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Gradient flow and quantum Markov semigroups with detailed balance

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Abstract

In this thesis we present a study of quantum Markov semigroups. In particular, we mainly consider quantum Markov semigroups with detailed balance that are defined on finite-dimensional C^*-algebras. They have an invariant density matrix ρ. Carlen and Maas showed that the evolution on the set of invertible density matrices that is given by such a semigroup is gradient flow for the relative entropy with respect to ρ for some Riemannian metric. This result is a non-commutative analog of certain diffusion equations that are gradient flow in the second order Wasserstein space. We provide a self-contained and accessible account to these issues. Moreover, we give a complete introduction to Tomita-Takesaki theory which has a close relation with quantum Markov semigroups satisfying detailed balance. Finally, we present some examples of these semigroups that arise from quantum theory.

Contents

1 Introduction

A natural problem that arises in the economic sector is optimal transportation. To elaborate on this and give a motivation, one can think for example of farms and bakeries. Suppose there are n farms where grains are grown, and there are n bakeries which use the grains to make bread. The grains that are harvested need to be transported to the bakeries and it needs to be done in such a way that the cost is minimized. Let A and B denote the sets consisting of the farms and bakeries, respectively. Then we may define a cost function $c : A \times B \to \mathbb{R}$, so that $c(a, b)$ is the cost of transporting one load of grains from farm a to factory b. For simplicity, suppose that each farm can only supply one factory of grains and each factory requires precisely one shipment of grains to operate. Then we may also define a transport map function $T : A \to B$ which is a bijection such that each farm $a \in A$ supplies exactly one factory $T(a) \in B$. The goal now is to find the optimal transport map T, that is, the map T whose total cost $c(T) := \sum_{a \in A} c(a, T(a))$ is minimized over all possible transport maps from A to B. This (easy) example brings a whole theory called (optimal) transportation theory and an exhaustive treatment can be found in [28].

An important topic within optimal transportation theory is about *gradient flows*. The gradient flow (for steepest descent) associated to a function $f : M \to \mathbb{R}$ (with M a Riemannian manifold) is the flow induced by the differential equation

$$\frac{dx}{dt} = -\mathrm{grad}_{x(t)} f,$$

whatever $\mathrm{grad}_{x(t)} f$ may mean. Heuristically, one may think of it as a flow which makes f decrease as fast as possible. An important classical result concerning gradient flows is that of Otto [18]. Otto showed that a large number of classical evolution equations could be viewed as gradient flow in a so called *2-Wasserstein metric* for certain functionals. Carlen and Maas studied a non-commutative analogy of this problem and considered M equal to invertible density matrices in a proper context involving *quantum Markov semigroups* [5]. In particular, Carlen and Maas were able to show non-commutative results in line with [18]. This thesis will mainly revolve around the results from [5].

The notion of a quantum Markov semigroup (QMS) can be viewed as a non-commutative analog of classical Markov semigroups motivated by the study of (open) quantum systems. A classical Markov semigroup $(P_t)_{t \geq 0}$ defined on $C_b(\mathbb{R})$ for example satisfies $P_t(1) = 1$ (conservation of probability) and $P_t(f) \geq 0$ (positivity) for all $t \geq 0$ and $f \geq 0$ by definition. In the non-commutative setting a quantum Markov semigroup needs to preserve the identity and has a property called "complete positivity" which shows the duality between a classical Markov semigroup and a quantum Markov semigroup.

The quantum Markov semigroups that we will discuss are *uniformly continuous* (or *norm continuous*). This is a condition which is *not* fulfilled in many infinite-dimensional applications. However, it is still important to study the form of a QMS satisfying the strong condition of uniform continuity. For example, in the finite dimensional setting all quantum Markov semigroups are uniformly continuous. Plenty can be said about generators of quantum Markov semigroups in this finite-dimensional setting but also in a more general setting while still assuming uniform continuity. Namely, the characterization of generators of quantum Markov semigroups on $M_n(\mathbb{C})$ of all $n \times n$ complex matrices was given by Gorini, Kossakowski and Sudershan [10]. And around the same time Lindblad [14] characterized the generators on *hyperfinite von Neumann algebras* but still assuming uniform continuity. (An example of a hyperfinite von Neumann algebra is $B(H)$ where H is an arbitrary separable Hilbert space.)

The main mathematical object in [5] that we will consider are quantum Markov semigroups satisfying a *(quantum) detailed balance condition* in a finite-dimensional setting. Detailed balance has a classical definition in terms of reversible Markov chains and we wish to extend this definition to the quantum setting. To be more precise, a classical Markov chain with transition matrix P satisfies the classical detailed balance equations if and only if P is self-adjoint with respect to the inner product $\langle v, w\rangle_\pi = \sum_{i=1}^n \pi_i v_i \overline{w_i}$ $(v, w \in \mathbb{C}^n)$, where $\pi = (\pi_i)_{i=1}^n$ is the invariant distribution for the Markov chain. There are a number of different ways to generalize this to the quantum setting and it will turn out that the definition we use for quantum detailed balance can be viewed as an extension of classical detailed balance.

A remarkable observation about quantum Markov semigroups with detailed balance is that they have an intimate relation with *Tomita-Takesaki theory* which is often not mentioned in the literature. Namely, such semigroups commute with the *modular operator* and *modular automorphism group*. As the name already suggests, Tomita introduced this theory in 1967 and Takesaki [24] published a slim volume elaborating Tomita's work as Tomita's work was hard to follow and mostly unpublished. Tomita-Takesaki theory (or *modular theory*) has a lot of applications in mathematical physics and is essential in the structure theory of von Neumann algebras (of type III) ([3, 4, 25]). A von Neumann algebra M is by definition a $*$-subalgebra of $B(H)$ with H a Hilbert space such that $M = M''$, where A' is the set of elements in $B(H)$ that commute with A for some subset $A \subseteq B(H)$. The structure of (type III) von Neumann algebras was quite intractable for some time, but with the introduction of Tomita-Takesaki theory it has led to a good structure theory.

Our aim of this thesis is to give a self-contained, in-depth and accessible exposure of [5] with some detours that involve Tomita-Takesaki theory and general (norm-continuous) quantum Markov semigroups. The first chapter is a short introduction in optimal transport and the emphasis is put on Wasserstein spaces. We will state a result (Theorem 2.3.2) involving these spaces and much later on a non-commutative form of this theorem will be given.

The aim of the third chapter is to present Tomita-Takesaki theory in an accessible way with detailed proofs. Nevertheless, the proof of the main theorem of Tomita-Takesaki will be referred to [26]. We will consider *σ-finite* von Neumann algebras but still in an infinite-dimensional setting. It starts with certain involution operators and by means of these operators we are able to construct a one parameter group of automorphisms defined on the von Neumann algebra. Moreover, it also gives a connection between the commutant and algebra itself. We are then able to show explicit computations with matrices that are important for later in the thesis. However, we will not discuss any structure theory of von Neumann algebras nor explicit applications in mathematical physics.

In Chapter 4 we start with complete positivity and study uniformly continuous quantum Markov semigroups on $M_n(\mathbb{C})$ but also on hyperfinite von Neumann algebras and in particular on $B(H)$ where separability is the only condition on the Hilbert space H. The emphasis is put on semigroups in a finite-dimensional setting with detailed balance. The main results consist of complete characterizations of generators of such quantum Markov semigroups. Subsequently, Chapter 5 compares classical detailed balance with quantum detailed balance and quantum detailed balance can be in fact seen as an extension of classical detailed balance.

The main results of this thesis are in Chapter 6.2 (Theorem 6.2.7 and 6.2.8). In particular, Theorem 6.2.8 shows that associated to any ergodic QMS satisfying detailed balance in a finite-dimensional setting, there is a *Riemannian metric* such that the flow on the set of invertible density matrices is gradient flow for the *relative entropy* induced by the dual generator.

Lastly, we give examples of quantum Markov semigroups with detailed balance that arise in quantum theory.

2 Optimal transport

Optimal transport theory came to light when mathematicians wanted to formalise the mathematics behind transporting mass from one location to another location with minimal cost. (Think about the farms and bakeries in the introduction.) In this section we give a short introduction on optimal transport theory and especially bring attention on Wasserstein spaces and gradient flows that will follow the one in [28].

We start with some conventions: When a measure space or measurable space is considered, we will usually not explicitly mention the associated σ-algebra. If $(\mathcal{X}, \mu)$ is a Polish (complete separable metric) probability space, then μ will always denote the Borel probability measure.

If μ is a measure on a measurable space $\mathcal{X}$ and $T : \mathcal{X} \to \mathcal{Y}$ is a measurable function from $\mathcal{X}$ to a measurable space $\mathcal{Y}$, then $T_*\mu$ stands for the push-forward measure of μ by T, that is, $(T_*\mu)(A) := \mu(T^{-1}(A))$ for measurable sets $A \subseteq \mathcal{Y}$.

2.1 Couplings

Definition 2.1.1. Let $(\mathcal{X}, \mu)$ and $(\mathcal{Y}, \nu)$ be two probability spaces. A *coupling* of μ and ν is a measure π on $\mathcal{X} \times \mathcal{Y}$ (with its tensor-product σ-algebra) such that π admits μ and ν as *marginals* on $\mathcal{X}$ and $\mathcal{Y}$ respectively, i.e. $\pi(A \times \mathcal{Y}) = \mu(A)$ and $\pi(\mathcal{X} \times B) = \nu(B)$ for all measurable sets $A \subseteq \mathcal{X}$, $B \subseteq \mathcal{Y}$. The set of all couplings of μ and ν is denoted by $\Pi(\mu, \nu)$. The coupling π is said to be *deterministic* if there exists a measurable function $T : \mathcal{X} \to \mathcal{Y}$ such that $\pi = (\mathrm{id}_{\mathcal{X}}, T)_*\mu$, where $(\mathrm{id}_{\mathcal{X}}, T)$ is the map $x \mapsto (x, T(x))$ for $x \in \mathcal{X}$. The function T is called the *transport map.*

Let $(\mathcal{X}, \mu)$ and $(\mathcal{Y}, \nu)$ be two probability spaces. If π is a deterministic coupling of μ and ν with transport map T, then it follows immediately that $T_*\mu = \nu$. This is seen by a direct computation:

$$\begin{aligned} T_*\mu(B) &= \mu(T^{-1}(B)) = \mu(\mathcal{X} \cap T^{-1}(B)) = \mu((\mathrm{id}_{\mathcal{X}}, T)^{-1}(\mathcal{X} \times B)) \\ &= ((\mathrm{id}_{\mathcal{X}}, T)_*\mu)(\mathcal{X} \times B) = \pi(\mathcal{X} \times B) = \nu(B) \end{aligned}$$

for all measurable sets $B \subseteq \mathcal{Y}$. So intuitively, one can say that T transports mass represented by the measure μ to the mass represented by the measure ν.

Note that there exists always a coupling, namely the product measure. This is the *trivial coupling.* However, unlike couplings, deterministic couplings do not always exist. (Take μ equal to Dirac measure and ν any other measure.)

One important example of coupling is *optimal coupling* or *optimal transport*: Let $(\mathcal{X}, \mu)$ and $(\mathcal{Y}, \nu)$ be two probability spaces, and define a measurable *cost function* $c : \mathcal{X} \times \mathcal{Y} \to [0, \infty]$ that can be interpreted as the work needed to move one unit of mass from location $x \in \mathcal{X}$ to $y \in \mathcal{Y}$. First assume that there exists a deterministic coupling of μ and ν. Then to minimize the cost, one can consider the following optimal transportation problem that is also know as *Monge's minimization problem*:

$$\inf \left\{ \int_{\mathcal{X}} c(x, T(x))\, d\mu(x) \;\middle|\; T : \mathcal{X} \to \mathcal{Y} \text{ is measurable and } T_*\mu = \nu \right\}.$$

The goal is now to find the transport map T that realizes this infimum. A transport map that attains this infimum is called an *optimal transport map.*

However, Monge's formulation of the optimal transport problem can be ill-posed, because a deterministic coupling does not always exist as we have already noted. Hence, we need to find a relaxation of this minimization problem if we want to consider the problem in a more general form.

One way to do this is using coupling measures. Then one considers the so called *Monge-Kantorovich minimization problem*:

$$\inf_{\pi\in\Pi(\mu,\nu)} \int_{\mathcal{X}\times\mathcal{Y}} c(x,y)\ d\pi(x,y).$$

In this context, a coupling π of μ and ν is also called a *transference plan* (or *transport plan*, or *transportation plan*). Those achieving the infimum are called *optimal transference plans* or *optimal couplings*.

Evidently, the solution of the Monge-Kantorovich minimization problem depends on the cost function c. If the probability spaces and the cost function are "nice" enough, then an optimal coupling exists which is stated in the next theorem.

Theorem 2.1.2. *Let $(\mathcal{X},\mu)$ and $(\mathcal{Y},\mu)$ be two Polish probability spaces. Let $a:\mathcal{X}\to\mathbb{R}\cup\{-\infty\}$ and $b:\mathcal{Y}\to\mathbb{R}\cup\{-\infty\}$ be two upper semi-continuous functions such that $a\in L^1(\mathcal{X},\mu)$ and $b\in L^1(\mathcal{Y},\nu)$. Let $c:\mathcal{X}\times\mathcal{Y}\to\mathbb{R}\cup\{\infty\}$ be a lower semi-continuous cost function such that $c(x,y)\geq a(x)+b(y)$ for all $x\in\mathcal{X}$ and $y\in\mathcal{Y}$. Then there is a coupling $\pi'\in\Pi(\mu,\nu)$ of μ and ν such that*

$$\int_{\mathcal{X}\times\mathcal{Y}} c(x,y)\ d\pi'(x,y) = \inf_{\pi\in\Pi(\mu,\nu)} \int_{\mathcal{X}\times\mathcal{Y}} c(x,y)\ d\pi(x,y).$$

Proof. Theorem 4.1 in [28]. □

2.2 Wasserstein distances

Assume that we are in charge of distributing products between producers and consumers and they are modeled by probability measures. We would like to summarize the cost of transporting these goods and minimize it. For that purpose it natural to consider the *optimal transport cost* between two probability measures, say μ and ν, that are defined on some probability spaces $\mathcal{X}$ and $\mathcal{Y}$ respectively:

$$C(\mu,\nu) = \inf_{\pi\in\Pi(\mu,\nu)} \int_{\mathcal{X}\times\mathcal{Y}} c(x,y)\ d\pi(x,y),$$

where $c(x,y)$ is the cost for transporting one unit of mass from x to y. This is just the Monge-Kantorovich minimization problem, but now we do not care about the minimizer (so much). We are more interested in the value of $C(\mu,\nu)$.

If we now suppose that $\mathcal{X}=\mathcal{Y}$, and $\mathcal{X}$ is a metric space with metric d, then an intuitive choice for the cost function c is the distance measured by d. This results in *Wasserstein distances*:

Definition 2.2.1. Let $(\mathcal{X},d)$ be a Polish metric space and let $p\in[1,\infty)$. For any two Borel probability measures μ, ν on X, the *Wasserstein distance of order p between μ and ν* is defined by the formula

$$W_p(\mu,\nu) := \left(\inf_{\pi\in\Pi(\mu,\nu)} \int_{\mathcal{X}\times\mathcal{X}} d(x,y)^p\ d\pi(x,y)\right)^{\frac{1}{p}}.$$

Example 2.2.2. Fix $a,b\in\mathcal{X}$, then $W_p(\delta_a,\delta_b)=d(a,b)$ where δ_a and δ_b are Dirac measures. To see this, we note every coupling $\pi\in\Pi(\delta_a,\delta_b)$ is a product measure of the form $\pi=\delta_a\times\delta_b$. Hence,

$$\begin{aligned} W_p(\delta_a,\delta_b) &= \left(\int_{\mathcal{X}\times\mathcal{X}} d(x,y)^p\ d(\delta_a\times\delta_b)(x,y)\right)^{\frac{1}{p}} = \left(\int_{\mathcal{X}}\int_{\mathcal{X}} d(x,y)^p\ d\delta_a(x)\ d\delta_b(y)\right)^{\frac{1}{p}} \\ &= \left(\int_{\mathcal{X}} d(a,y)^p\ d\delta_b(y)\right)^{\frac{1}{p}} = d(a,b). \end{aligned}$$

Definition 2.2.3. Let $p \in [1, \infty)$ and take a Polish metric space $(\mathcal{X}, d)$. The space of Borel probability measures on $\mathcal{X}$ is denoted by $P(\mathcal{X})$. The *Wasserstein space of order* p is defined as

$$P_p(\mathcal{X}) := \left\{ \mu \in P(\mathcal{X}) : \int_{\mathcal{X}} d(x_0, x)^p \, d\mu(x) < \infty \right\},$$

where $x_0 \in \mathcal{X}$ is arbitrary and note that $P_p(\mathcal{X})$ does not depend on the choice of x_0.

It is not directly clear that W_p defines a metric since it might take the value $+\infty$. But when restricted to $P_p(\mathcal{X})$ it becomes a metric as it will be checked now using the Gluing lemma.

Lemma 2.2.4 (Gluing)**.** *Let $(\mathcal{X}_i, \mu_i)$, $i = 1, 2, 3$ be Polish probability spaces. If $\pi_{1,2} \in \Pi(\mu_1, \mu_2)$ and $\pi_{2,3} \in \Pi(\mu_2, \mu_3)$ are couplings then there exists a Borel probability measure μ on $\mathcal{X}_1 \times \mathcal{X}_2 \times \mathcal{X}_3$ such that μ has marginals $\pi_{1,2}$ and $\pi_{2,3}$ on $\mathcal{X}_1 \times \mathcal{X}_2$ and $\mathcal{X}_2 \times \mathcal{X}_3$, respectively. Moreover, the marginal of μ to $\mathcal{X}_1 \times \mathcal{X}_3$ is a coupling between μ_1 and μ_3.*

Proof. Lemma 5.3.2 and Remark 5.3.3 in [2] □

Proposition 2.2.5. *Let $(\mathcal{X}, d)$ be a Polish metric space and let $p \in [1, \infty)$. Then the Wasserstein space $(P_p(\mathcal{X}), W_p)$ equipped with the Wasserstein distance is a metric space.*

Proof. To show that W_p is finite on $P_p(\mathcal{X})$, we let $x_0 \in \mathcal{X}$ and $\mu, \nu \in P_p(\mathcal{X})$. Let $\pi \in \Pi(\mu, \nu)$ be a coupling between μ and ν. Then, since

$$d(x,y)^p \leq (d(x,x_0) + d(x_0,y))^p \leq 2^p \left(\frac{1}{2} d(x,x_0) + \frac{1}{2} d(x_0,y) \right)^p \leq 2^{p-1}(d(x,x_0)^p + d(x_0,y)^p)$$

using the convexity of $t \mapsto t^p$, we have

$$\begin{aligned} W_p(\mu,\nu)^p &\leq \int_{\mathcal{X}\times\mathcal{X}} d(x,y)^p \, d\pi(x,y) \leq 2^{p-1} \left(\int_{\mathcal{X}\times\mathcal{X}} d(x,x_0)^p \, d\pi(x,y) + \int_{\mathcal{X}\times\mathcal{X}} d(x_0,y)^p \, d\pi(x,y) \right) \\ &= 2^{p-1} \left(\int_{\mathcal{X}} d(x,x_0)^p \, d\mu(x) + \int_{\mathcal{X}} d(x_0,y)^p \, d\nu(y) \right) < \infty. \end{aligned}$$

Thus, W_p in finite on $P_p(\mathcal{X})$.

