] and the references therein). Here, for simplicity, the system space is finite-dimensional $\mathsf{h} = \mathbb{C}^n$ with orthonormal basis $(e_j)_{0\le j\le n-1}$, the operators L_ℓ, in this case labeled by a double index (ℓ, m) with $\ell \neq m$, are

$$L_{\ell m} = \gamma_{\ell m}^{1/2} \left|e_m\right\rangle \left\langle e_\ell\right|$$

where are $\gamma_{\ell m} \ge 0$ positive constants and the effective Hamiltonian H is a self-adjoint operator diagonal in the given basis whose explicit form is not needed here because it does not affect the entropy production. The generator $\mathcal{L}$ is

$$\mathcal{L}(x) = \mathrm{i}[H, x] + \frac{1}{2}\sum_{\ell\neq m}\left(-L_{\ell m}^* L_{\ell m} x + 2L_{\ell m}^* x L_{\ell m} - x L_{\ell m}^* L_{\ell m}\right), \tag{32}$$

therefore

$$G = -\frac{1}{2}\sum_{\ell\neq m} L_{\ell m}^* L_{\ell m} - \mathrm{i}H = -\frac{1}{2}\sum_{\ell}\left(\sum_{\{m\,|\,m\neq\ell\}}\gamma_{\ell m}\right)\left|e_\ell\right\rangle\left\langle e_\ell\right| - \mathrm{i}H$$

is diagonal in the given basis and the condition $\rho^{1/2}\theta G^*\theta = G\rho^{1/2}$ holds. Moreover, for any given faithful normal state (even if it is *not* an invariant state) $\rho = \sum_{j=0}^n \left|e_j\right\rangle\left\langle e_j\right|$ we have

$$L_{\ell m}\rho^{1/2} = \rho_\ell^{1/2}\gamma_{\ell m}^{1/2}\left|e_m\right\rangle\left\langle e_\ell\right|, \qquad \rho^{1/2}\theta L_{\ell m}^*\theta = \rho_\ell^{1/2}\gamma_{\ell m}^{1/2}\left|e_\ell\right\rangle\left\langle e_m\right|.$$

It follows that the linear span of operators $L_{\ell m}\rho^{1/2}$ coincides with the linear span of operators $\rho^{1/2}\theta L_{\ell m}^*\theta$ if and only if $\gamma_{\ell m} > 0$ implies $\gamma_{m\ell} > 0$ for all ℓ, m. Under this assumption (**FBS**) clearly holds.

The restriction of $\mathcal{L}$ to the algebra of diagonal matrices coincides with the generator of a time continuous Markov chain with states $0, 1, \ldots, n-1$ and jump rates $\gamma_{\ell m}$. As a consequence, if $\gamma_{\ell m} > 0$ implies $\gamma_{m\ell} > 0$ for all ℓ, m the classical time-continuous Markov chain can be realised as a union of its irreducible classes each one of them admitting a unique strictly positive invariant probability density. Any convex combination of these probability densities with all non-zero coefficients yields and invariant probability density $(\rho_j)_{0\le j\le n-1}$ for the whole Markov chain with $\rho_j > 0$ for all j. It is easy to check that the diagonal matrix with eigenvalues $(\rho_j)_{0\le j\le n-1}$ is an invariant state for the quantum Markov semigroup generated by $\mathcal{L}$.

Straightforward computations give the following formulae:

$$\overrightarrow{\Phi}_*(D) = \sum_{\{(\ell,m)\,|\,\gamma_{\ell m}>0\}} \rho_\ell\,\gamma_{\ell m}\left|e_\ell\otimes e_m\right\rangle\left\langle e_\ell\otimes e_m\right|$$

$$\overleftarrow{\Phi}_*(D) = \sum_{\{(\ell,m)\,|\,\gamma_{\ell m}>0\}} \rho_m\gamma_{m\ell}\left|e_\ell\otimes e_m\right\rangle\left\langle e_\ell\otimes e_m\right|$$

Therefore the entropy production is

$$\frac{1}{2}\sum_{\{(\ell,m)\,|\,\gamma_{\ell m}>0\}}\left(\rho_\ell\,\gamma_{\ell m} - \rho_m\gamma_{m\ell}\right)\log\left(\frac{\rho_\ell\,\gamma_{\ell m}}{\rho_m\gamma_{m\ell}}\right).$$

This formula shows immediately that the entropy production is zero if and only if the classical detailed balance condition $\rho_\ell \gamma_{\ell m} = \rho_m \gamma_{m\ell}$ for all ℓ, m holds. Here again, entropy production coincides with the entropy production of the classical QMS obtained by restriction to the commutative subalgebra of diagonal matrices. Moreover, it is not difficult to show that, if there is a $\gamma_{\ell m} > 0$ with $\gamma_{m\ell} = 0$ and the classical Markov chain is irreducible, the invariant state is faithful but the entropy production is infinite.