Symmetry of W_p is clear. Now let $\mu \in P(\mathcal{X})$ and we show that $W_p(\mu, \mu) = 0$. Define $\nu := f_* \mu$ with $f : \mathcal{X} \to \Delta$ given by $f(x) = (x, x)$, i.e. Δ is the diagonal of $\mathcal{X} \times \mathcal{X}$. Now define a Borel measure π on $\mathcal{X} \times \mathcal{X}$ by $\pi(M) = \nu(M \cap \Delta)$ for all Borel sets M. Then for all Borel sets $A \subseteq \mathcal{X}$ we have $\pi(A \times X) = \mu(f^{-1}(A \times \mathcal{X} \cap \Delta)) = \mu(A)$ as $f(A) = \{(a, a) \times \mathcal{X} : a \in A\} = \{(a, x) : a \in A, x \in \mathcal{X}\} \cap \Delta = A \times \mathcal{X} \cap \Delta$. And since we have $A \times \mathcal{X} \cap \Delta = \mathcal{X} \times A \cap \Delta$, we also have $\pi(\mathcal{X} \times A) = \mu(A)$. It follows that $\pi \in \Pi(\mu, \mu)$. Combined with the facts that $d(\Delta) = \{0\}$ and $\pi(\Delta^c) = 0$, we obtain

$$W_p(\mu,\mu) \leq \int_{\mathcal{X}\times\mathcal{X}} d(x,y)^p \, d\pi(x,y) = \int_{\Delta} d(x,y)^p \, d\pi(x,y) + \int_{\Delta^c} d(x,y)^p \, d\pi(x,y) = 0 + 0 = 0,$$

and this obviously implies that $W_p(\mu, \mu) = 0$.

Conversely, suppose that $W_p(\mu, \nu) = 0$. Let $\gamma \in \Pi(\mu, \nu)$ be an optimal coupling with respect to d^p between μ and ν. With the same definition for Δ, we see that

$$0 \leq \int_{\Delta^c} d(x,y)^p \, d\gamma(x,y) \leq \int_{\mathcal{X}\times\mathcal{X}} d(x,y)^p \, d\gamma(x,y) = W_p(\mu,\nu) = 0.$$

Thus, $\gamma(\Delta^c) = 0$ as $d(x,y)^p > 0$ for all $x \neq y$. It then follows that $\mu(A) = \gamma(A \times \mathcal{X}) = \gamma(A \times \mathcal{X} \cap \Delta) = \gamma(\mathcal{X} \times A \cap \Delta) = \gamma(\mathcal{X} \times A) = \nu(A)$ for all Borel sets $A \subseteq \mathcal{X}$ by the marginal properties of γ and the fact that the support of γ lies in Δ. Therefore, $\mu = \nu$.

Note that there exists an optimal coupling with respect to the continuous cost function $c = d^p$ for each pair $\mu, \nu \in P(\mathcal{X})$ by Theorem 2.1.2. To prove the triangle inequality, let $\mu_1, \mu_2, \mu_3 \in P_p(\mathcal{X})$ with optimal couplings $\pi_{1,2} \in \Pi(\mu_1, \mu_2)$ and $\pi_{2,3} \in \Pi(\mu_2, \mu_3)$ with respect to the cost function d^p. Then, by Lemma 2.2.4, there exists a Borel probability measure μ on $\mathcal{X} \times \mathcal{X} \times \mathcal{X}$ such that μ has marginals $\pi_{1,2}$ and $\pi_{2,3}$ on $\mathcal{X} \times \mathcal{X}$ to the "left" and "right", respectively. And, we denote the marginal of μ to $\mathcal{X} \times \mathcal{X}$ (first and third $\mathcal{X}$) by $\pi_{1,3} \in \Pi(\mu_1, \mu_3)$ which is a coupling between μ_1 and μ_3. It follows, by the marginal properties and Minkowski inequality in $L^p(\mathcal{X}^3, \mu)$, that

$$\begin{aligned}
W_p(\mu_1, \mu_3) &\leq \left(\int_{\mathcal{X} \times \mathcal{X}} d(x,z)^p \, d\pi_{1,3}(x,z) \right)^{\frac{1}{p}} = \left(\int_{\mathcal{X} \times \mathcal{X} \times \mathcal{X}} d(x,z)^p \, d\mu(x,y,z) \right)^{\frac{1}{p}} \\
&\leq \left(\int_{\mathcal{X} \times \mathcal{X} \times \mathcal{X}} (d(x,y) + d(y,z))^p \, d\mu(x,y,z) \right)^{\frac{1}{p}} \\
&\leq \left(\int_{\mathcal{X} \times \mathcal{X} \times \mathcal{X}} d(x,y)^p \, d\mu(x,y,z) \right)^{\frac{1}{p}} + \left(\int_{\mathcal{X} \times \mathcal{X} \times \mathcal{X}} d(y,z)^p \, d\mu(x,y,z) \right)^{\frac{1}{p}} \\
&= \left(\int_{\mathcal{X} \times \mathcal{X}} d(x,y)^p \, d\pi_{1,2}(x,y) \right)^{\frac{1}{p}} + \left(\int_{\mathcal{X} \times \mathcal{X}} d(y,z)^p \, d\pi_{2,3}(y,z) \right)^{\frac{1}{p}} \\
&= W_p(\mu_1, \mu_2) + W_p(\mu_2, \mu_3).
\end{aligned}$$

□

From now on, all Wasserstein spaces are endowed with their corresponding Wasserstein distance. The Wasserstein space has many convergence and topological properties. For example, $(P_p(\mathcal{X}), W_p)$ is a Polish space again when $\mathcal{X}$ is Polish (Theorem 6.18 in [28]). For other results we refer to Chapter 6 in [28].

2.3 Gradient flows in Wasserstein space

Definition 2.3.1. Let (M, g) be a Riemannian manifold and let $f : M \to \mathbb{R}$ be continuously differentiable. The *Riemannian gradient of f at $p \in M$*, denoted by $\text{grad}_p f$ or $\nabla_p f$, is the unique tangent vector in T_pM satisfying the equation

$$\frac{d}{dt}\Big|_{t=0} f(\gamma(t)) = g_p(\text{grad}_p f, \dot{\gamma}(0))$$

for all smooth curves $\gamma : (-\epsilon, \epsilon) \to M$ such that $\gamma(0) = p$.

Let (M, g) be a Riemannian manifold and let $f : M \to \mathbb{R}$ continuously differentiable. Fix $p \in M$. Then one might ask for which smooth curve $\gamma : (-\epsilon, \epsilon) \to M$ with $\gamma(0) = p$ the derivative $\frac{d}{dt}\big|_{t=0} f(\gamma(t))$ is as large or as small as possible. By the definition of the Riemannian gradient, we see that we need to choose γ such that $\dot{\gamma}(0)$ and $\text{grad}_p f$ are linearly dependent. So essentially, $\text{grad}_p f$ indicates the direction in which f increases and decreases most rapidly. The corresponding *gradient flow equation for strongest ascent* associated to f is the flow induced by the differential equation

$$\dot{\gamma}(t) = \text{grad}_{\gamma(t)} f, \quad \gamma(0) = p.$$

Similarly, the *gradient flow equation for steepest descent* associated to f is the flow induced by the differential equation

$$\dot{\gamma}(t) = -\text{grad}_{\gamma(t)} f, \quad \gamma(0) = p.$$

The gradient flow for steepest descent is most important for us. Henceforth, when we write "gradient flow" it will always mean the gradient flow for steepest descent. Heuristically, one may think of the gradient flow as a flow which makes f *decrease as fast a possible.*

Every Riemannian manifold has a metric space structure that is induced by the *geodesic distance.* Keeping this in mind, we boldly state the next theorem that identifies certain diffusion equations as gradient flows in the Wasserstein space of order 2.

Theorem 2.3.2. *Let M be a compact separable Riemannian manifold equipped with a reference measure ν. Let $V \in C^2(M)$ and let $L = \Delta - \nabla V \cdot \nabla$ where Δ is the Laplace operator on M. Let $\mu_0 \in P_2(M)$ and define a path $(\mu_t)_{t>0}$ in $P_2(M)$ by $\mu_t(A) = \int_A \rho_t \, d\nu$ where ρ_t satisfies*

$$\frac{\partial \rho_t}{\partial t} = L\rho_t.$$

Then $(\mu_t)_{t>0}$ is a trajectory of the gradient flow associated with the energy functional

$$H_\nu(\mu) = \int_M \frac{d\mu}{d\nu} \log\left(\frac{d\mu}{d\nu}\right) d\nu \qquad \left(\frac{d\mu}{d\nu} \text{ is the Radon-Nikodym derivative}\right)$$

in the Wasserstein space $P_2(M)$.

Proof. Theorem 23.19 and Corollary 23.23 in [28]. □

Much later in this thesis, we will consider a non-commutative form of this theorem involving *quantum Markov semigroups with detailed balance* and *relative entropy.*

3 Tomita-Takesaki Theory

In the theory of von Neumann algebras, Tomita-Takesaki theory is a method for constructing a one parameter group of automorphisms on a (σ-finite) von Neumann algebra from the polar decomposition of a certain involution. It also gives a connection between the algebra itself and its commutant.

Definition 3.0.1. Let τ be a positive linear functional on a von Neumann algebra M. Then τ is called

- a *state*, if $\|\tau\| = 1$;
- *pure*, if τ is a state and is an extreme point of the set of states on M;
- *faithful*, if $\tau(a^*a) = 0$ implies that $a = 0$;
- *tracial*, if $\tau(ab) = \tau(ba)$ for all $a, b \in M$;
- *normal*, if $\tau(\sup_\lambda a_\lambda) = \sup_\lambda \tau(a_\lambda)$ for all increasing nets (a_λ) in M^+ with an upper bound.

3.1 Von Neumann algebras with faithful normal tracial state

Theorem 3.1.1. *Let ϕ be a bounded linear functional on a von Neumann algebra $M \subseteq B(H)$. The following conditions are equivalent:*

1. *ϕ is normal;*
2. *ϕ is weakly continuous on the unit ball of M;*
3. *ϕ is σ-weakly continuous;*
4. *There exists a trace-class operator $u \in L^1(H)$ such that $\phi(a) = \mathrm{Tr}(au)$ for all $a \in M$.*

Proof. Theorem 2.4.21 in [3] or Theorem 3.6.4 in [20]. □

Proposition 3.1.2. *Let M be a von Neumann algebra with a faithful normal state ϕ. Let $(H_\phi, \pi_\phi, \xi_\phi)$ be the GNS representation of M associated to ϕ. Then $\pi_\phi(M) \subseteq B(H_\phi)$ is a von Neumann algebra and M is $*$-isomorphic to $\pi_\phi(M)$. Moreover, $\pi_\phi(M)$ admits a vector which is separating and cyclic.*

Proof. First, let (a_λ) be an increasing net in M^+ which is bounded. Then (a_λ) is strongly convergent to $a := \sup_\lambda a_\lambda \in M^+$ by Vigier. Now, since ϕ is normal, we have for all $b \in M$ that

$$\begin{aligned}\lim_\lambda \langle \pi_\phi(a_\lambda)\pi_\phi(b)\xi_\phi, \pi_\phi(b)\xi_\phi\rangle &= \lim_\lambda \langle \pi_\phi(b^* a_\lambda b)\xi_\phi, \xi_\phi\rangle \\ &= \lim_\lambda \phi(b^* a_\lambda b) \\ &= \phi(b^* a b) \\ &= \langle \pi_\phi(a)\pi_\phi(b)\xi_\phi, \pi_\phi(b)\xi_\phi\rangle.\end{aligned}$$

So, using polarization and the facts that ξ_ϕ is cyclic for $\pi_\phi(M)$ and $(\pi_\phi(a_\lambda))$ is bounded, we obtain $\pi_\phi(a_\lambda) \to \pi_\phi(a)$ weakly. But then also $\pi_\phi(a_\lambda) \to \pi_\phi(a)$ σ-weakly as the weak (operator) topology coincides with the σ-weak topology on bounded sets. Hence, $\lim_\lambda \omega(\pi_\phi(a_\lambda)) = \omega(\pi_\phi(a))$ for all σ-weakly continuous states ω on $B(H_\phi)$, or equivalently by Theorem 3.1.1, for all normal states ω on $B(H_\phi)$. But this implies that $\omega \circ \pi_\phi$ is normal for all normal states ω on $B(H_\phi)$. Or, equivalently by Theorem 3.1.1 once again, $\omega \circ \pi_\phi$ is a σ-weakly continuous state on M for all σ-weakly continuous states ω on $B(H_\phi)$. Now, every σ-weakly continuous linear functional on $B(H_\phi)$ is of the form $\mathrm{Tr}(\cdot u)$ for some $u \in L^1(H_\phi)$. Moreover, every σ-weakly continuous linear functional is a linear combination of σ-weakly continuous states. Therefore, $\pi_\phi : M \to B(H_\phi)$ is σ-weakly continuous.

It clear that π_ϕ is injective since ϕ is faithful. Thus, π_ϕ is isometric. It follows that $\pi_\phi(M_{\leq 1}) = \pi_\phi(M)_{\leq 1}$. But we know that $M_{\leq 1}$ is σ-weakly compact and π_ϕ is σ-weakly continuous. Therefore, $\pi_\phi(M)_{\leq 1}$ is σ-weakly compact and also weakly compact. And, in particular, $\pi_\phi(M)_{\leq 1}$ is weakly closed. But then we also have that $\pi_\phi(M)_{\leq 1}$ is strongly closed as $\pi_\phi(M)_{\leq 1}$ is convex. Consequently, by the Kaplansky density theorem, $\left(\overline{\pi_\phi(M)}^{\mathrm{SOT}}\right)_{\leq 1} = \overline{\pi_\phi(M)_{\leq 1}}^{\mathrm{SOT}} = \pi_\phi(M)_{\leq 1}$. So, if $a \in \overline{\pi_\phi(M)}^{\mathrm{SOT}}$, then $\frac{a}{\|a\|} \in \left(\overline{\pi_\phi(M)}^{\mathrm{SOT}}\right)_{\leq 1} = \pi_\phi(M)_{\leq 1}$ which implies that $a \in \pi_\phi(M)$. In other words, $\pi_\phi(M)$ is strongly closed and we see that $\pi_\phi(M)$ is a von Neumann algebra such that M is $*$-isomorphic to it.

We already know that $\xi_\phi \in H_\phi$ is cyclic for $\pi_\phi(M)$. So suppose that $\pi_\phi(a)\xi_\phi = 0$ for some $a \in M$. Then $\phi(a^*a) = \langle \pi_\phi(a^*a)\xi_\phi, \xi_\phi \rangle = \|\pi_\phi(a)\xi_\phi\|^2 = 0$. Hence, $a = 0$ since ϕ is faithful. Therefore, ξ_ϕ is also a separating vector for $\pi_\phi(M)$. □

Let M be a von Neumann algebra with a faithful normal tracial state τ defined on M. Denote the pair (H_τ, π_τ) as the GNS representation of M associated to τ. To be more precise, H_τ is the Hilbert space completion of M with respect to the inner product $\langle a, b \rangle := \tau(b^*a)$. This inner product is well defined since τ is faithful. Furthermore, the operator $\pi(a) \in B(M)$ with $a \in M$ defined by $\pi(a)b = ab$ for $b \in M$ can be uniquely extended to a bounded operator $\pi_\tau(a)$ on H_τ by density. And the map

$$\pi_\tau : M \to B(H_\tau), \quad a \mapsto \pi_\tau(a)$$

is a faithful $*$-homomorphism. Note, by Proposition 3.1.2, that $\pi_\tau(M)$ is a von Neumann algebra because τ is a faithful normal state.

Denote $\xi_0 := 1 \in M$ and the set $\pi(M)\xi_0 := \{\pi_\tau(a)\xi_0 : a \in M\} = M$ lies dense in H_τ by construction of H_τ. So ξ_0 is cyclic for $\pi_\tau(M)$. Moreover, ξ_0 is also separating for $\pi_\tau(M)$ since $\pi_\tau(a)\xi_0 = 0$ implies $a = 0$ for all $a \in M$. Now identify M with the von Neumann algebra $\pi_\tau(M)$ and we can do this because π_τ is injective. We may therefore also write $\tau(a) = \langle a\xi_0, \xi_0 \rangle$ for all $a \in M$ in view of $\tau(a) = \langle \pi_\tau(a)\xi_0, \xi_0 \rangle$ formally speaking. In particular,

$$\langle ab\xi_0, \xi_0 \rangle = \langle ba\xi_0, \xi_0 \rangle, \quad \text{for all } \ a, b \in M$$

as τ is tracial. The map

$$J_0 : M\xi_0 \to M\xi_0, \quad J_0(a\xi_0) = a^*\xi_0$$

is a well-defined map because ξ_0 is separating for M. It also clear that J_0 is conjugate linear. In addition,

$$\|J_0(a\xi_0)\|^2 = \langle aa^*\xi_0, \xi_0 \rangle = \langle a^*a\xi_0, \xi_0 \rangle = \|a\xi_0\|^2$$

so that J_0 is an isometry (and hence bounded). Let J be the unique extension of J_0 to $H_\tau = \overline{M\xi_0}$. Since $J_0^2 = \mathrm{id}_{M\xi_0}$, one also has $J^2 = \mathrm{id}_{H_\tau}$ by density and continuity.

Lemma 3.1.3. *Suppose that M is a von Neumann algebra on a Hilbert space H. Then $\xi \in H$ is cyclic for M if and only if ξ is separating for M'.*

Proof. Assume that $\xi \in H$ is cyclic M and let $a' \in M'$ such that $a'\xi = 0$. Then $a'a\xi = aa'\xi = 0$ for all $a \in M$, i.e. $a'M\xi = \{0\}$. Therefore, $a'H = \{0\}$ since $\overline{M\xi} = H$ (cyclicity of ξ for M) and continuity of a'. Thus $a' = 0$.

Now suppose that ξ is separating for M'. Let p be the projection onto $\overline{M\xi}$. Now note $p \in M'$ if and only if $p(H)$ is invariant for M. It is clear that $p(H) = \overline{M\xi}$ is invariant for M. Thus, $p \in M'$. Using the fact that $\xi \in \overline{M\xi}$, it follows that $p\xi = \xi = \mathrm{id}_H\xi$. Consequently, $p = \mathrm{id}_H$ as ξ is separating for M' which implies that $\overline{M\xi} = H$. □

Corollary 3.1.4. *Suppose that M is a von Neumann algebra on a Hilbert space H. Then $\xi \in H$ is cyclic and separating for M if and only if ξ is cyclic and separating for M'.*

Proof. This follows almost immediately from Lemma 3.1.3. Use that $M'' = M$ and that M' is also a von Neumann algebra. □

Proposition 3.1.5. *Let J and M be as above, then $JMJ \subseteq M'$.*

Proof. Let $a, b, c \in M$. Then

$$\begin{aligned} JaJ(bc\xi_0) &= J(ac^*b^*\xi_0) \\ &= bca^*\xi_0 \\ &= bJ(ac^*\xi_0) \\ &= bJaJc\xi_0. \end{aligned}$$

Hence, $JaJb$ and $bJaJ$ coincide on $M\xi_0$ which is dense in H_τ by cyclicity of ξ_0. Thus, $JaJb = bJaJ$ by continuity and therefore $JaJ \in M'$ which gives $JMJ \subseteq M'$. □

Theorem 3.1.6. *Let J and M be as above, then $JMJ = M'$.*

Proof. Let $a, b \in M$ and $a' \in M'$. Then

$$\langle Ja\xi_0, b\xi_0\rangle = \langle a^*\xi_0, b\xi_0\rangle = \langle b^*\xi_0, a\xi_0\rangle = \langle Jb\xi_0, a\xi_0\rangle = \langle J^*a\xi_0, b\xi_0\rangle,$$

where the second equality comes from the fact that ξ_0 is a *tracial* vector and the last equality is the definition of the adjoint of an conjugate linear operator. Consequently, $J = J^*$ using density of $M\xi_0$ in H_τ twice. It follows that

$$\langle Ja'\xi_0, a\xi_0\rangle = \langle J^*a\xi_0, a'\xi_0\rangle = \langle Ja\xi_0, a'\xi_0\rangle = \langle a^*\xi_0, a'\xi_0\rangle = \langle (a')^*\xi_0, a\xi_0\rangle.$$

And here the first equality is the definition of J^*, the second equality is $J^* = J$ and the last equality is the tracial property. Therefore, $Ja'\xi_0 = (a')^*\xi_0$ for all $a' \in M'$ using density of $M\xi_0$ in H_τ once again.

Remember that ξ_0 is cyclic and separating for M. Thus, ξ_0 is also cyclic and separating for M' by Corollary 3.1.4 . So there exists a well defined operator $J' \in B(H_\tau)$ with $J'(a'\xi_0) = (a')^*\xi_0$ for all $a' \in M'$. But then $J'M'J' \subseteq M'' = M$ by applying Proposition 3.1.5 with J' and M'. Note that $J = J'$ such that $JM'J \subseteq M$. Lastly, since $J^2 = \mathrm{id}_{H_\tau}$, we obtain $M' = J(JM'J)J \subseteq JMJ$ and together with Proposition 3.1.5 this results in $JMJ = M'$. □

3.2 Von Neumann algebras with faithful normal state

Definition 3.2.1. A von Neumann algebra M is *σ-finite* if each collection of mutually orthogonal nonzero projections in M is countable.

Proposition 3.2.2. *Let $M \subseteq B(H)$ be a von Neumann algebra. Then M is σ-finite if and only if M has a faithful normal state.*

Proof. Suppose that M is σ-finite. An application of Zorn's lemma shows that there exists a maximal family of units vectors (ξ_λ) in H such that the spaces $\overline{M'\xi_\lambda}$ and $\overline{M'\xi_{\lambda'}}$ are orthogonal whenever $\lambda \neq \lambda'$. Let p_λ be the projections onto $\overline{M'\xi_\lambda}$. Then $p_\lambda \in M$ for all λ as $p_\lambda(H)$ is invariant for M'. Thus, p_λ is countable since we have assumed that M is σ-finite. We may therefore consider the sequence $(p_n)_{n\in\mathbb{N}}$ of mutually orthogonal projections with $p_n(H) = \overline{M'\xi_n}$ such that $(p_n)_{n\in\mathbb{N}}$ is maximal and $\|\xi_n\| = 1$ for all $n \in \mathbb{N}$. Now let $\xi \in \left(\bigcup_{n\in\mathbb{N}} \overline{M'\xi_n}\right)^\perp$. Then $\langle a'\xi, b'\xi_n\rangle = \langle \xi, (a')^* b'\xi_n\rangle = 0$ for all $a', b' \in M'$ and $n \in \mathbb{N}$. This implies that $\overline{M'\xi}$ and $\overline{M'\xi_n}$ are orthogonal for all $n \in \mathbb{N}$. It follows from maximality that $\xi = 0$. Hence, $H = \overline{\bigcup_{n=1}^\infty p_n(H)}$. ($H$ is the orthogonal direct sum of the spaces $p_n(H) = \overline{M'\xi_n}$.)
Define the state $\phi(x) := \sum_{n=1}^\infty 2^{-n}\langle x\xi_n, \xi_n\rangle$ for $x \in M$. It is clear that ϕ is σ-weakly continuous, hence normal by Theorem 3.1.1. Now if $\phi(x^*x) = 0$, then $\|x\xi_n\|^2 = \langle x^*x\xi_n, \xi_n\rangle = 0$ for all $n \in \mathbb{N}$. But then $xM'\xi_n = M'x\xi_n = \{0\}$ which implies that $x(p_n(H)) = x(\overline{M'\xi_n}) = \{0\}$ by continuity. Consequently, $x\Big(\bigcup_{n=1}^\infty p_n(H)\Big) = \bigcup_{n=1}^\infty x(p_n(H)) = \{0\}$ and using continuity once again, we obtain $x(H) = x\Big(\overline{\bigcup_{n=1}^\infty p_n(H)}\Big) = \{0\}$. This means that $x = 0$ and hence ϕ is also faithful.

Conversely, assume that M has a faithful normal state ϕ. Let (p_λ) be a collection of mutually orthogonal nonzero projections in M. Let $(H_\phi, \pi_\phi, \xi_\phi)$ be the GNS representation of M associated to ϕ. Then $\xi_\phi \in H_\phi$ is cyclic and separating for $\pi_\phi(M)$ by Proposition 3.1.2. Set $p = \sum_\lambda p_\lambda \in M$ with convergence in the σ-strong topology (Vigier) and hence also in the σ-weak topology. Remember that we have shown in the proof of Proposition 3.1.2 that π_ϕ is σ-weakly continuous. Therefore,

$$\begin{aligned}\sum_\lambda \|\pi_\phi(p_\lambda)\xi_\phi\|^2 &= \sum_{\lambda,\lambda'}\langle \pi_\phi(p_\lambda)\xi_\phi, \pi_\phi(p_{\lambda'})\xi_\phi\rangle \\ &= \langle \pi_\phi(p)\xi_\phi, \pi_\phi(p)\xi_\phi\rangle \\ &= \|\pi_\phi(p)\xi_\phi\|^2 < \infty.\end{aligned}$$

Therefore, only a countable number of $(\pi_\phi(p_\lambda)\xi_\phi)$ is nonzero and thus the same is true for (p_λ). □

One of the goals is to extend Theorem 3.1.6 to von Neumann algebras with a faithful normal state or, equivalently by Proposition 3.2.2, to σ-finite von Neumann algebras. Let M be a σ-finite von Neumann algebra. Using Proposition 3.1.2, we may assume that M acts on Hilbert space H such that M admits a cyclic and separating vector $\xi_0 \in H$ (and thus also for M'). So we may define:

$$\begin{aligned} S_0 &: M\xi_0 \to M\xi_0, \quad a\xi_0 \mapsto a^*\xi_0; \\ F_0 &: M'\xi_0 \to M'\xi_0, \quad a'\xi_0 \mapsto (a')^*\xi_0. \end{aligned}$$

Lemma 3.2.3. *Adopting the foregoing definitions. It follows that $\langle S_0\xi, \eta\rangle = \overline{\langle \xi, F_0\eta\rangle}$ for all $\xi \in D(S_0) = M\xi$ and for all $\eta \in D(F_0) = M'\xi_0$.*

Proof. Let $a \in M$ and $a' \in M'$, then

$$\langle S_0 a\xi_0, a'\xi_0\rangle = \langle a^*\xi_0, a'\xi_0\rangle = \langle \xi_0, aa'\xi_0\rangle = \langle \xi_0, a'a\xi_0\rangle = \langle (a')^*\xi_0, a\xi_0\rangle = \overline{\langle a\xi_0, F_0 a'\xi_0\rangle},$$

where the third equality comes from the fact that a and a' commute since $a \in M$ and $a' \in M'$. $\square$

"Easy" case: Assume that $\mathbf{S_0}$ is *bounded* on its domain.
(This happens if $M = M_n(\mathbb{C})$ for example, which will be important later on.)

Let S be the unique (continuous) extension of S_0 to H. Then S^* coincides with F_0 on $M'\xi_0$ by Lemma 3.2.3. In particular, F_0 is bounded on its domain and therefore has a unique (continuous) extension F to H. Moreover, $S^* = F$ by the uniqueness of extension. Note that S and F are conjugate linear bounded operators. Define the *modular operator*

$$\Delta := S^*S = FS.$$

It is clear that Δ is positive. Moreover, Δ is invertible with $\Delta^{-1} = SS^* = SF$ because $S^2 = I$ and $F^2 = I$. Write S in the left and right polar decomposition:

$$S = J|S| = |S^*|J, \quad \text{or}$$
$$S = J\Delta^{\frac{1}{2}} = \Delta^{-\frac{1}{2}}J,$$

where J is a conjugate linear partial isometry. Note that $J = S\Delta^{-\frac{1}{2}} = \Delta^{\frac{1}{2}}S$ such that $J^2 = S\Delta^{-\frac{1}{2}}\Delta^{\frac{1}{2}}S = I$. In particular, J is invertible (with $J^{-1} = J$) and hence $\ker(J) = \{0\}$. Therefore, J is isometric on $\ker(J)^{\perp} = H$ which implies that J is a conjugate linear unitary operator.

Lemma 3.2.4. *Let S and F be as mentioned above. Then $SMS = M'$, $SM'S = M$, $FMF = M'$ and $FM'F = M$.*

Proof. First note that it will be sufficient to prove the inclusion "$\subseteq$" at each place since the other inclusion follows (almost) directly using $S^2 = F^2 = I$.
Let $a, b, c \in M$, then

$$SaSbc\xi_0 = Sac^*b^*\xi_0 = bca^*\xi_0 = bSac^*\xi_0 = bSaSc\xi_0.$$

Consequently, $SaSb$ and $bSaS$ coincide on $M\xi_0$ which is dense in H by cyclicity of ξ_0. Thus, $SaSb = bSaS$ by continuity and therefore $SaS \in M'$ which gives $SMS \subseteq M'$. But then, $FaF = S^*aS^* = (Sa^*S)^* \in (M')^* = M'$, so also $FMF \subseteq M'$.

In the same way as in the last part of the proof of Theorem 3.1.6, it is possible to exchange M with M' in order to obtain $SM'S \subseteq M'' = M$ and $FM'F \subseteq M'' = M$. The details are omitted. $\square$

Corollary 3.2.5. $\Delta^n M \Delta^{-n} = M$ *for all* $n \in \mathbb{Z}$.

Proof. It is clear for $n = 0$ and for $n \in \{1, -1\}$:

$$\Delta M \Delta^{-1} = FSMSF = FM'F = M,$$
$$\Delta^{-1} M \Delta = SFMFS = SM'S = M$$

by Lemma 3.2.4 and using $\Delta = FS$, $\Delta^{-1} = SF$. Now use induction or iterate to obtain the result. $\square$

Lemma 3.2.6. *Let h be a bounded analytic function on the open unit disk $\{z \in \mathbb{C} : |z| < 1\}$ with $h \neq 0$. If $\alpha_1, \alpha_2, \alpha_3, ...$ are the zeros of h, then*

$$\sum_{n=1}^{\infty}(1 - |\alpha_n|) < \infty.$$

Proof. Theorem 15.23 in [21]. □

Lemma 3.2.7. *Let f, g be analytic functions in the right open half-plane $\{z \in \mathbb{C} : \Re(z) > 0\}$. Assume that*

1. *$f(n) = g(n)$ for all $n \in \mathbb{N}_{\geq 1}$;*
2. *$|f(z) - g(z)| \leq c_1 e^{c_2 \Re(z)}$ for some constants $c_1, c_2 > 0$.*

Then $f = g$.

Proof. Define $F(z) := f(z)e^{-c_2 z}$ and $G(z) := g(z)e^{-c_2 z}$ and let $H := F - G$. Then

$$|H(z)| = |F(z) - G(z)| = |f(z) - g(z)| \cdot |e^{-c_2 z}| = |f(z) - g(z)|e^{-c_2 \Re(z)} \leq c_1$$

by assumption 2. Hence, H is a bounded analytic function on $\{z \in \mathbb{C} : \Re(z) > 0\}$ with $H(n) = 0$ for all $n \in \mathbb{N}_{\geq 1}$ by assumption 1.

Define $\Phi : \{z \in \mathbb{C} : |z| < 1\} \to \{z \in \mathbb{C} : \Re(z) > 0\}$ by $\Phi(z) = \frac{1+z}{1-z}$. Then Φ is a bijection with $\Phi^{-1}(w) = \frac{w-1}{w+1}$. Let $h := H \circ \Phi$. It is clear that h is well-defined bounded analytic function on $\{z \in \mathbb{C} : |z| < 1\}$ and h is zero on $\Phi^{-1}(\mathbb{N}_{\geq 1})$ since $h(\Phi^{-1}(\mathbb{N}_{\geq 1})) = H(\mathbb{N}_{\geq 1}) = \{0\}$. However,

$$\sum_{n=1}^{\infty}\left(1 - |\Phi^{-1}(n)|\right) = \sum_{n=1}^{\infty}\left(1 - \frac{n-1}{n+1}\right) = \sum_{n=1}^{\infty}\frac{2}{n+1} = \infty.$$

Therefore, $h = 0$ by Lemma 3.2.6. (Note that h may contain more zeros but it will only have a positive contribution to the sum). It follows that $H = 0$ which implies that $f = g$. □

Lemma 3.2.8. *Let $\Delta = S^*S = FS$ be the modular operator. Then $\Delta^\alpha M \Delta^{-\alpha} \subseteq M$ for all $\alpha \in \mathbb{C}$.*

Proof. First fix $\alpha \in \{z \in \mathbb{C} : \Re(z) > 0\}$. Define the continuous functions $\tilde{f}, \tilde{g} \in C(\sigma(\Delta))$ by $\tilde{f}(t) = t^\alpha$ and $\tilde{g}(t) = t^{-\alpha}$. Note that $\|\Delta^{-1}\| = \|SS^*\| = \|S^*\|^2 = \|S\|^2 = \|S^*S\| = \|\Delta\|$ using the C^*-identity. Now, $\sigma(\Delta) \subseteq (0, \|\Delta\|]$ such that $\sigma(\Delta^{-1}) \subseteq [\|\Delta\|^{-1}, \|\Delta^{-1}\|]$ by the spectral mapping theorem and therefore $\sigma(\Delta) \subseteq [\|\Delta\|^{-1}, \|\Delta\|]$ using the spectral mapping theorem once again and the fact that $\|\Delta^{-1}\| = \|\Delta\|$. Consequently,

$$\|\tilde{f}\|_\infty = \sup_{t\in\sigma(\Delta)} |t^\alpha| = \sup_{t\in\sigma(\Delta)} t^{\Re(\alpha)} = \|\Delta\|^{\Re(\alpha)}, \quad \text{and}$$

$$\|\tilde{g}\|_\infty = \sup_{t\in\sigma(\Delta)} |t^{-\alpha}| = \sup_{t\in\sigma(\Delta)} \left(\frac{1}{t}\right)^{\Re(\alpha)} = \|\Delta\|^{\Re(\alpha)}.$$

Now let $a \in M$, $a' \in M'$ and $\phi \in B(H)^*$. Define $f, g : \mathbb{C} \to \mathbb{C}$ by $f(\alpha) = \phi((\Delta^\alpha a \Delta^{-\alpha})a')$ and $g(\alpha) = \phi(a'(\Delta^\alpha a \Delta^{-\alpha}))$.

It follows that for all $\alpha \in \{z \in \mathbb{C} : \Re(z) > 0\}$,

$$\begin{aligned} |f(\alpha) - g(\alpha)| &\leq |f(\alpha)| + |g(\alpha)| \\ &\leq 2\|\phi\|\|a\|\|a'\|\|\Delta^{\alpha}\|\|\Delta^{-\alpha}\| \\ &= 2\|\phi\|\|a\|\|a'\|\|\tilde{f}(\Delta)\|\|\tilde{g}(\Delta)\| \\ &= 2\|\phi\|\|a\|\|a'\|\|\tilde{f}\|_{\infty}\|\tilde{g}\|_{\infty} \\ &= 2\|\phi\|\|a\|\|a'\|\|\Delta\|^{2\Re(\alpha)} \\ &= 2\|\phi\|\|a\|\|a'\|e^{2\log(\|\Delta\|)\Re(\alpha)}. \end{aligned}$$

where the isometry property of continuous functional calculus and the values for $\|\tilde{f}\|_{\infty}$ and $\|\tilde{g}\|_{\infty}$ have been used. Moreover, $\Delta^n a \Delta^{-n} \in M$ for all $n \in \mathbb{N}_{\geq 1}$ by Corollary 3.2.5 which implies that $f(n) = \phi((\Delta^n a \Delta^{-n})a') = \phi(a'(\Delta^n a \Delta^{-n})) = g(n)$ as $a' \in M'$. But then $f = g$ when restricted to $\{z \in \mathbb{C} : \Re(z) > 0\}$ by Lemma 3.2.7. This implies that $f = g$ on $\mathbb{C}$ by uniqueness of analytic continuation. Now since $\phi \in B(H)^*$ was arbitrary,

$$(\Delta^{\alpha} a \Delta^{-\alpha})a' = a'(\Delta^{\alpha} a \Delta^{-\alpha}), \quad \text{for all } \alpha \in \mathbb{C}$$

by Hahn-Banach theorem. But this implies that $\Delta^{\alpha} M \Delta^{-\alpha} \subseteq M'' = M$. □

Theorem 3.2.9. *The following two statements hold:*

1. $\Delta^{\alpha} M \Delta^{-\alpha} = M$ *for all* $\alpha \in \mathbb{C}$*;*
2. $JMJ = M'$.

Proof. Statement 1 follows almost directly from Lemma 3.2.8:

$$M = \Delta^{\alpha}(\Delta^{-\alpha} M \Delta^{\alpha})\Delta^{-\alpha} \subseteq \Delta^{\alpha} M \Delta^{-\alpha} \subseteq M, \quad \text{for all } \alpha \in \mathbb{C}.$$

But then, using this, Lemma 3.2.4 and that $J = S\Delta^{-\frac{1}{2}} = \Delta^{\frac{1}{2}}S$, we obtain

$$JMJ = S\Delta^{-\frac{1}{2}} M \Delta^{\frac{1}{2}} S = SMS = M'.$$

□

General case: What if $\mathbf{S_0}$ is *unbounded*?

First, for the sake of completeness, we give the definition of the adjoint a densely defined conjugate linear operator.

Definition 3.2.10. Let H and K be Hilbert spaces and let $T : H \supseteq D(T) \to K$ be a densely defined conjugate linear operator. Then the domain of T^* is

$$D(T^*) := \{\eta \in K \mid \exists \zeta \in H \text{ such that } \forall \xi \in D(T) : \langle T\xi, \eta \rangle = \overline{\langle \xi, \zeta \rangle}\},$$

and we set $T^*\eta := \zeta$ for $\eta \in D(T^*)$. (Note that that there is at most one such ζ for a given η since $D(T)$ is dense in H.)

The following proposition will be frequently used.

Proposition 3.2.11. *Let H and K be Hilbert spaces. If $T : H \supseteq D(T) \to K$ is a densely defined (conjugate) linear operator, then:*

1. *T^* is a closed operator;*
2. *T^* is densely defined if and only if T is closable;*
3. *if T is closable, then its closure is T^{**}.*

Proof. Proposition X.1.6 in [7]. □

Let M be a von Neumann algebra with a faithful normal state, or what is the same, a σ-finite von Neumann algebra. Once again, using Proposition 3.1.2, we may assume that M acts on Hilbert space H such that M admits a cyclic and separating vector $\xi_0 \in H$ (and thus also for M'). Define again:

$$\begin{aligned} S_0 : M\xi_0 \to M\xi_0, &\quad a\xi_0 \mapsto a^*\xi_0; \\ F_0 : M'\xi_0 \to M'\xi_0, &\quad a'\xi_0 \mapsto (a')^*\xi_0, \end{aligned}$$

but now we do *not* assume that S_0 is bounded on its domain.

Remark 3.2.12. Remember that $\langle S_0\xi, \eta\rangle = \overline{\langle \xi, F_0\eta\rangle}$ for all $\xi \in D(S_0) = M\xi$ and for all $\eta \in D(F_0) = M'\xi_0$ from Lemma 3.2.3. But this implies that $F_0 \subseteq S_0^*$ (S_0^* is an extension of F_0) and $S_0 \subseteq F_0^*$ (F_0^* is an extension of S_0). In particular, S_0^* and F_0^* are densely defined which implies that S_0 and F_0 are closable by Proposition 3.2.11. Let $S := \overline{S_0}$ be the closure of S_0, that is, $\mathrm{G}(S) = \overline{\mathrm{G}(S_0)}$ where $\mathrm{G}(T)$ is the graph of a linear operator T. Similarly, let $F := \overline{F_0}$ be the closure of F_0. Then $F_0 \subseteq S_0^* = S^*$ and $S_0 \subseteq F_0^* = F^*$ so that $F \subseteq S^*$ and $S \subseteq F^*$ where we used the fact that $T^* = (\overline{T})^*$ whenever T is a densely defined closable operator and the fact that S^* and F^* are closed operators (by Proposition 3.2.11).