7.3. Two-level system. Let $\mathcal{T}$ be the QMS on $\mathcal{B}(\mathbb{C}^2)$ with generator $\mathcal{L}$ represented in a GKSL form with

$$L_1 = |e_1\rangle\langle e_2|, \quad L_2 = |e_2\rangle\langle e_1|, \quad H = \mathrm{i}\kappa\left(|e_2\rangle\langle e_1| - |e_1\rangle\langle e_2|\right), \quad \kappa \in \mathbb{R} - \{0\}.$$

The normalised trace $\rho = \mathbb{1}/2$ is a faithful invariant state and the above operator give a special GKSL representation of $\mathcal{L}$.

The semigroup $\mathcal{T}$ satisfies the SQDB condition by Theorem 2. Indeed

$$\rho^{1/2} L_1^* = L_2\, \rho^{1/2}, \qquad \rho^{1/2} L_2^* = L_1\, \rho^{1/2}$$

so that we can choose as self-adjoint unitary in (5) the flip $ue_1 = e_2,\ ue_2 = e_1$.

The SQBD-Θ condition, however, does not hold because

$$\rho^{1/2}\theta G^*\theta - G\rho^{1/2} = 2\mathrm{i}H\rho^{1/2} \neq 0.$$

Computing $[G, L_1] = [G, L_2] = \kappa\left(|e_1\rangle\langle e_1| - |e_2\rangle\langle e_2|\right)$ and noting that

$$(\mathbb{1} \otimes L_1)r = e_2 \otimes e_1/\sqrt{2}, \qquad (\mathbb{1} \otimes L_2)r = e_1 \otimes e_2/\sqrt{2},$$
$$(\mathbb{1} \otimes [G, L_1])r = \kappa(e_1 \otimes e_1 - e_2 \otimes e_2)/\sqrt{2},$$

by the invertibility of $\mathbb{1} \otimes P_t$, we find immediately that the support of $\overrightarrow{D}_t$ is the whole $\mathbb{C}^2 \otimes \mathbb{C}^2$ by Theorem 7. The support of $\overleftarrow{D}_t$ is the same since $\overleftarrow{D}_t = F\, \overrightarrow{D}_t F$ where F is the unitary flip $Fe_j \otimes e_k = e_k \otimes e_j$. Therefore the assumption (**FBS**) holds.

A simple computation yields

$$\overrightarrow{\Phi}_*(D) = \overleftarrow{\Phi}_*(D) = \frac{1}{2}\left(|e_1 \otimes e_2\rangle\langle e_1 \otimes e_2| + |e_2 \otimes e_1\rangle\langle e_2 \otimes e_1|\right),$$

thus the entropy production is zero.

8. Conclusions and Outlook

We showed that strict positivity of entropy production characterises non equilibrium invariant states of quantum Markov semigroups, irrespectively of the chosen notion of quantum detailed balance and commutation with the modular group. The entropy production rate only depends on the completely positive part of the generator of a QMS that can be regarded as its truly irreversible part.

States with finite entropy production form a promising class of non equilibrium invariant states. Indeed, they satisfy an operator version (Theorem 8) of the necessary condition for finiteness of classical entropy production $\gamma_{jk} > 0$ if and only if $\gamma_{kj} > 0$, where γ_{jk} are transition rates. Moreover, dependence of entropy production on the completely positive part of the generator of a QMS only might allow us to extend cycle decompositions of QMS like those obtained in [1,7,18] to QMS non commuting with the modular group. These directions will be explored in forthcoming papers.

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Appendix

Proposition 7. *If the state ρ and θ commute there exists an orthonormal basis $(e_j)_{j\geq 1}$ of h of eigenvectors of ρ that are all invariant under θ.*

Proof. Let $(e_j)_{j\geq 1}$ of h of eigenvectors of ρ and let $\rho = \sum_{j\geq 1} |e_j\rangle\langle e_j|$ be a spectral decomposition of ρ with $\rho_j > 0$ for all $j \geq 1$ because ρ is faithful. Since θ commutes with ρ we have $\rho\theta e_j = \theta\rho e_j = \rho_j\theta e_j$, and eigenspaces of ρ are θ-invariant. Now, for each j such that $\theta e_j \neq -e_j$, the normalised vector $f_j = (e_j + \theta e_j)/\left\| e_j + \theta e_j \right\|$ is θ-invariant and is still an eigenvector of ρ as well as $f_j = \mathrm{i} e_j$ if $\theta e_j = -e_j$. Noting that scalar products $\langle f_j, f_k\rangle$ are real, since $\langle f_j, f_k\rangle = \langle \theta f_k, \theta f_j\rangle = \langle f_k, f_j\rangle$, by a standard Gram-Schmidt orthogonalisation process we can find an orthonormal basis of the eigenspace of ρ_j of θ-invariant vectors. □

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