Definition 3.2.13. A closed densely defined operator T is said to be *affiliated* with a von Neumann algebra M if $U'T(U')^* = T$ for each unitary $U' \in M'$.

The polar decomposition of unbounded operators is required from here on. We refer to ([12], Theorem 6.1.11) for more background and other properties.

Lemma 3.2.14. *Assume that T is affiliated with a von Neumann algebra $M \subseteq B(H)$. If $T = U|T|$ is the (unbounded) polar decomposition of T, then U and the spectral projections of $|T|$ lie in M.*

Proof. Let $U' \in M'$ be unitary. Then $\widetilde{U} := U'U(U')^*$ is a partial isometry and $\widetilde{|T|} := U'|T|(U')^*$ is positive such that

$$\widetilde{U}\widetilde{|T|} = U'U((U')^*U')|T|(U')^* = U'U|T|(U')^* = U'T(U')^* = T,$$

where the third equality is the polar decomposition of T and the last equality is the fact that T is affiliated with M. It follows, therefore, from the uniqueness of the polar decomposition that $\widetilde{U} = U$ and $\widetilde{|T|} = |T|$. Or equivalently, $U'U(U')^* = U$ and $U'|T|(U')^* = |T|$. Note M' is a C^*-algebra. So in particular, the unitaries linearly span M'. Now since U commutes with U', U commutes with all elements in M' as $U' \in M'$ was arbitrary. Hence, $U \in M'' = M$.

Now let E be the resolution of the identity for $|T|$. Then $\widetilde{E}(\cdot) := U'E(\cdot)(U')^*$ defines a spectral measure on the Borel sets of $\sigma(|T|)$: First note that for all Borel sets $A \subseteq \sigma(|T|)$, $\widetilde{E}(A)$ is a projection because $E(A)$ is projection. Clearly, $\widetilde{E}(\emptyset) = 0$ and $\widetilde{E}(\sigma(|T|)) = 1$. And, $\widetilde{E}(A_1 \cap A_2) = U'E(A_1 \cap A_2)(U')^* = U'E(A_1)E(A_2)(U')^* = U'E(A_1)(U')^*U'E(A_2)(U')^* = \widetilde{E}(A_1)\widetilde{E}(A_2)$ for Borel sets $A_1, A_2 \subseteq \sigma(|T|)$. Moreover, if $(A_i)_{i=1}^{\infty} \subseteq \sigma(|T|)$ are pairwise disjoint Borel sets, then

$\widetilde{E}(\bigcup_{i=1}^{\infty} A_i) = U'E(\bigcup_{i=1}^{\infty} A_i)(U')^* = \sum_{i=1}^{\infty} U'E(A_i)(U')^* = \sum_{i=1}^{\infty} \widetilde{E}(A_i)$ where the convergence is in the strong operator topology (SOT).

Let $\xi, \eta \in H$ and $A \subseteq \sigma(|T|)$ be a Borel set, then

$$E_{(U')^*\xi,(U')^*\eta}(A) = \langle E(A)(U')^*\xi, (U')^*\eta\rangle = \langle U'E(A)(U')^*\xi, \eta\rangle = \widetilde{E}_{\xi,\eta}(A)$$

so that $E_{(U')^*\xi,(U')^*\eta} = \widetilde{E}_{\xi,\eta}$. But then, using this, it follows that

$$\langle U'(\textstyle\int zdE)(U')^*\xi, \eta\rangle = \langle(\textstyle\int zdE)(U')^*\xi, (U')^*\eta\rangle = \displaystyle\int_{\sigma(|T|)} z\, dE_{(U')^*\xi,(U')^*\eta}(z) = \int_{\sigma(|T|)} z\, d\widetilde{E}_{\xi,\eta}(z)$$

which implies that $U'(\int zdE)(U')^* = \int zd\widetilde{E}$. Consequently, by the spectral decomposition for $|T|$ and the fact that $U'|T|(U')^* = |T|$, we obtain

$$|T| = U'|T|(U')^* = U'\Big(\int z\, dE\Big)(U')^* = \int z\, d\widetilde{E}.$$

This implies that $E = \widetilde{E}$ by the uniqueness of the resolution of the identity for $|T|$. Hence, $E(A) = U'E(A)(U')^*$ for all Borel sets $A \subseteq \sigma(|T|)$. Using the same argument to deduce that U lies in M, we also see that the spectral projections of $|T|$ lie in $M'' = M$. □

Theorem 3.2.15. *S_0 and F_0 are closable with closures, say, S and F respectively such that $S^* = F$ and $F^* = S$.*

Proof. Due to Remark 3.2.12, it is sufficient to show that $S^* \subseteq F$ and $F^* \subseteq S$. But to prove this theorem it will actually be enough to show that $F^* \subseteq S$ because then $F^* = S$ which implies $F = F^{**} = S^*$.

So let $\xi \in D(F^*)$ and $\eta := F^*\xi$. Then $\langle F\sigma, \xi\rangle = \overline{\langle \sigma, \eta\rangle}$ for all $\sigma \in D(F)$ by definition. Consequently, using the definition of F, $\langle (a')^*\xi_0, \xi\rangle = \overline{\langle a'\xi_0, \eta\rangle}$ for all $a' \in M'$. Define the densely defined operators $a, b : M'\xi_0 \to H$ by $a(x'\xi_0) = x'\xi$ and $b(y'\xi_0) = y'\eta$. In particular, $a\xi_0 = \xi$ and $b\xi_0 = \eta$. It follows that for all $x', y' \in M'$,

$$\langle a(x'\xi_0), y'\xi_0'\rangle = \langle x'\xi, y'\xi_0\rangle = \langle \xi, (x')^*y'\xi_0\rangle = \langle ((x')^*y')^*\xi_0, \eta\rangle = \langle x'\xi_0, y'\eta\rangle = \langle x'\xi_0, b(y'\xi_0)\rangle$$

where the third equality is that $\langle (a')^*\xi_0, \xi\rangle = \overline{\langle a'\xi_0, \eta\rangle}$ for all $a' \in M'$. This implies that $b \subseteq a^*$ and $a \subseteq b^*$. In particular, a^* and b^* are densely defined which implies that a and b are closable by Proposition 3.2.11. Let $c := \overline{a}$ be the closure of a, then $c\xi_0 = \xi$. Additionally, $c^* = a^* \supseteq b$ such that $c^*\xi_0 = b\xi_0 = \eta$.

Now let $u' \in M'$ be an arbitrary unitary operator. Note that $u'(D(a)) \subseteq D(a)$ such that $D(a) \subseteq D(u'a(u')^*)$. But also, if $\zeta \in D(u'a(u')^*)$, then $(u')^*\zeta \in D(a)$ and it follows that $\zeta = u'((u')^*\zeta) \in D(a)$. Hence, $D(a) = D(u'a(u')^*)$. Moreover, for all $x' \in M'$,

$$u'a(u')^*x'\xi_0 = u'(u')^*x'\xi = x'\xi = a(x'\xi_0)$$

and this, together with the equality of domains, implies that $u'a(u')^* = a$. Hence, a is affiliated with M. But then also, $u'\overline{a}(u')^* = \overline{a}$, so c is also affiliated with M.

Let $c = u|c|$ be the (unbounded) polar decomposition for c. Then u and the spectral projections of $|c|$ lie in M by Lemma 3.2.14, i.e. u, $1_{[0,n]}(|c|) \in M$. It follows that $f(|c|) \in M$ for every bounded Borel function f on $[0, \infty)$ because bounded Borel functions can be uniformly approximated by simple functions, the fact that $\|f(|c|)\| \leq \|f\|_\infty$ and M is norm closed. Also note that u is isometric on the closure of the range of $|c|$. Define the bounded Borel functions $f_n : [0,\infty) \to \mathbb{R}$ by $f_n(t) = t1_{[0,n]}(t)$ for $n \in \mathbb{N}$ and let $c_n := uf_n(|c|) \in M$. Then

$$\begin{aligned}\|\xi - c_n\xi_0\| &= \|(c - c_n)\xi_0\| \\ &= \|(u|c| - uf_n(|c|))\xi_0\| \\ &= \|(|c| - f_n(|c|))\xi_0\| \\ &= \|(1 - 1_{[0,n]}(|c|))|c|\xi_0\| \to 0, \quad \text{as } n \to \infty.\end{aligned}$$

since $1_{[0,n]}(|c|) \to 1$ as $n \to \infty$ in the strong operator topology by Theorem 4.1.2. in [16]. Similarly,

$$\begin{aligned}\|\eta - c_n^*\xi_0\| &= \|(c^* - c_n^*)\xi_0\| \\ &= \|(|c|u^* - f_n(|c|)u^*)\xi_0\| \\ &= \|(|c| - f_n(|c|))u^*\xi_0\| \\ &= \|(1 - 1_{[0,n]}(|c|))|c|u^*\xi_0\| \to 0, \quad \text{as } n \to \infty.\end{aligned}$$

Thus, $(\xi,\eta) \in \overline{\mathrm{G}(S_0)} = \mathrm{G}(S)$ as $\mathrm{G}(S_0) = \{(a\xi_0, a^*\xi_0) : a \in M\}$ and with that we have shown that $F^* \subseteq S$. □

Theorem 3.2.16 (Tomita-Takesaki)**.** *Let $\Delta := S^*S = FS$ be the modular operator with $S := \overline{S_0}$ and $F := \overline{F_0}$. Then Δ is positive, self adjoint and injective, and $\Delta^{-1} = SS^* = SF$. Let $S = J\Delta^{\frac{1}{2}} = \Delta^{-\frac{1}{2}}J$ be the left and right polar decomposition of S. Then:*

1. *$J^2 = I$;*
2. *J is a conjugate linear isometry ("unitary");*
3. *$JMJ = M$';*
4. *$\Delta^{it}M\Delta^{-it} = M$ for all $t \in \mathbb{R}$.*

Proof. Theorem VI.1.19 in [26] □

The operator J in Theorem 3.2.16 is often called the *modular conjugation.* Also note, as a consequence of this theorem, that the map

$$\sigma_t : M \to M, \quad a \mapsto \Delta^{it}a\Delta^{-it}$$

defines a $*$-automorphism on M for each $t \in \mathbb{R}$. And it is clear that $\sigma_{t+s} = \sigma_t\sigma_s$ for all $t, s \in \mathbb{R}$ by the properties of the functional calculus. Therefore, $(\sigma_t)_{t\in\mathbb{R}}$ is a *one parameter group of automorphisms* on M. In addition, $(\sigma_t)_{t\in\mathbb{R}}$ is pointwise strongly continuous which will be shown in the next proposition.

Definition 3.2.17. Let M be a σ-finite von Neumann algebra. Let ϕ be a faithful normal state on M and identify M with the von Neumann algebra $\pi_\phi(M) \subseteq B(H_\phi)$ where (H_ϕ, π_ϕ) is the GNS representation of M associated to ϕ. Let Δ be the corresponding modular operator. The one parameter group of $*$-automorphisms $(\sigma_t^\phi)_{t\in\mathbb{R}}$ on M defined by $\sigma_t^\phi(a) = \Delta^{it}a\Delta^{-it}$ is called the *modular automorphism group* associated with ϕ.

If the dependence on ϕ is clear, we may write $\sigma_t = \sigma_t^\phi$.

Proposition 3.2.18. *The modular automorphism group $(\sigma_t)_{t\in\mathbb{R}}$ on a (σ-finite) von Neumann algebra M is pointwise strongly continuous, i.e. $t \mapsto \sigma_t(a)$ is strongly continuous for a fixed $a \in M$.*

Proof. Fix $a \in M$. Let $\xi \in H$ and let E be the resolution of the identity for Δ. Note that $|x^{is} - x^{it}|^2 \leq 4$ for all $x, s, t \in \mathbb{R}$. Moreover, $\int_{\sigma(\Delta)} 4 \, dE_{\xi,\xi}(x) = 4E_{\xi,\xi}(\sigma(\Delta)) = 4\|\xi\|^2 < \infty$. So, by the Dominated Convergence Theorem,

$$\lim_{t\to s} \|(\Delta^{is} - \Delta^{it})\xi\|^2 = \lim_{t\to s} \int_{\sigma(\Delta)} |x^{is} - x^{it}|^2 \, dE_{\xi,\xi}(x) = 0.$$

And, similarly, $\lim_{t\to s} \|(\Delta^{-is} - \Delta^{-it})\xi\|^2 = 0$. Hence, the maps

$$\begin{aligned} \mathbb{R} &\to (B(H), \text{ SOT}), & \mathbb{R} &\to (B(H), \text{ SOT}), \\ t &\mapsto \Delta^{it}; & t &\mapsto \Delta^{-it} \end{aligned}$$

are continuous. But then, using the fact that Δ^{it} is unitary for all $t \in \mathbb{R}$ and therefore $\|\Delta^{it}\| = 1$, we obtain

$$\begin{aligned} \lim_{t\to s} \|(\sigma_s(a) - \sigma_t(a))\xi\| &= \lim_{t\to s} \|(\Delta^{is} a \Delta^{-is} - \Delta^{it} a \Delta^{-it})\xi\| \\ &\leq \lim_{t\to s} \|(\Delta^{is} - \Delta^{it}) a \Delta^{-is}\xi\| + \lim_{t\to s} \|\Delta^{it} a (\Delta^{-is} - \Delta^{-it})\xi\| \\ &\leq \lim_{t\to s} \|(\Delta^{is} - \Delta^{it}) a \Delta^{-is}\xi\| + \|a\| \lim_{t\to s} \|(\Delta^{-is} - \Delta^{-it})\xi\| \\ &= 0. \end{aligned}$$

□

3.3 Tomita-Takesaki for $M_n(\mathbb{C})$

Let ϕ be a faithful normal state on $M_n(\mathbb{C})$. Then there exists a unique invertible *density matrix* $h \in M_n(\mathbb{C})$ (a density matrix is a positive operator with trace equal to 1) such that $\phi(x) = \mathrm{Tr}(xh)$ for all $x \in M_n(\mathbb{C})$. Without loss of generality we may assume that h is a diagonal matrix with positive diagonal entries such that $\mathrm{Tr}(h) = 1$ by changing to an appropriate basis. Let (H_ϕ, π_ϕ) be the GNS representation of $M_n(\mathbb{C})$ associated with ϕ. In particular, $H_\phi = M_n(\mathbb{C})$ equipped with the inner product $\langle x, y\rangle = \phi(y^*x)$ for $x, y \in M_n(\mathbb{C})$. Note that this inner product is well-defined as ϕ is faithful and that completion is not needed since $M_n(\mathbb{C})$ is finite-dimensional. Moreover, $\pi_\phi : M_n(\mathbb{C}) \to B(H_\phi)$ is defined by $\pi_\phi(x)y = xy$. It is clear that $1_{H_\phi} \in H_\phi$ is the cyclic and separating vector for $\pi_\phi(M)$.

It is important to note that the theory of Tomita-Takesaki does not work on $M_n(\mathbb{C}) \cong B(\mathbb{C}^n)$ for $n \geq 2$. Suppose on the contrary that it does work on $B(\mathbb{C}^n)$, then we would obtain

$$n^2 = \dim(JB(\mathbb{C}^n)J) = \dim(B(\mathbb{C}^n)') = \dim(\mathbb{C}\mathrm{id}_{\mathbb{C}^n}) = 1$$

by Theorem 3.2.16 which is of course a contradiction. It is necessary to proceed on the image of the GNS representation $\pi_\phi(M_n(\mathbb{C})) \subseteq B(H_\phi)$ (which we have always implicitly done in the preceding sections!).

Theorem 3.3.1. *Let $\phi(\cdot) = \mathrm{Tr}(\cdot h)$ be a faithful normal state on $M_n(\mathbb{C})$ with $h \in M_n(\mathbb{C})$ an invertible density matrix. Let $(H_\phi, \pi_\phi, 1_{H_\phi})$ be the GNS representation of $M_n(\mathbb{C})$ associated with ϕ. Then the modular operator, the modular conjugation and the modular automorphism group are respectively given by:*

1. $\Delta : H_\phi \to H_\phi,\ \ \Delta(x) = hxh^{-1}$*;*

2. $J : H_\phi \to H_\phi,\ \ J(x) = h^{\frac{1}{2}}x^*h^{-\frac{1}{2}}$*;*

3. $\sigma_t^\phi : \pi_\phi(M_n(\mathbb{C})) \to \pi_\phi(M_n(\mathbb{C})),\ \ \sigma_t^\phi(\pi_\phi(x)) = \pi_\phi(h^{it}xh^{-it})$ *for* $x \in M_n(\mathbb{C})$*.*

Proof. First of all, we can assume that $h = \mathrm{diag}(\lambda_1, ..., \lambda_n)$ with $\lambda_i > 0$ for $i = 1, ..., n$ by changing to an appropriate basis. Note that $\pi_\phi(M_n(\mathbb{C}))1_{H_\phi} = H_\phi$ such that $S : H_\phi \to H_\phi$ is defined by $S(x) = x^*$. Consequently, for all $x, y \in H_\phi$,

$$\begin{aligned}\langle S^*S(x), y\rangle &= \langle S(y), S(x)\rangle = \langle y^*, x^*\rangle = \phi(xy^*)\\ &= \mathrm{Tr}(xy^*h) = \mathrm{Tr}(y^*hx) = \mathrm{Tr}(y^*hxh^{-1}h)\\ &= \phi(y^*hxh^{-1}) = \langle hxh^{-1}, y\rangle.\end{aligned}$$

Hence, $\Delta(x) = S^*S(x) = hxh^{-1}$ for all $x \in H_\phi$.

Now let $(E_{k,l})_{1\leq k,l\leq n}$ be the matrix units of H_ϕ. Then for all $k, l \in \{1, ..., n\}$ we obtain

$$\Delta(E_{k,l}) = hE_{k,l}h^{-1} = \lambda_k\lambda_l^{-1}E_{k,l},$$

which implies that $E_{k,l}$ is an eigenvector of Δ with eigenvalue $\lambda_k\lambda_l^{-1}$. Therefore, $f(\Delta)E_{k,l} = f(\lambda_k\lambda_l^{-1})E_{k,l}$ for all $f \in C(\sigma(\Delta))$ by the continuous functional calculus. In particular, using the fact that h is a diagonal matrix,

$$\begin{aligned}&\Delta^{it}E_{k,l} = (\lambda_k\lambda_l^{-1})^{it}E_{k,l} = \lambda_k^{it}\lambda_l^{-it}E_{k,l} = h^{it}E_{k,l}h^{-it} \quad \text{and similarly,}\\ &\Delta^{-it}E_{k,l} = h^{-it}E_{k,l}h^{it},\\ &\Delta^{\frac{1}{2}}E_{k,l} = h^{\frac{1}{2}}E_{k,l}h^{-\frac{1}{2}}.\end{aligned}$$

Then, by linearity, $\Delta^{it}(x) = h^{it}xh^{-it}$, $\Delta^{-it}(x) = h^{-it}xh^{it}$ and $\Delta^{\frac{1}{2}}x = h^{\frac{1}{2}}xh^{-\frac{1}{2}}$ for all $x \in H_\phi$. It follows that the modular conjugation $J = \Delta^{\frac{1}{2}}S$ is given by

$$J(x) = \Delta^{\frac{1}{2}}Sx = \Delta^{\frac{1}{2}}x^* = h^{\frac{1}{2}}x^*h^{-\frac{1}{2}}$$

for all $x \in H_\phi$. In addition, for all $y \in H_\phi$,

$$\begin{aligned}\sigma_t^\phi(\pi_\phi(x))y &= \Delta^{it}\pi_\phi(x)(\Delta^{-it}y) = \Delta^{it}\pi_\phi(x)(h^{-it}yh^{it})\\ &= \Delta^{it}(xh^{-it}yh^{it}) = h^{it}xh^{-it}yh^{it}h^{-it} = h^{it}xh^{-it}y\\ &= \pi_\phi(h^{it}xh^{-it})y.\end{aligned}$$

So indeed, $\sigma_t^\phi(\pi_\phi(x)) = \pi_\phi(h^{it}xh^{-it})$ for all $x \in M_n(\mathbb{C})$. □

Remark 3.3.2. Note that $S_0 = S$ is bounded on H_ϕ as H_ϕ is finite dimensional. So it possible to invoke Theorem 3.2.9 to give a stronger statement than the one in Theorem 3.2.16.(4). Namely, $\Delta^\alpha\pi_\phi(M_n(\mathbb{C}))\Delta^{-\alpha} = \pi_\phi(M_n(\mathbb{C}))$ for all $\alpha \in \mathbb{C}$. However, $\pi_\phi(a) \mapsto \Delta^\alpha\pi_\phi(a)\Delta^{-\alpha}$ is not necessarily a $*$-automorphism on $\pi_\phi(M_n(\mathbb{C}))$ anymore. It is a $*$-automorphism if and only if $\Re(\alpha) = 0$.

Remark 3.3.3. The modular automorphism group σ_t^ϕ is defined on $\pi_\phi(M_n(\mathbb{C}))$. It is actually possible to define a 'new' modular automorphism group α_t^ϕ on $M_n(\mathbb{C})$ via $\alpha_t^\phi : M_n(\mathbb{C}) \to M_n(\mathbb{C})$, $\alpha_t^\phi(x) := \pi_\phi^{-1}(\sigma_t^\phi(\pi_\phi(x)))$. (This also works for the general theory of Tomita-Takesaki on σ-finite von Neumann algebras.) But then, $\alpha_t^\phi(x) = \pi_\phi^{-1}(\pi_\phi(h^{it}xh^{-it})) = h^{it}xh^{-it}$ for all $x \in M_n(\mathbb{C})$ by Theorem 3.3.1. Hence, without loss of generality, we may consider σ_t^ϕ on $M_n(\mathbb{C})$ defined by $\sigma_t^\phi(x) = h^{it}xh^{-it}$.

3.4 KMS state and Connes' Cocycle

We now continue with general von Neumann algebras again.

Definition 3.4.1. Let $t \mapsto \sigma_t$ be a pointwise strongly continuous one parameter group of automorphisms on a von Neumann algebra M. Let ϕ be a normal state on M. Then ϕ satisfies the *KMS*[1]*-condition* with respect to σ_t (or is called σ_t-*KMS*) if $\phi \circ \sigma_t = \phi$, and for all $x, y \in M$ there exists a bounded continuous function $F : \{z \in \mathbb{C} : 0 \leq \operatorname{Im}(z) \leq 1\} \to \mathbb{C}$, such that

1. F is analytic on $\{z \in \mathbb{C} : 0 < \operatorname{Im}(z) < 1\}$;
2. $F(t) = \phi(\sigma_t(x)y)$ for all $t \in \mathbb{R}$;
3. $F(t + i) = \phi(y\sigma_t(x))$ for all $t \in \mathbb{R}$.

Theorem 3.4.2. *Let M be a von Neumann algebra with a faithful normal state ϕ. Then:*

1. *ϕ is KMS with respect to the modular automorphism group σ_t^ϕ;*
2. *If ϕ is KMS with respect to a pointwise strongly continuous one parameter group of $*$-automorphisms σ_t, then $\sigma_t = \sigma_t^\phi$.*

Proof. We first prove 1. Let ξ_0 be the separating and cyclic vector for M from the GNS representation associated to ϕ where we identify M with its GNS image. First, note that $\Delta\xi_0 = FS\xi_0 = \xi_0$ by definition of S and F. In other words, ξ_0 is an eigenvector of Δ with eigenvalue 1. So ξ_0 is an eigenvector of Δ^{-it} with eigenvalue $1^{-it} = 1$ because if E is the resolution of the identity for Δ, then

$$\begin{aligned}
\|\Delta^{-it}\xi_0 - \xi_0\|^2 &= \int_{\sigma(\Delta)} |z^{-it} - 1|^2 \, dE_{\xi_0,\xi_0}(z) = \int_{\sigma(\Delta)\setminus\{1\}} |z^{-it} - 1|^2 \, dE_{\xi_0,\xi_0}(z) \\
&\leq 4E_{\xi_0,\xi_0}(\sigma(\Delta) \setminus \{1\}) = 4\langle E(\sigma(\Delta) \setminus \{1\}\xi_0, \xi_0\rangle \\
&= 4\langle E(\sigma(\Delta) \setminus \{1\})E(\{1\})\xi_0, \xi_0\rangle = 4\langle E(\emptyset)\xi_0, \xi_0\rangle \\
&= 0,
\end{aligned}$$

where we used the fact that $E(\{1\})$ is the projection onto $\ker(\Delta - I)$ and $\xi_0 \in \ker(\Delta - I)$. Consequently, for all $x \in M$,

$$\phi(\sigma_t^\phi(x)) = \langle \sigma_t^\phi(x)\xi_0, \xi_0\rangle = \langle \Delta^{it}x\Delta^{-it}\xi_0, \xi_0\rangle = \langle x\Delta^{-it}\xi_0, \Delta^{-it}\xi_0\rangle = \langle x\xi_0, x\xi_0\rangle = \phi(x).$$

Therefore, $\phi \circ \sigma_t^\phi = \phi$ for all $t \in \mathbb{R}$.

Now let $x, y \in M$. Then, using the fact that $\Delta^{-it}\xi_0 = \xi_0$ once again,

$$\phi(\sigma_t^\phi(x)y) = \langle \sigma_t^\phi(x)y\xi_0, \xi_0\rangle = \langle y\xi_0, \sigma_t^\phi(x^*)\xi_0\rangle = \langle y\xi_0, \Delta^{it}x^*\Delta^{-it}\xi_0\rangle = \langle y\xi_0, \Delta^{it}x^*\xi_0\rangle = \langle \Delta^{-it}y\xi_0, x^*\xi_0\rangle,$$

and, also using the polar decomposition $S = J\Delta^{\frac{1}{2}}$, we see that

$$\begin{aligned}
\phi(y\sigma_t^\phi(x)) &= \langle y\sigma_t^\phi(x)\xi_0, \xi_0\rangle = \langle \sigma_t^\phi(x)\xi_0, y^*\xi_0\rangle = \langle S\sigma_t^\phi(x^*)\xi_0, Sy\xi_0\rangle \\
&= \langle J\Delta^{\frac{1}{2}}\Delta^{it}x^*\Delta^{-it}\xi_0, J\Delta^{\frac{1}{2}}y\xi_0\rangle = \langle J\Delta^{\frac{1}{2}}\Delta^{it}x^*\xi_0, J\Delta^{\frac{1}{2}}y\xi_0\rangle \\
&= \langle \Delta^{\frac{1}{2}}y\xi_0, \Delta^{\frac{1}{2}+it}x^*\xi_0\rangle = \langle \Delta^{\frac{1}{2}-it}y\xi_0, \Delta^{\frac{1}{2}}x^*\xi_0\rangle.
\end{aligned}$$

[1] Kubo-Martin-Schwinger

Let $\xi := y\xi_0$ and $\eta := x^*\xi_0$ for convenience. Then

$$\phi(\sigma_t^\phi(x)y) = \langle \Delta^{-it}\xi, \eta\rangle \quad \text{and} \quad \phi(y\sigma_t^\phi(x)) = \langle \Delta^{\frac{1}{2}-it}\xi, \Delta^{\frac{1}{2}}\eta\rangle.$$

Define the Borel functions $f_n : [0,\infty) \to \mathbb{C}$ by $f_n(t) = t1_{[0,n]}(t)$ for $n \in \mathbb{N}$. Let $p_n := 1_{[\frac{1}{n},n]}(\Delta)$ be the spectral projections for Δ corresponding to the interval $\left[\frac{1}{n}, n\right]$. Now note that $f_n(\Delta)$ is bounded since f_n is bounded. In other words, Δ restricted to $p_n(H)$ is bounded and the same is true for Δ^{-1}. Hence, we can define entire functions $F_n : \mathbb{C} \to \mathbb{C}$ by $F_n(z) := \langle \Delta^{-iz}p_n\xi, \eta\rangle$ for $n \in \mathbb{N}$. It follows that $F_n(t) = \langle \Delta^{-it}p_n\xi, \eta\rangle$ and $F_n(t+i) = \langle \Delta^{1-it}p_n\xi, \eta\rangle = \langle \Delta^{\frac{1}{2}-it}p_n\xi, \Delta^{\frac{1}{2}}\eta\rangle$ for $t \in \mathbb{R}$. Hence, since $\|\Delta^{it}\| = 1$ for $t \in \mathbb{R}$, we obtain for all $t \in \mathbb{R}$:

$$\begin{aligned}|F_n(t) - \phi(\sigma_t^\phi(x)y)| &= |\langle \Delta^{-it}(p_n - 1)\xi, \eta\rangle| \leq \|(p_n - 1)\xi\|\|\eta\| \quad \text{and} \\ |F_n(t+i) - \phi(y\sigma_t^\phi(x))| &= |\langle \Delta^{\frac{1}{2}-it}(p_n - 1)\xi, \Delta^{\frac{1}{2}}\eta\rangle| \leq |\langle \Delta^{\frac{1}{2}}(p_n - 1)\xi, \Delta^{\frac{1}{2}}\eta\rangle| \\ &= |\langle (p_n - 1)\Delta^{\frac{1}{2}}\xi, \Delta^{\frac{1}{2}}\eta\rangle| \leq \|(p_n - 1)\Delta^{\frac{1}{2}}\xi\|\|\Delta^{\frac{1}{2}}\eta\|.\end{aligned}$$

This implies that $\lim_{n\to\infty} F_n(t) = \phi(\sigma_t^\phi(x)y)$ and $\lim_{n\to\infty} F_n(t+i) = \phi(y\sigma_t^\phi(x))$ uniformly for $t \in \mathbb{R}$ since $p_n \to 1$ strongly. So F_n converges uniformly on ∂S where $S := \{z \in \mathbb{C} : 0 \leq \mathrm{Im}(z) \leq 1\}$. By a maximal modulus argument (Phragmén-Lindelöf theorem) and completeness, it follows that F_n converges uniformly to a continuous bounded function F on S. Moreover, F is analytic in $\mathrm{int}(S)$ because F_n is analytic in $\mathrm{int}(S)$ for each $n \in \mathbb{N}$ and the convergence is uniform. Furthermore,

$$F(t) = \lim_{n\to\infty} F_n(t) = \phi(\sigma_t^\phi(x)y) \quad \text{and} \quad F(t+i) = \lim_{n\to\infty} F_n(t+i) = \phi(y\sigma_t^\phi(x)).$$

Therefore, ϕ is σ_t^ϕ-KMS.

The proof of statement 2 can be found in [26], Theorem VIII.1.2. □

If ϕ is a positive faithful normal functional, then S, F, J, Δ and σ_t^ϕ can be defined in the same way.

Lemma 3.4.3. *Let M be a von Neumann algebra with a positive faithful normal functional ϕ. Let $a \in M$. If $\phi(ax) = \phi(xa)$ for all $x \in M$, then $\sigma_t^\phi(a) = a$ for all $t \in \mathbb{R}$.*

Proof. Let ξ_0 be the separating and cyclic vector for M from the GNS representation associated to ϕ where we identify M with its GNS image. Suppose that $\phi(ax) = \phi(xa)$ for all $x \in M$. Then for all $x \in M$,

$$\begin{aligned}\langle S_0x\xi_0, a\xi_0\rangle = \langle x^*\xi_0, a\xi_0\rangle = \langle \xi_0, xa\xi_0\rangle = \overline{\phi(xa)} = \overline{\phi(ax)} \\ = \overline{\langle ax\xi_0, \xi_0\rangle} = \overline{\langle x\xi_0, a^*\xi_0\rangle} = \overline{\langle x\xi_0, S_0a\xi_0\rangle}.\end{aligned}$$

Using this and the fact that $S_0^* = S^* = F$, it follows that $a\xi_0 \in D(S_0^*) = D(F)$ and $Fa\xi_0 = S^*a\xi_0 = S_0^*a\xi_0 = S_0a\xi_0 = Sa\xi_0$. But $F = F^{-1}$, so $Sa\xi_0 = Fa\xi_0 \in D(F)$ and $\Delta a\xi_0 = FSa\xi_0 = F^2a\xi_0 = a\xi_0$. In other words, $a\xi_0$ is an eigenvector of Δ with eigenvalue 1. So $a\xi_0$ is an eigenvector of Δ^{it} with eigenvalue $1^{it} = 1$ by the same argument that was used in the proof of Theorem 3.4.2. The details are omitted for this case.

Moreover, we have already shown that $\Delta^{-it}\xi_0 = \xi_0$ in the proof of Theorem 3.4.2. It follows that

$$\sigma_t^\phi(a)\xi_0 = \Delta^{it}a\Delta^{-it}\xi_0 = \Delta^{it}a\xi_0 = a\xi_0,$$

and since ξ_0 is separating for M, we conclude that $\sigma_t^\phi(a) = a$ for all $t \in \mathbb{R}$. □

Let $M_2(M)$ denote the set of 2×2 matrices with entries in a von Neumann algebra M. Then $M_2(M)$ is a von Neumann algebra again. Let ϕ_1 and ϕ_2 be two positive faithful normal functionals on M. Define $\phi : M_2(M) \to \mathbb{C}$ by

$$\phi \begin{pmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{pmatrix} := \phi_1(x_{11}) + \phi_2(x_{22}).$$

Then ϕ is a positive faithful normal functional on $M_2(M)$ and Tomita-Takesaki theory also works for $M_2(M)$ with ϕ. Let $e := \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$, and let $x \in M_2(M)$. Then

$$\phi(ex) = \begin{pmatrix} x_{11} & x_{12} \\ 0 & 0 \end{pmatrix} = \phi_1(x_{11}) \quad \text{and} \quad \phi(xe) = \begin{pmatrix} x_{11} & 0 \\ x_{21} & 0 \end{pmatrix} = \phi_1(x_{11})$$

so that $\sigma_t^{\phi}(e) = e$ for all $t \in \mathbb{R}$ by Lemma 3.4.3. Using this, we can consider

$$\begin{aligned} \sigma_t^{\phi} \begin{pmatrix} x_{11} & 0 \\ 0 & 0 \end{pmatrix} &= \sigma_t^{\phi} \left(e \begin{pmatrix} x_{11} & 0 \\ 0 & 0 \end{pmatrix} e \right) = \sigma_t^{\phi}(e) \sigma_t^{\phi} \begin{pmatrix} x_{11} & 0 \\ 0 & 0 \end{pmatrix} \sigma_t^{\phi}(e) \\ &= e \sigma_t^{\phi} \begin{pmatrix} x_{11} & 0 \\ 0 & 0 \end{pmatrix} e = \begin{pmatrix} \alpha_t(x_{11}) & 0 \\ 0 & 0 \end{pmatrix}, \end{aligned}$$

and

$$\begin{aligned} \sigma_t^{\phi} \begin{pmatrix} 0 & x_{12} \\ 0 & 0 \end{pmatrix} &= \sigma_t^{\phi} \left(e \begin{pmatrix} 0 & x_{12} \\ 0 & 0 \end{pmatrix} (1-e) \right) = \sigma_t^{\phi}(e) \sigma_t^{\phi} \begin{pmatrix} 0 & x_{12} \\ 0 & 0 \end{pmatrix} \sigma_t^{\phi}(1-e) \\ &= e \sigma_t^{\phi} \begin{pmatrix} 0 & x_{12} \\ 0 & 0 \end{pmatrix} (1-e) = \begin{pmatrix} 0 & \beta_t(x_{12}) \\ 0 & 0 \end{pmatrix}. \end{aligned}$$

By similar computations and linearity, we get that $\sigma_t^{\phi} \begin{pmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{pmatrix} = \begin{pmatrix} \alpha_t(x_{11}) & \beta_t(x_{12}) \\ \gamma_t(x_{21}) & \delta_t(x_{22}) \end{pmatrix}$ for some $\alpha_t, \beta_t, \gamma_t, \delta_t \in B(M)$ (as $\sigma_t^{\phi}(x) \in M_2(M)$ for all $x \in M_2(M)$).

Lemma 3.4.4. *Following the above-mentioned computations, we have that*

$$\sigma_t^{\phi} \begin{pmatrix} x_{11} & 0 \\ 0 & x_{22} \end{pmatrix} = \begin{pmatrix} \sigma_t^{\phi_1}(x_{11}) & 0 \\ 0 & \sigma_t^{\phi_2}(x_{22}) \end{pmatrix}, \quad \textit{for all } t \in \mathbb{R} \textit{ and } x_{11}, x_{22} \in M$$

Proof. By symmetry, we can assume that $x_{22} = 0$. Since $\sigma_t^{\phi} \begin{pmatrix} x & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} \alpha_t(x) & 0 \\ 0 & 0 \end{pmatrix}$, it can be (easily) seen that α_t is a pointwise strongly continuous one parameter group of $*$-automorphisms on M as σ_t^{ϕ} is one on $M_2(M)$. Moreover, using Theorem 3.4.2, it will be sufficient to prove that ϕ_1 is KMS with respect to α_t. We check this. Let $x \in M$. Note ϕ is σ_t^{ϕ}-KMS by Theorem 3.4.2, in particular $\phi = \phi \circ \sigma_t^{\phi}$. It follows that $\phi_1(x) = \phi \begin{pmatrix} x & 0 \\ 0 & 0 \end{pmatrix} = \phi \circ \sigma_t^{\phi} \begin{pmatrix} x & 0 \\ 0 & 0 \end{pmatrix} = \phi \begin{pmatrix} \alpha_t(x) & 0 \\ 0 & 0 \end{pmatrix} = \phi_1(\alpha_t(x))$, i.e. $\phi_1 = \phi_1 \circ \alpha_t$.

Now let $x, y \in M$. Using the fact that ϕ is σ_t^{ϕ}-KMS once again, there exists a bounded continuous function $F : \{z \in \mathbb{C} : 0 \leq \mathrm{Im}(z) \leq 1\} \to \mathbb{C}$ which is analytic in $\{z \in \mathbb{C} : 0 < \mathrm{Im}(z) < 1\}$ such that $F(t) = \phi \left(\left(\sigma_t^{\phi} \begin{pmatrix} x & 0 \\ 0 & 0 \end{pmatrix} \right) \begin{pmatrix} y & 0 \\ 0 & 0 \end{pmatrix} \right)$ and $F(t+i) = \phi \left(\begin{pmatrix} y & 0 \\ 0 & 0 \end{pmatrix} \sigma_t^{\phi} \begin{pmatrix} x & 0 \\ 0 & 0 \end{pmatrix} \right)$ for all $t \in \mathbb{R}$. But now writing out the matrix multiplications, we obtain $F(t) = \phi(\alpha_t(x)y)$ and $F(t+i) = \phi(y\alpha_t(x))$ for all $t \in \mathbb{R}$. Hence, ϕ_1 is α_t-KMS which was sufficient to prove the lemma. $\square$

Lemma 3.4.5. *Define for $t \in \mathbb{R}$ the bounded operator $u_t \in M$ by $\begin{pmatrix} 0 & 0 \\ u_t & 0 \end{pmatrix} = \sigma_t^\phi \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$ (which is possible by the computations preceding Lemma 3.4.4). Then u_t is unitary for each $t \in \mathbb{R}$.*

Proof. Using the fact that σ_t^ϕ is a $*$-homomorphism and $\sigma_t^\phi(e) = e$,

$$\begin{aligned}
\begin{pmatrix} u_t^* u_t & 0 \\ 0 & 0 \end{pmatrix} &= \begin{pmatrix} 0 & u_t^* \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ u_t & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ u_t & 0 \end{pmatrix}^* \begin{pmatrix} 0 & 0 \\ u_t & 0 \end{pmatrix} \\
&= \left(\sigma_t^\phi \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \right)^* \sigma_t^\phi \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \sigma_t^\phi \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \sigma_t^\phi \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \\
&= \sigma_t^\phi \left(\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \right) = \sigma_t^\phi(e) = e = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}.
\end{aligned}$$

Now by a similar computation, we get that $\begin{pmatrix} 0 & 0 \\ 0 & u_t u_t^* \end{pmatrix} = \sigma_t^\phi(1-e) = 1 - e = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$. □

Proposition 3.4.6. *Let u_t be defined as in the previous lemma. Then the following two statements hold:*

1. *$u_{s+t} = u_s \sigma_s^{\phi_1}(u_t)$ for all $s, t \in \mathbb{R}$;*
2. *$\sigma_t^{\phi_2}(x) = u_t \sigma_t^{\phi_1} u_t^*(x)$ for all $t \in \mathbb{R}$ and all $x \in M$.*

Proof. Using the definition of u_t, Lemma 3.4.4 and the fact that σ_t^ϕ is a one parameter group of $*$-automorphisms, we see that

$$\begin{aligned}
\begin{pmatrix} 0 & 0 \\ u_{s+t} & 0 \end{pmatrix} &= \sigma_{s+t}^\phi \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \sigma_s^\phi \sigma_t^\phi \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \sigma_s^\phi \begin{pmatrix} 0 & 0 \\ u_t & 0 \end{pmatrix} \\
&= \sigma_s^\phi \left(\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} u_t & 0 \\ 0 & 0 \end{pmatrix} \right) = \sigma_s^\phi \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \sigma_s^\phi \begin{pmatrix} u_t & 0 \\ 0 & 0 \end{pmatrix} \\
&= \begin{pmatrix} 0 & 0 \\ u_s & 0 \end{pmatrix} \begin{pmatrix} \sigma_s^{\phi_1}(u_t) & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ u_s \sigma_s^{\phi_1}(u_t) & 0 \end{pmatrix},
\end{aligned}$$

which shows statement 1. Now we show statement 2:

$$\begin{aligned}
\begin{pmatrix} 0 & 0 \\ 0 & \sigma_t^{\phi_2}(x) \end{pmatrix} &= \sigma_t^\phi \begin{pmatrix} 0 & 0 \\ 0 & x \end{pmatrix} = \sigma_t^\phi \left(\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} x & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \right) \\
&= \sigma_t^\phi \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \sigma_t^\phi \begin{pmatrix} x & 0 \\ 0 & 0 \end{pmatrix} \left(\sigma_t^\phi \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \right)^* \\
&= \begin{pmatrix} 0 & 0 \\ u_t & 0 \end{pmatrix} \begin{pmatrix} \sigma_s^{\phi_1}(x) & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & u_t^* \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & u_t \sigma_t^{\phi_1} u_t^*(x) \end{pmatrix}.
\end{aligned}$$

□

Definition 3.4.7. Let M be a von Neumann algebra with two positive faithful normal functionals ϕ_1 and ϕ_2 on M. Define a positive faithful normal functional ϕ on $M_2(M)$ by

$$\phi \begin{pmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{pmatrix} := \phi_1(x_{11}) + \phi_2(x_{22}).$$

Then $(D\phi_2 : D\phi_1)_t := u_t \in M$ defined by $\begin{pmatrix} 0 & 0 \\ u_t & 0 \end{pmatrix} = \sigma_t^{\phi} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$ is called *Connes' cocycle Radon-Nikodym derivative.*

Obviously, a Connes' cocycle Radon-Nikodym derivative $(D\phi_2 : D\phi_1)_t$ is unitary for each $t \in \mathbb{R}$ and satisfies the properties in Proposition 3.4.6.

Example 3.4.8. Let $M = M_n(\mathbb{C})$ and let ϕ_1 and ϕ_2 be two positive faithful normal functionals on M. Then there exist unique invertible positive matrices $h_1, h_2 \in M_n(\mathbb{C})$ such that $\phi_j(\cdot) = \mathrm{Tr}(\cdot h_j)$ and we have $\sigma_t^{\phi_j}(x) = h_j^{it} x h_j^{-it}$ for $j = 1, 2$ by Theorem 3.3.1 (and Remark 3.3.3). Define a positive faithful normal functional ϕ on $M_2(M) \cong M_{2n}(\mathbb{C})$ by

$$\phi \begin{pmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{pmatrix} := \phi_1(x_{11}) + \phi_2(x_{22}), \quad \text{with } x_{ij} \in M_n(\mathbb{C}).$$

Then for all $x = \begin{pmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{pmatrix} \in M_{2n}(\mathbb{C})$ with $x_{ij} \in M_n(\mathbb{C})$, we have

$$\phi(x) = \phi_1(x_{11}) + \phi_2(x_{22}) = \mathrm{Tr}(x_{11}h_1) + \mathrm{Tr}(x_{22}h_2) = \mathrm{Tr} \begin{pmatrix} x_{11}h_1 & 0 \\ 0 & x_{22}h_2 \end{pmatrix} = \mathrm{Tr}(xh)$$

where $h := \begin{pmatrix} h_1 & 0 \\ 0 & h_2 \end{pmatrix}$. It follows that the modular automorphism group associated with ϕ is given by $\sigma_t^{\phi}(x) = h^{it} x h^{-it}$ for $x \in M_{2n}(\mathbb{C})$. But then,

$$\begin{aligned} \begin{pmatrix} 0 & 0 \\ u_t & 0 \end{pmatrix} = \sigma_t^{\phi} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} &= \begin{pmatrix} h_1 & 0 \\ 0 & h_2 \end{pmatrix}^{it} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} h_1 & 0 \\ 0 & h_2 \end{pmatrix}^{-it} \\ &= \begin{pmatrix} h_1^{it} & 0 \\ 0 & h_2^{it} \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} h_1^{-it} & 0 \\ 0 & h_2^{-it} \end{pmatrix} \\ &= \begin{pmatrix} 0 & 0 \\ h_2^{it} h_1^{-it} & 0 \end{pmatrix}, \end{aligned}$$

i.e. $(D\phi_2 : D\phi_1)_t = h_2^{it} h_1^{-it}$ is the Connes' cocycle Radon-Nikodym derivative.

4 Quantum Markov semigroups and their generators

Before we give the definition of a quantum Markov semigroup and analyze their generator, a (short) introduction on completely positive maps is necessary. It turns out that positive maps are not sufficient to have a physical interpretation and we must demand the stronger property of complete positivity. The focus in this section will be on *uniformly continuous* quantum Markov semigroups and particular emphasis is put on such semigroups with *detailed balance*.

4.1 Completely positive maps

Let A be a C^*-algebra. Then $M_n(A)$, the $*$-algebra of all $n \times n$ matrices with entries in A, admits a unique norm making it a C^*-algebra. If $\Phi : A \to B$ is a linear map between C^*-algebras, then for $n \in \mathbb{N}_{\geq 1}$ define the extensions $\Phi^{(n)} : M_n(A) \to M_n(B)$ through

$$\Phi^{(n)} : \begin{pmatrix} a_{11} & \dots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{n1} & \dots & a_{nn} \end{pmatrix} \mapsto \begin{pmatrix} \Phi(a_{11}) & \dots & \Phi(a_{1n}) \\ \vdots & \ddots & \vdots \\ \Phi(a_{n1}) & \dots & \Phi(a_{nn}) \end{pmatrix}.$$

In other words, if $M_n(A)$ is identified with $M_n(\mathbb{C}) \otimes A$ and $M_n(B)$ with $M_n(\mathbb{C}) \otimes B$, then

$$\Phi^{(n)} = \mathrm{id}_n \otimes \Phi : M_n(\mathbb{C}) \otimes A \to M_n(\mathbb{C}) \otimes B.$$

Definition 4.1.1. A linear map $\Phi : A \to B$ between C^*-algebras is said to be *completely positive* if $\Phi^{(n)}$ is positive for all $n \geq 1$.

Let $\Phi : A \to B$ be completely positive. Then it follows immediately from the definition that $\Phi^{(n)} : M_n(A) \to M_n(B)$ is completely positive for all $n \in \mathbb{N}$. Moreover, $\Phi^{(n)}(a)^* = \Phi^{(n)}(a^*)$ for all $a \in A$ and $n \in \mathbb{N}$ since

$$\begin{aligned} \Phi^{(n)}(a)^* &= \Phi^{(n)}(\Re(a) + i\Im(a))^* = \Phi^{(n)}(\Re(a)^+ - \Re(a)^- + i\Im(a)^+ - i\Im(a)^-)^* \\ &= \Phi^{(n)}(\Re(a)^+)^* - \Phi^{(n)}(\Re(a)^-)^* - i\Phi^{(n)}(\Im(a)^+)^* + i\Phi^{(n)}(\Im(a)^-)^* \\ &= \Phi^{(n)}(\Re(a)^+) - \Phi^{(n)}(\Re(a)^-) - i\Phi^{(n)}(\Im(a)^+) + i\Phi^{(n)}(\Im(a)^-) \\ &= \Phi^{(n)}(\Re(a) - i\Im(a)) = \Phi^{(n)}(a^*) \end{aligned}$$

where the third equality is the fact that $\Phi^{(n)}$ is positive.

Remark 4.1.2. Suppose now only that $\Phi : A \to B$ is a linear map between C*-algebras and there exists $M > 0$ such that $\|\Phi(a)\| \leq M$ for all $a \in A^+ \cap A_{\leq 1}$. Then Φ is bounded with norm $\|\Phi\| \leq 4M$. We show this: First assume that $a \in A_{sa}$ such that $\|a\| \leq 1$. Then also, a^+, a^- are positive elements of the closed unit ball of A, and therefore $\|\Phi(a)\| = \|\Phi(a^+) - \Phi(a^-)\| \leq \|\Phi(a^+)\| + \|\Phi(a^-)\| \leq 2M$. Now let $a \in A_{\leq 1}$ arbitrary, then write $a = b + ic$ with $b, c \in A_{sa}$. Note that $\|b\|, \|c\| \leq 1$. Then we obtain $\|\Phi(a)\| \leq \|\Phi(b)\| + \|\Phi(c)\| \leq 2M + 2M = 4M$. Thus, Φ is bounded with $\|\Phi\| \leq 4M$.

Proposition 4.1.3. *If $\Phi : A \to B$ is a positive linear map between C^*-algebras, then it is bounded.*

Proof. Suppose Φ is not bounded. Then by the preceding remark $\sup_{a \in S} \|\Phi(a)\| = \infty$, where S is the set of all positive elements of A of norm not greater than 1. Therefore, we can find a sequence $(a_n)_{n \geq 1} \subseteq S$ such that $4^n \leq \|\Phi(a_n)\|$ for all $n \in \mathbb{N}$. Define $a := \sum_{n \geq 1} 2^{-n} a_n \in A$. Note that a is indeed an element of A because the sum is absolutely convergent and A is a Banach space. But now, for all $n \in \mathbb{N}$, we obtain $a - 2^{-n}a_n = \sum_{\substack{j\geq 1\\ j\neq n}} 2^{-j}a_j \geq 0$ because $2^{-j}a_j \geq 0$, the sum of positive elements is a positive element and using the fact that A^+ is norm closed in A. But then, $\Phi(a) \geq 2^{-n}\Phi(a_n) \geq 0$ for all $n \in \mathbb{N}$ as Φ is positive. Consequently, $\|\Phi(a)\| \geq 2^{-n}\|\Phi(a_n)\| \geq 2^{-n} \cdot 4^n = 2^n$ for all $n \in \mathbb{N}$ by Theorem 2.2.5(3) in [16]. This is a contradiction since $\|\Phi(a)\| < \infty$ and we conclude that Φ is bounded. □

Remark 4.1.4. Let $\Phi : A \to B$ be a completely positive map between unital C^*-algebras. There is actually an easier way to show that Φ is bounded with $\|\Phi\| = \|\Phi(1)\|$ using the *Kadison-Schwarz inequality*: $\Phi(a)^*\Phi(a) \leq \|\Phi(1)\|\Phi(a^*a)$ for all $a \in A$. We show this: Let $a \in A$. Then the inequality $a^*a \leq \|a^*a\|1$ follows from the Gelfand duality applied to the commutative C^*-algebra generated by 1 and a^*a. Hence, $\|\Phi(a)\|^2 = \|\Phi(a)^*\Phi(a)\| \leq \|\Phi(1)\|\|\Phi(a^*a)\| \leq \|\Phi(1)\|^2\|a^*a\| = \|\Phi(1)\|^2\|a\|^2$ where we repeatedly used Theorem 2.2.5(3) in [16], the Kadison-Schwarz inequality and the fact that Φ is positive. But then, Φ is bounded with $\|\Phi\| \leq \|\Phi(1)\|$ which directly implies that $\|\Phi\| = \|\Phi(1)\|$.

There exists a canonical decomposition of completely positive maps due to Stinespring.

Theorem 4.1.5 (Stinespring)**.** *Let A and $B \subseteq B(H)$ be unital C^*-algebras. Then $\Phi : A \to B$ is completely positive if and only if there is a representation $\pi : A \to B(K)$ for some Hilbert space K and a bounded linear map $V : H \to K$ such that*

$$\Phi(a) = V^*\pi(a)V \quad \textit{for all } a \in A.$$

Moreover, $\|V\|^2 \leq \|\Phi\|$.

Proof. Theorem 1 in [23]. □

If $A = B(H)$, then there exists another decomposition which is called the *Kraus decomposition* or *Choi canonical form* on the condition that the completely positive map is also σ-weakly continuous.

Theorem 4.1.6 (Kraus)**.** *$\Phi : B(H) \to B(H)$ is σ-weakly continuous (normal) and completely positive if and only if there exists a family of operators $(a_i) \subseteq B(H)$ such that*

$$\Phi(x) = \sum_i a_i^* x a_i \quad \textit{for all } x \in B(H),$$

and the series $\sum_i a_i^* x a_i$ converges in strong operator topology.

Proof. Theorem 3.3 in [13]. □

4.2 Generators of uniformly continuous quantum Markov semigroups

Firstly, we state the definition of a general quantum Markov semigroup (QMS).

Definition 4.2.1. Let $M \subseteq B(H)$ be a von Neumann algebra. A *quantum Markov semigroup (QMS)* is a one parameter family $(\Phi_t)_{t\geq 0}$ of linear maps of M into itself satisfying the following five properties:

(a) Φ_t is completely positive for all $t \geq 0$;

(b) $\Phi_t(\mathrm{id}_H) = \mathrm{id}_H$ for all $t \geq 0$;

(c) $\Phi_{s+t} = \Phi_s\Phi_t$ for all $s, t \geq 0$;

(d) $\lim_{t\downarrow 0} \Phi_t(x) = x$ in the σ-weak topology for all $x \in M$;

(e) Φ_t is σ-weakly continuous (normal) for all $t \geq 0$.

The *infinitesimal generator*, or briefly *generator*, of $(\Phi_t)_{t\geq 0}$ is the (generally unbounded) linear operator L with domain $D(L) \subseteq M$ defined by

$$D(L) = \left\{ x \in M : (\sigma\text{-weak})\text{-}\lim_{t\downarrow 0} t^{-1}(\Phi_t(x) - x) \text{ exists} \right\};$$

$$L(x) = \lim_{t\downarrow 0} \frac{\Phi_t(x) - x}{t}, \ x \in D(L) \text{ with the limit taken in the } \sigma\text{-weak topology.}$$

The usual assumption that Φ_0 is the identity for (semi)groups is in fact redundant as it follows from the other properties: $\Phi_0(x) = \Phi_0(\lim_{t\downarrow 0} \Phi_t(x)) = \lim_{t\downarrow 0} \Phi_0(\Phi_t(x)) = \lim_{t\downarrow 0} \Phi_t(x) = x$ for all $x \in M$ where the limits are taken in the σ-weak sense. The first equality is property (d), the second equality is property (e), the third equality is property (c) and the fourth equality is property (d) again. Hence, $\Phi_0 = \mathrm{id}_M$.

The purpose of this subsection is to derive an explicit form for the generator of a quantum Markov semigroup that is *uniformly/norm continuous*, i.e. $\lim_{t\downarrow 0} \|\Phi_t - \mathrm{id}_M\| = 0$. This is a condition which is *not* fulfilled in many applications. Nevertheless, a QMS defined on a finite dimensional C^*-algebra is always uniformly continuous since its generator is bounded. The main result of this subsection is Corollary 4.2.10 and is due to the works of Lindblad [14].
So let $(\Phi_t)_{t\geq 0}$ be a uniformly continuous QMS on a von Neumann algebra M. Then there exists a unique bounded linear operator $L : M \to M$ such that

$$\Phi_t = e^{tL}, \ t \geq 0 \quad \text{and} \quad \lim_{t\downarrow 0} \|L - t^{-1}(\Phi_t - \mathrm{id}_M)\| = 0,$$

with L the generator of $(\Phi_t)_{t\geq 0}$ by Corollary 1.4 in [19]. Now, from the fact that the set of σ-weakly continuous (normal) functionals on M is norm closed it follows that the set of σ-weakly continuous linear maps of M into itself is norm closed ([8], section 1.3.3). This, combined with $\lim_{t\downarrow 0} \|L - t^{-1}(\Phi_t - \mathrm{id}_M)\| = 0$ and property (e), we also have that L is σ-weakly continuous. It is actually possible to characterize exactly which maps generate a uniformly continuous QMS and this will be stated in Theorem 4.2.4.

Definition 4.2.2. Let M be a von Neumann algebra. A bounded linear map $L : M \to M$ is called *completely dissipative* if

1. $L(\mathrm{id}_H) = 0$;
2. $L(x)^* = L(x^*)$ for all $x \in M$;
3. $D(L^{(n)}; x, x) \geq 0$ for all $n \in \mathbb{N}$ and $x \in M_n(M)$,

where $D(L^{(n)}; x, y) := L^{(n)}(x^*y) - L^{(n)}(x^*)y - x^*L^{(n)}(y)$ for $x, y \in M_n(M)$ (and $n \in \mathbb{N}$).

Example 4.2.3. Let $\Phi_t = e^{tL}$ be a uniformly continuous QMS on a von Neumann algebra M, then the bounded generator L is a σ-weakly continuous, completely dissipative map. Indeed,

$$L(\mathrm{id}_H) = \lim_{t\downarrow 0} \frac{\Phi_t(\mathrm{id}_H) - \mathrm{id}_H}{t} = \lim_{t\downarrow 0} \frac{\mathrm{id}_H - \mathrm{id}_H}{t} = 0, \quad L(x)^* = \left(\lim_{t\downarrow 0} \frac{\Phi_t(x) - x}{t} \right)^* = \lim_{t\downarrow 0} \frac{\Phi_t(x)^* - x^*}{t}$$
$$= \lim_{t\downarrow 0} \frac{\Phi_t(x^*) - x^*}{t} = L(x^*) \quad (x \in M)$$

where the limits can be either taken in the σ-weak topology or norm topology.

Now fix $n \in \mathbb{N}$ and $x \in M_n(M)$ arbitrary. Note that $\Phi_t^{(n)} = e^{tL^{(n)}}$ for $t \geq 0$. Define $f(t) := \Phi_t^{(n)}(x^*)\Phi_t^{(n)}(x)$ and $g(t) := \Phi_t^{(n)}(x^*x)$ for $t \geq 0$. Then $f(t) \leq g(t)$ for all $t \geq 0$ by Kadison-Schwarz inequality. Moreover, f and g are differentiable at $t = 0$ with

$$\begin{aligned} L^{(n)}(x^*)x + x^*L^{(n)}(x) = f'(0) &= \lim_{h\downarrow 0} \frac{f(h) - f(0)}{h} \\ &= \lim_{h\downarrow 0} \frac{f(h) - g(0)}{h} \leq \lim_{h\downarrow 0} \frac{g(h) - g(0)}{h} = g'(0) = L^{(n)}(x^*x), \end{aligned}$$

and this exactly means that $D(L^{(n)}; x, x) \geq 0$. Hence, L is completely dissipative and the fact that L is σ-weakly continuous has already been shown due to the remark(s) prior to Definition 4.2.2.

Theorem 4.2.4. $(\Phi_t)_{t\geq 0}$ *is a uniformly continuous QMS defined on a von Neumann algebra* M *if and only if* $\Phi_t = e^{tL}$ *with* $L : M \to M$ *a* σ*-weakly continuous completely dissipative map.*

Proof. $\Longrightarrow$: This is Example 4.2.3.
$\Longleftarrow$: It is clear that $(\Phi_t)_{t\geq 0}$ is uniformly continuous as L is bounded. Moreover, Φ_t is σ-weakly continuous for all $t \geq 0$ as $\Phi_t = \sum_{n=0}^{\infty} \frac{(tL)^n}{n!}$ can be approximated in norm by σ-weakly continuous maps $\left(\sum_{n=0}^{N} \frac{(tL)^n}{n!}\right)_{N\in\mathbb{N}}$ and using the fact that the set of σ-weakly continuous linear maps of M into itself is norm closed ([8], section 1.3.3). We have $\lim_{t\downarrow 0} \Phi_t(x) = x$ in norm for all $x \in M$. So, in particular, $\lim_{t\downarrow 0} \Phi_t(x) = x$ in the σ-weak topology for all $x \in M$. And, $\Phi_{t+s} = \Phi_t\Phi_s$ for all $s, t \geq 0$ by (continuous) functional calculus. Since $L(\mathrm{id}_H) = 0$, we see that id_H is an eigenvector of L with eigenvalue 0. It follows that id_H is a eigenvector of $\Phi_t = e^{tL}$ with eigenvalue $e^{t\cdot 0} = 1$ by (continuous) functional calculus. Therefore, $\Phi_t(\mathrm{id}_H) = \mathrm{id}_H$ for all $t \geq 0$. The only thing left to prove is that Φ_t is completely positive for all $t \geq 0$.
To this end, we will use the result that L generates a semigroup of contraction operators if and only if

$$\Theta(L) := \lim_{t\downarrow 0} t^{-1}(\|\mathrm{id}_H + tL\| - 1) \leq 0,$$

see Theorem 2.1. in [15]. Moreover, from Corollary 1 in [22] we obtain

$$\|\mathrm{id}_H + tL\| = \sup_{u\in U(M)} \|u + tL(u)\|,$$

where $U(M)$ is the set of unitary elements in M. Now since L is completely dissipative, we have for all $u \in U(M)$ and $t \geq 0$,

$$\begin{aligned} \|u + tL(u)\|^2 &= \|(u^* + tL(u^*))(u + tL(u))\| = \|\mathrm{id}_H + t(L(u^*)u + u^*L(u)) + t^2L(u^*)L(u)\| \\ &= \|\mathrm{id}_H + t(L(u^*)u + u^*L(u) - L(u^*u)) + t^2L(u^*)L(u)\| \\ &\leq \|\mathrm{id}_H + t^2L(u^*)L(u)\| \leq 1 + t^2\|L\|^2. \end{aligned}$$

From this, it follows that $\|u + tL(u)\| \leq \sqrt{1 + t^2\|L\|^2} \leq 1 + t^2\|L\|^2$ such that

$$t^{-1}(\|u + tL(u)\| - 1) \leq t\|L\|^2, \quad \text{for all } u \in U(M) \text{ and } t \geq 0.$$

Hence, $\Theta(L) = \lim_{t\downarrow 0} t^{-1}(\|\mathrm{id}_H + tL\| - 1) \leq \lim_{t\downarrow 0} t\|L\|^2 = 0$ and this implies that $\|\Phi_t\| \leq 1$ for all $t \geq 0$. And we have already shown that $\Phi_t(\mathrm{id}_H) = \mathrm{id}_H$ and thus $\|\Phi_t\| = 1$ for all $t \geq 0$. Corollary 1 in [22] also states that Φ_t is positive if and only if $\|\Phi_t\| = 1$ on the condition that $\Phi_t(\mathrm{id}_H) = \mathrm{id}_H$ and that is the case. Thus, Φ_t is positive. We can repeat this same argument to $L^{(n)}$ for each $n \in \mathbb{N}$ and conclude that $\Phi_t^{(n)}$ is positive, i.e. Φ_t is completely positive. □

We shall give an implicit form for σ-weakly continuous completely dissipative maps defined on a special class of von Neumann algebras, namely the *hyperfinite* ones.

Definition 4.2.5. A *uniformly hyperfinite algebra* or *UHF algebra* is a unital C^* algebra A which has in increasing sequence $(A_n)_{n=1}^{\infty}$ of finite dimensional simple C^*-subalgebras each containing the unit of A such that $\bigcup_{n=1}^{\infty} A_n$ is dense in A.

A von Neumann algebra $M \subseteq B(H)$ is *hyperfinite* if it has a weakly dense C^*-subalgebra that is a UHF algebra and whose unit is id_H.

Example 4.2.6. If H is a separable Hilbert space, then $B(H)$ is hyperfinite. This is clear if H is finite dimensional. To prove the infinite dimensional case, we let A be an infinite dimensional UHF algebra. In particular, there exists a non-zero irreducible representation $(\tilde{H}, \pi)$ of A (Theorem 5.1.12 in [16]). Since A is simple (Theorem 21, page 88 in [27]), π is a $*$-isomorphism from A onto $\pi(A) \subseteq B(\tilde{H})$, so $\pi(A)$ is also a UHF algebra (use that π is isometric). Now let $x \in \tilde{H}$ be any non-zero vector. Then x is cyclic for $(\tilde{H}, \pi)$, that is, $\overline{\pi(A)x} = \tilde{H}$ by irreducibility (Theorem 5.1.5(2) in [16]). This shows that $\tilde{H}$ is separable as A is separable and it is already clear that $\tilde{H}$ is infinite dimensional since A is infinite-dimensional. Therefore, H is isometrically isomorphic to $\tilde{H}$ as they both are separable and infinite dimensional. It follows that $B(H) \cong B(\tilde{H})$ as an isometric isomorphism. Moreover, $\pi(A)' = \mathbb{C}\mathrm{id}_{\tilde{H}}$ as $(\tilde{H}, \pi)$ is irreducible using Theorem 5.1.5(1) in [16]. But then $\pi(A)'' = B(\tilde{H})$ or, equivalently, $\pi(A)$ is weakly dense in $B(\tilde{H})$ by the double commutant theorem. Hence, $B(\tilde{H})$ is hyperfinite and so is $B(H)$.

Proposition 4.2.7. *Let $M \subseteq B(H)$ be a hyperfinite von Neumann algebra. If $L : M \to M$ is a σ-weakly continuous completely dissipative map, then there exists a σ-weakly continuous completely positive map $\Psi : M \to M$ and a self-adjoint $h \in M$ such that*

$$L(x) = \Psi(x) - \frac{1}{2}\{\Psi(\mathrm{id}_H), x\} + i[h, x] \quad \textit{for all} \;\; x \in M.$$

Proof. Since M is hyperfinite, there exists an increasing sequence $(M_j)_{j\geq 1} \subseteq M$ of finite-dimensional simple C^*-subalgebras each containing id_H such that $\overline{\bigcup_{j=1}^{\infty} M_j}^{\mathrm{WOT}} = \overline{\bigcup_{j=1}^{\infty} M_j}^{\mathrm{SOT}} = M$. Fix $j \in \mathbb{N}$ and let $U(M_j)$ be the set of unitary elements in M_j. Then $U(M_j)$ forms a compact (topological) group. So there exists a (unique) Haar measure μ on $U(M_j)$ with $\mu(U(M_j)) = 1$ (see Section 2.2 in [9] for more details and background on Haar measure).

Now define $\varphi_j : H^2 \to \mathbb{C}$ by $\varphi_j(\xi, \eta) = \int_{U(M_j)} \langle L(u^*)u\xi, \eta\rangle d\mu(u)$. It is clear that φ_j is sesquilinear. It is also bounded, because

$$\begin{aligned} |\varphi_j(\xi, \eta)| &\leq \int_{U(M_j)} |\langle L(u^*)u\xi, \eta\rangle| \, d\mu(u) \leq \|L\|\|\xi\|\|\eta\| \int_{U(M_j)} \|u^*\|\|u\| \, d\mu(u) \\ &= \|L\|\|\xi\|\|\eta\|\mu(U(M_j)) = \|L\|\|\xi\|\|\eta\| \end{aligned}$$

Therefore, there exists a unique operator $k_j \in B(H)$ such that

$$\langle k_j\xi, \eta\rangle = \int_{U(M_j)} \langle L(u^*)u\xi, \eta\rangle d\mu(u), \quad \xi, \eta \in H$$

by Theorem 2.3.6 in [16]. Moreover, $\|k_j\| = \|\varphi\| \leq \|L\|$. We actually have $k_j \in M$ because for all

$x' \in M'$ and $\xi, \eta \in H$ we have

$$\langle x'k_j\xi, \eta\rangle = \langle k_j\xi, (x')^*\eta\rangle = \int_{U(M_j)} \langle L(u^*)u\xi, (x')^*\eta\rangle \, d\mu(u) = \int_{U(M_j)} \langle x'L(u^*)u\xi, \eta\rangle \, d\mu(u)$$
$$= \int_{U(M_j)} \langle L(u^*)ux'\xi, \eta\rangle \, d\mu(u) = \langle k_jx'\xi, \eta\rangle$$

where in the third equality we used that $L(u^*), u \in M$ for all $u \in U(M_j)$. So indeed, $k_j \in M'' = M$. Define $f_{\xi,\eta} : U(M_j) \to \mathbb{C}$ by $f_{\xi,\eta}(u) = \langle L(u^*)u\xi, \eta\rangle$ for convenience. But then for a $v \in U(M_j)$,

$$\langle k_jv\xi, \eta\rangle = \int_{U(M_j)} \langle L(u^*)uv\xi, \eta\rangle \, d\mu(u) = \int_{U(M_j)} f_{v\xi,\eta}(u) \, d\mu(u) = \int_{U(M_j)} f_{v\xi,\eta}(uv^*) \, d\mu(u)$$
$$= \int_{U(M_j)} \langle L(vu^*)uv^*v\xi, \eta\rangle \, d\mu(u) = \int_{U(M_j)} \langle L(vu^*)u\xi, \eta\rangle \, d\mu(u),$$

where third equality is the invariance of the Haar integral. And since $U(M_j)$ spans M_j, we obtain $\langle k_jx\xi, \eta\rangle = \int_{U(M_j)} \langle L(xu^*)u\xi, \eta\rangle d\mu(u)$ for all $x \in M_j$. Consequently, using the fact that L is $*$-preserving, we have for all $x, y \in M_j$ and $\xi, \eta \in H$

$$\langle x^*yk_j^*\xi, \eta\rangle = \langle \xi, k_jy^*x\eta\rangle = \overline{\langle k_jy^*x\eta, \xi\rangle} = \int_{U(M_j)} \overline{\langle L(y^*u^*)ux\eta, \xi\rangle} \, d\mu(u)$$
$$= \int_{U(M_j)} \overline{\langle \eta, x^*u^*L(uy)\xi\rangle} \, d\mu(u) = \int_{U(M_j)} \langle x^*u^*L(uy)\xi, \eta\rangle \, d\mu(u).$$

Using these observations, we have for all $x, y \in M_j$ and $\xi, \eta \in H$ that

$$\begin{aligned}
\int_{U(M_j)} \langle D(L; ux, uy)\xi, \eta\rangle \, d\mu(u) &= \int_{U(M_j)} \langle \big(L(x^*u^*uy) - L(x^*u^*)uy - x^*u^*L(uy)\big)\xi, \eta\rangle \, d\mu(u) \\
&= \int_{U(M_j)} \langle L(x^*y)\xi, \eta\rangle \, d\mu(u) - \int_{U(M_j)} \langle L(x^*u^*)uy\xi, \eta\rangle \, d\mu(u) - \\
&\quad \int_{U(M_j)} \langle x^*u^*L(uy)\xi, \eta\rangle \, d\mu(u) \\
&= \langle L(x^*y)\xi, \eta\rangle - \langle k_jx^*y\xi, \eta\rangle - \langle x^*yk_j^*\xi, \eta\rangle \\
&= \langle \big(L(x^*y) - k_jx^*y - x^*yk_j^*\big)\xi, \eta\rangle.
\end{aligned}$$

Define for each $k \in M$ the linear map $\Psi_k : M \to M$ by

$$\Psi_k(x) = L(x) - kx - xk^*.$$

Then, as L is completely dissipative, we have for $x \in M_j$

$$\langle \Psi_{k_j}(x^*x)\xi, \xi\rangle = \langle \big(L(x^*x) - k_jx^*x - x^*xk_j^*\big)\xi, \xi\rangle = \int_{U(M_j)} \langle D(L; ux, ux)\xi, \xi\rangle \, d\mu(u) \geq 0,$$

which implies that $\Psi_{k_j}|_{M_j}$ is positive. We can repeat this same argument to $M_n(M_j) \cong M_n(\mathbb{C}) \otimes M_j$ for every $n \in \mathbb{N}$ since $D(L^{(n)}; ux, ux) \geq 0$. It follows that $\Psi_{k_j}|_{M_j}$ is completely positive as a map from M_j into M.

Define the set

$$\Gamma_j := \{k \in M : \Psi_k|_{M_j} \text{ is completely positive as a map from } M_j \text{ into } M \text{ and } \|k\| \leq \|L\|\}.$$

We have shown that $k_j \in \Gamma_j$ so that $\Gamma_j \neq \emptyset$ for all $j \in \mathbb{N}$. Moreover, $\Gamma_{j+1} \subseteq \Gamma_j$ as $M_j \subseteq M_{j+1}$ for every $j \in \mathbb{N}$ and hence any finite intersection of Γ_j's is nonempty.

Claim: Γ_j is weakly closed. To show this we let $(k_\lambda) \subseteq \Gamma_j$ be a net such that $k_\lambda \to k \in M$ in the weak operator topology. Then for all $n \in \mathbb{N}$, $x \in M_n(M_j)$ and $\xi \in H^{(n)}$,

$$\begin{aligned}\langle \Psi_k^{(n)}(x^*x)\xi, \xi\rangle &= \langle \big(L^{(n)}(x^*x) - (k \otimes \mathrm{id}_n)x^*x - x^*x(k \otimes \mathrm{id}_n)\big)\xi, \xi\rangle \\ &= \lim_\lambda \langle \big(L^{(n)}(x^*x) - (k_\lambda \otimes \mathrm{id}_n)x^*x - x^*x(k_\lambda \otimes \mathrm{id}_n)\big)\xi, \xi\rangle \\ &= \lim_\lambda \langle \Psi_{k_\lambda}^{(n)}(x^*x)\xi, \xi\rangle \geq 0\end{aligned}$$

such that $\Psi_k|_{M_j}$ is completely positive as a map from M_j into M. Moreover,

$$|\langle k\xi, \eta\rangle| = \lim_\lambda |\langle k_\lambda \xi, \eta\rangle| \leq \sup_\lambda \|k_\lambda\|\|x\|\|y\| \leq \|L\|\|x\|\|y\| \quad \text{for all } \xi, \eta \in H$$

such that $\|k\| \leq \|L\|$. So indeed, $k \in \Gamma_j$ and thus Γ_j is closed in the weak operator topology.
As a consequence, Γ_j is compact in the weak operator topology since the unit ball in M is compact in the weak operator topology. Thus, $\Gamma := \bigcap_{j=1}^\infty \Gamma_j \neq \emptyset$ by a standard topology argument. So there exists a $\tilde{k} \in \Gamma$. It follows that $\Psi := \Psi_{\tilde{k}}$ is completely positive on $\bigcup_{j=1}^\infty M_j$. Moreover, Ψ is σ-weakly continuous as L is σ-weakly continuous and the maps $x \mapsto \tilde{k}x$, $x \mapsto x\tilde{k}^*$ are σ-weakly continuous.

To show that Ψ is completely positive on M, we first note that the closed unit ball of $\left(\bigcup_{j=1}^\infty M_j\right)^+$ is strongly dense in the closed unit ball of $\left(\overline{\bigcup_{j=1}^\infty M_j}^{\mathrm{SOT}}\right)^+ = M^+$ by Kaplansky density theorem and by hyperfiniteness. The closed unit ball is convex so that the closed unit ball of $\left(\bigcup_{j=1}^\infty M_j\right)^+$ is weakly dense in the closed unit ball of M^+. Furthermore, the weak operator topology and the σ-weak topology coincide on the unit ball which implies that the closed unit ball of $\left(\bigcup_{j=1}^\infty M_j\right)^+$ is σ-weakly dense in the closed unit ball of M^+. Now let $x \in M^+$, then $\frac{x}{\|x\|}$ is an element of the closed unit ball of M^+. So there exists a net $(y_\lambda) \subseteq \left(\bigcup_{j=1}^\infty M_j\right)^+$ with $\|y_\lambda\| \leq 1$ such that $\lim_\lambda y_\lambda = \frac{x}{\|x\|}$ in the σ-weak topology. Now using the σ-weak continuity of Ψ, positivity of Ψ and the fact that the set of positive elements is σ-weakly closed, we obtain $\frac{1}{\|x\|}\Psi(x) = \lim_\lambda \Psi(y_\lambda) \geq 0$. Hence, $\Psi(x) \geq 0$ and this means that Ψ is positive on M. We can repeat this argument to $\Psi^{(n)}$ and $M_n(M)$ to conclude that Ψ is completely positive on M.

Obviously, $\Psi(\mathrm{id}_H) = -\tilde{k} - \tilde{k}^*$ as $L(\mathrm{id}_H) = 0$. So setting $h := \frac{1}{2}i(\tilde{k}^* - k) \in M_{sa}$ results in

$$\begin{aligned}\Psi(x) - \frac{1}{2}\{\Psi(\mathrm{id}_H), x\} + i[h, x] &= L(x) - \tilde{k}x - x\tilde{k}^* - \frac{1}{2}(-\tilde{k}x - \tilde{k}^*x - x\tilde{k} - x\tilde{k}^*) + \\ &\quad i \cdot \frac{i}{2}(\tilde{k}^*x - \tilde{k}x - (x\tilde{k}^* - x\tilde{k})) \\ &= L(x) - \tilde{k}x - x\tilde{k}^* + \frac{1}{2}(\tilde{k}x + \tilde{k}^*x + x\tilde{k} + x\tilde{k}^*) + \frac{1}{2}(\tilde{k}x - \tilde{k}^*x - x\tilde{k} + x\tilde{k}^*) \\ &= L(x)\end{aligned}$$

for all $x \in M$, which gives the statement. □

The converse is also true on any von Neumann algebra:

Lemma 4.2.8. *Let M be a von Neumann algebra. If $\Psi : M \to M$ is completely positive and $h \in M$ is self-adjoint, then $L : M \to M$ defined by $L(x) = \Psi(x) - \frac{1}{2}\{\Psi(\mathrm{id}_H), x\} + i[h, x]$ is completely dissipative. Moreover, L is σ-weakly continuous if Ψ is σ-weakly continuous.*

Proof. It is clear that L is bounded as Ψ is bounded and multiplication operators are bounded. We have

$$L(\mathrm{id}_H) = \Psi(\mathrm{id}_H) - \frac{1}{2}(\Psi(\mathrm{id}_H) + \Psi(\mathrm{id}_H)) + i(h - h) = 0,$$

and

$$\begin{aligned}
L(x)^* &= \Psi(x)^* - \frac{1}{2}(\Psi(\mathrm{id}_H)x + x\Psi(\mathrm{id}_H))^* - i(hx - xh)^* \\
&= \Psi(x^*) - \frac{1}{2}(x^*\Psi(\mathrm{id}_H) + \Psi(\mathrm{id}_H)x^*) - i(x^*h - hx^*) \\
&= \Psi(x^*) - \frac{1}{2}\{\Psi(\mathrm{id}_H), x^*\} + i[h, x^*] \\
&= L(x^*).
\end{aligned}$$

Let $\Psi(x) = V^*\pi(x)V$ be the Stinespring decomposition (Theorem 4.1.5). We may choose π such that $\pi(\mathrm{id}_H) = \mathrm{id}_H$. Then, for all $x \in M$, we have

$$\begin{aligned}
D(L; x, x) &= L(x^*x) - L(x^*)x - x^*L(x) \\
&= \Psi(x^*x) - \frac{1}{2}(\Psi(\mathrm{id}_H)x^*x + x^*x\Psi(\mathrm{id}_H)) + i(hx^*x - x^*xh) - \\
&\quad (\Psi(x^*) - \frac{1}{2}(\Psi(\mathrm{id}_H)x^* + x^*\Psi(\mathrm{id}_H)) + i(hx^* - x^*h))x - \\
&\quad x^*(\Psi(x) - \frac{1}{2}(\Psi(\mathrm{id}_H)x + x\Psi(\mathrm{id}_H)) + i(hx - xh)) \\
&= \Psi(x^*x) - \Psi(x^*)x - x^*\Psi(x) + x^*\Psi(\mathrm{id}_H)x \\
&= V^*\pi(x^*x)V - V^*\pi(x^*)Vx - x^*V^*\pi(x)V + x^*V^*Vx \\
&= (\pi(x)V - Vx)^*(\pi(x)V - Vx) \\
&\geq 0.
\end{aligned}$$

Now the same argument applied to $L^{(n)}$ and $\Psi^{(n)}$ shows that $D(L^{(n)}; x, x) \geq 0$ for all $x \in M_n(M)$ and $n \in \mathbb{N}$. Consequently, L is completely dissipative. Furthermore, L is σ-weakly continuous if Ψ is σ-weakly continuous since $x \mapsto \frac{1}{2}\{\Psi(\mathrm{id}_H), x\} + i[h, x]$ is a σ-weakly continuous map. □

If we consider the full algebra $B(H)$ for some separable Hilbert space H, then the σ-weakly continuous completely dissipative maps can be entirely characterized.

Theorem 4.2.9. *Let H be a separable Hilbert space. Then $L : B(H) \to B(H)$ is completely dissipative and σ-weakly continuous if and only if there exists a family of operators $(a_j) \subseteq B(H)$ and a self-adjoint $h \in B(H)$ such that*

$$L(x) = \sum_j \left(a_j^* x a_j - \frac{1}{2}\{a_j^* a_j, x\}\right) + i[h, x] \quad \text{for all } x \in B(H),$$

and the series converges in the strong operator topology.

Proof. $\Longrightarrow$: This follows from Proposition 4.2.7 (note that $B(H)$ is hyperfinite) and Kraus decomposition (Theorem 4.1.6).
$\Longleftarrow$: This follows from Lemma 4.2.8 and Kraus decomposition (Theorem 4.1.6) again. $\square$

Corollary 4.2.10 (Lindblad)**.** *Let H be a separable Hilbert space. Then $(\Phi_t)_{t\geq 0}$ is a uniformly continuous quantum Markov semigroup defined on $B(H)$ if and only if $\Phi_t = e^{tL}$ and $L : B(H) \to B(H)$ can be represented in the form*

$$L(x) = \sum_j \left(a_j^* x a_j - \frac{1}{2}\{a_j^* a_j, x\} \right) + i[h, x] \quad \textit{for all } \ x \in B(H),$$

where $(a_j) \subseteq B(H)$ is a family of operators and $h \in B(H)$ self-adjoint such that the series in the formula for L converges in the strong operator topology.

Proof. This follows from Theorem 4.2.4 and Theorem 4.2.9. $\square$

4.3 Detailed balance

An important observation in physics is that many equations (e.g. kinetic systems) are valid regardless of whether time goes forwards or backwards. The principle of *detailed balance* plays a central role in here and can be defined through Markov chains.

Let $X = (X_n)_{0\leq n\leq N}$ be a discrete time Markov chain taking values in a finite state space $S = \{x_1, ..., x_n\}$ with transition matrix $P = (p_{i,j})_{i,j\in S}$. Moreover, assume that X is irreducible and positive recurrent so that it has a unique invariant distribution $\pi = (\pi_i)_{i\in S}$. If X_0 has distribution π (so that X_n has distribution π for every n), then the 'reversed chain' $Y = (Y_n)_{0\leq n\leq N}$ defined by $Y_n := X_{N-n}$ is an irreducible Markov chain with transition matrix $\widetilde{P} = (\tilde{p}_{i,j})_{i,j\in S}$ given by

$$\tilde{p}_{i,j} = \frac{\pi_j}{\pi_i} p_{j,i} \quad \text{for } i, j \in S,$$

and with invariant distribution π (see Theorem 12.109 in [11]). We say that X is *reversible* if X and Y have the same transition matrices, that is,

$$\pi_i p_{i,j} = \pi_j p_{j,i} \quad \text{for all } i, j \in S$$

and these equations are called the *detailed balance equations*. If the detailed balance conditions are satisfied we might also say that P satisfies the *detailed balance condition with respect to* π and it characterizes *time reversal invariance* of X.

There is another way to characterize the detailed balance equations via self-adjointness: the matrix P satisfies the detailed balance condition with respect to π if and only if P is self-adjoint on $\mathbb{C}^n$ equipped with the inner product $\langle v, w\rangle_\pi = \sum_{i=1}^n \pi_i v_i \overline{w_i}$ $(v, w \in \mathbb{C}^n)$. One might want to generalize this inner product to the quantum setting and therefore have a notion of *(quantum) detailed balance* defined through self-adjointness. Hence, matrix algebras will be considered and in this subsection A will always denote a unital C^*-subalgebra of some matrix algebra $M_n(\mathbb{C})$ with $1_A = \mathrm{id}_{\mathbb{C}^n}$.

Definition 4.3.1. A *density matrix* or *density operator* $\rho \in M_n(\mathbb{C})$ is a positive operator on $\mathbb{C}^n$ with $\mathrm{Tr}(\rho) = 1$. We denote the set of invertible density matrices belonging to a C^*-subalgebra $A \subseteq M_n(\mathbb{C})$ by $\mathfrak{S}_+(A)$ and we write $\mathfrak{S}_+$ for $\mathfrak{S}_+(M_n(\mathbb{C}))$. (It should be emphasized that the density matrices in $\mathfrak{S}_+$ are invertible.)

Definition 4.3.2. An inner product $\langle\cdot,\cdot\rangle$ on A is *compatible* with $\rho \in \mathfrak{S}_+(A)$ in case $\mathrm{Tr}(\rho a) = \langle a, 1\rangle$ for all $a \in A$, where $1 = \mathrm{id}_{\mathbb{C}^n}$.

Definition 4.3.3. Let $\rho \in \mathfrak{S}_+$ be an invertible density matrix. For each $s \in \mathbb{R}$ and each $a, b \in A$, define the inner product $\langle\cdot,\cdot\rangle_{\rho,s}$ on A by

$$\langle a, b\rangle_{\rho,s} := \mathrm{Tr}\left((\rho^{(1-s)/2} b \rho^{s/2})^*(\rho^{(1-s)/2} a \rho^{s/2})\right) = \mathrm{Tr}\left(\rho^s b^* \rho^{1-s} a\right).$$

Note that for all $s \in \mathbb{R}$ the inner product $\langle\cdot,\cdot\rangle_{\rho,s}$ is compatible with $\rho \in \mathfrak{S}_+(A)$.

Definition 4.3.4. A quantum Markov semigroup $(\Phi_t)_{t\geq 0}$ on a A satisfies the *(quantum) detailed balance condition (DBC)* with respect to $\rho \in \mathfrak{S}_+(A)$ if for each $t > 0$, Φ_t is self-adjoint in the ρ-GNS inner product $\langle\cdot,\cdot\rangle_{\rho,1}$. We say that the QMS $(\Phi_t)_{t\geq 0}$ satisfies the ρ-DBC.

By applying Theorem 3.3.1 to $A \subseteq M_n(\mathbb{C})$ and $\mathrm{Tr}(\cdot\rho)$ on A for some $\rho \in \mathfrak{S}_+(A)$, we obtain the modular operator Δ_ρ and the modular automorphism group $(\sigma_t^\rho)_{t\in\mathbb{R}}$ on A given by

$$\Delta_\rho(x) = \rho x \rho^{-1} \quad \text{and} \quad \sigma_t^\rho(x) = \rho^{it} x \rho^{-it} \quad \text{for } x \in A.$$

Then, by continuous functional calculus, we have $\langle a, b\rangle_{\rho,s} = \mathrm{Tr}(b^* \Delta_\rho^{1-s}(a)\rho)$ for $a, b \in A$ and $s \in \mathbb{R}$. More generally, given any function $f : (0,\infty) \to (0,\infty)$ (which is automatically continuous on every discrete spectrum of an invertible positive operator), define the inner product on A by

$$\langle a, b\rangle_{\rho,f} := \mathrm{Tr}(b^* f(\Delta_\rho)(a)\rho) \quad \text{for } a, b \in A.$$

It should be clear from the context when we use this definition or Definition 4.3.3 and we notice that $\langle\cdot,\cdot\rangle_{\rho,1}$ is the ρ-GNS inner product whether 1 is interpreted as a number, or as the constant function $f(t) = 1$. It turns out that self-adjointness with respect to the ρ-GNS inner product $\langle\cdot,\cdot\rangle_{\rho,1}$ implies self-adjointness with respect to $\langle\cdot,\cdot\rangle_{\rho,f}$ for every $f : (0,\infty) \to (0,\infty)$. As a direct consequence, a QMS satisfying the ρ-DBC is self-adjoint with respect to $\langle\cdot,\cdot\rangle_{\rho,f}$ for every $f : (0,\infty) \to (0,\infty)$ and as a by-product the QMS commutes with the modular operator Δ_ρ and the modular automorphism group $(\sigma_t^\rho)_{t\in\mathbb{R}}$. We will show this.

Note that since A finite-dimensional, σ_t^ρ is an automorphism on A for all $t \in \mathbb{C}$ and we refer to $(\sigma_t^\rho)_{t\in\mathbb{C}}$ also as the modular automorphism group. Keep in mind that σ_t^ρ will only be a $*$-automorphism if and only if $t \in \mathbb{R}$ (see Remark 3.3.2).

Lemma 4.3.5. *Let $s \in \mathbb{R}$ and $\rho \in \mathfrak{S}_+(A)$. Then for all $t \in \mathbb{R}$ and $a, b \in A$,*

$$\langle \sigma_{-it}^\rho(a), b\rangle_{\rho,s} = \langle a, b\rangle_{s-t} = \langle a, \sigma_{-it}^\rho(b)\rangle_{\rho,s}$$

In particular, σ_{-it}^ρ is self-adjoint with respect to $\langle\cdot,\cdot\rangle_{\rho,s}$.

Proof. Using the definitions we obtain

$$\langle \sigma_{-it}^\rho(a), b\rangle_{\rho,s} = \mathrm{Tr}(\rho^s b^* \rho^{1-s} \rho^t a \rho^{-t}) = \mathrm{Tr}(\rho^{s-t} b^* \rho^{1-(s-t)} a) = \langle a, b\rangle_{s-t}, \quad \text{and}$$
$$\langle a, \sigma_{-it}^\rho(b)\rangle_{\rho,s} = \mathrm{Tr}(\rho^s (\rho^t b \rho^{-t})^* \rho^{1-s} a) = \mathrm{Tr}(\rho^{s-t} b^* \rho^{1-(s-t)} a) = \langle a, b\rangle_{s-t}.$$ □

Lemma 4.3.6. *Let $\rho \in \mathfrak{S}_+(A)$ and let K be any linear operator on A that is self-adjoint with respect to $\langle\cdot,\cdot\rangle_{\rho,1}$ and such that $K(a)^* = K(a^*)$ for all $a \in A$. Then K commutes with Δ_ρ and σ_t^ρ for all $t \in \mathbb{C}$.*

Proof. For all $a, b \in A$, we have

$$\begin{aligned}\langle K(\sigma_{-i}^{\rho}(a)), b\rangle_{\rho,1} &= \langle \sigma_{-i}^{\rho}(a), K(b)\rangle_{\rho,1} = \mathrm{Tr}(\rho K(b)^* \rho a \rho^{-1}) = \mathrm{Tr}(K(b^*)\rho a) \\ &= \mathrm{Tr}(\rho a K(b^*)) = \langle K(b^*), a^*\rangle_{\rho,1} = \langle b^*, K(a)^*\rangle_{\rho,1} \\ &= \mathrm{Tr}(\rho K(a) b^*) = \mathrm{Tr}(b^* \rho K(a)) = \langle K(a), b\rangle_{\rho,0}.\end{aligned}$$

Now apply Lemma 4.3.5 with $s = t = 1$ to obtain $\langle \sigma_{-i}^{\rho}(K(a)), b\rangle_{\rho,1} = \langle K(a), b\rangle_{\rho,0}$. It follows that $\langle K(\sigma_{-i}^{\rho}(a)), b\rangle_{\rho,1} = \langle \sigma_{-i}^{\rho}(K(a)), b\rangle_{\rho,1}$ for all $a, b \in A$ and this implies that

$$K\Delta_\rho = K\sigma_{-i}^{\rho} = \sigma_{-i}^{\rho} K = \Delta_\rho K.$$

Since K commutes with Δ_ρ, K commutes with every polynomial in the self-adjoint operator Δ_ρ. By Stone-Weierstrass, K commutes with $f(\Delta_\rho)$ for every continuous function $f : \sigma(\Delta_\rho) \to \mathbb{C}$. In particular, K commutes with σ_t^{ρ} for every $t \in \mathbb{C}$ (choose $f(x) = x^{it}$). ☐

Lemma 4.3.7. *Let $\rho \in \mathfrak{S}_+(A)$. Let K be any linear operator on A such that $K\sigma_t^{\rho} = \sigma_t^{\rho} K$ for all $t \in \mathbb{C}$, or equivalently, $K\Delta_\rho = \Delta_\rho K$. If K is self-adjoint with respect to the inner product $\langle \cdot, \cdot \rangle_{\rho,f}$ for some function $f : (0, \infty) \to (0, \infty)$, then the same holds for every function $f : (0, \infty) \to (0, \infty)$.*

Proof. Suppose that K is self-adjoint with respect to the inner product $\langle \cdot, \cdot \rangle_{\rho,f}$ for some function $f : (0, \infty) \to (0, \infty)$. Let $g : (0, \infty) \to (0, \infty)$ be arbitrary and set $h := g/f$. Since K commutes with Δ_ρ, it commutes with $h(\Delta_\rho)$ (by Stone-Weierstrass). Consequently, using the definitions and multiplicativity of the continuous functional calculus, we have for all $a, b \in A$ that

$$\begin{aligned}\langle K(a), b\rangle_{\rho,g} &= \mathrm{Tr}(b^* g(\Delta_\rho)(K(a))\rho) = \mathrm{Tr}(b^* f(\Delta_\rho) h(\Delta_\rho)(K(a))\rho) = \mathrm{Tr}(b^* f(\Delta_\rho) K h(\Delta_\rho)(a)\rho) \\ &= \langle K h(\Delta_\rho)(a), b\rangle_{\rho,f} = \langle h(\Delta_\rho)(a), K(b)\rangle_{\rho,f} = \mathrm{Tr}(K(b)^* f(\Delta_\rho) h(\Delta_\rho)(a)\rho) \\ &= \mathrm{Tr}(K(b)^* g(\Delta_\rho)(a)\rho) = \langle a, K(b)\rangle_{\rho,g}.\end{aligned}$$

This give the desired result. ☐

Theorem 4.3.8. *Let $\rho \in \mathfrak{S}_+(A)$ and let K be any linear operator on A. If K is self-adjoint with respect to the GNS inner product $\langle \cdot, \cdot \rangle_{\rho,1}$ and $K(a)^* = K(a^*)$ for all $a \in A$, then K commutes with Δ_ρ and σ_t^{ρ} for all $t \in \mathbb{C}$. Moreover, K is self-adjoint with respect to $\langle \cdot, \cdot \rangle_{\rho,f}$ for all $f : (0, \infty) \to (0, \infty)$.*

Proof. This follows immediately from Lemma 4.3.6 and Lemma 4.3.7. ☐

Corollary 4.3.9. *Let $\rho \in \mathfrak{S}_+(A)$ and let $\Phi_t = e^{tL}$ be a QMS on A satisfying the ρ-DBC. Then $(\Phi_t)_{t \geq 0}$ and L both commute with the modular operator Δ_ρ and the modular automorphism group $(\sigma_t^{\rho})_{t \in \mathbb{C}}$. Moreover, for all $t \geq 0$, Φ_t and L are self-adjoint with respect to $\langle \cdot, \cdot \rangle_{\rho,f}$ for all $f : (0, \infty) \to (0, \infty)$.*

Proof. Since Φ_t is (completely) positive for all $t \geq 0$, it is also $*$-preserving: $\Phi_t(a)^* = \Phi_t(a^*)$ for all $a \in A$. Therefore, $\Phi_t \Delta_\rho = \Delta_\rho \Phi_t$ and $\Phi_t \sigma_{t'}^{\rho} = \sigma_{t'}^{\rho} \Phi_t$ for all $t \geq 0$ and $t' \in \mathbb{C}$ by Theorem 4.3.8 as Φ_t is self-adjoint with respect to $\langle \cdot, \cdot \rangle_{\rho,1}$ for all $t \geq 0$. Moreover,

$$L\Delta_\rho = \lim_{t \downarrow 0} t^{-1}(\Phi_t - \mathrm{id}_A)\Delta_\rho = \lim_{t \downarrow 0} t^{-1}(\Phi_t \Delta_\rho - \Delta_\rho) = \lim_{t \downarrow 0} t^{-1}(\Delta_\rho \Phi_t - \Delta_\rho) = \Delta_\rho L,$$

where the limits are norm limits. The same computation for σ_t^{ρ} yields $L\sigma_t^{\rho} = \sigma_t^{\rho} L$ for all $t \in \mathbb{C}$.

Let $f : (0, \infty) \to (0, \infty)$ be arbitrary. It is clear that for all Φ_t is self-adjoint with respect to $\langle \cdot, \cdot \rangle_{\rho,f}$ for all $t \geq 0$ by Theorem 4.3.8. Let $K^{*_{\rho,f}}$ be the adjoint of K with respect to $\langle \cdot, \cdot \rangle_{\rho,f}$ for any operator K on A. Then, using $\Phi_t^{*_{\rho,f}} = \Phi_t$ for all $t \geq 0$, we obtain

$$L^{*_{\rho,f}} = \left(\lim_{t \downarrow 0} t^{-1}(\Phi_t - \mathrm{id}_A) \right)^{*_{\rho,f}} = \lim_{t \downarrow 0} t^{-1} \left(\Phi_t^{*_{\rho,f}} - \mathrm{id}_A \right) = \lim_{t \downarrow 0}, t^{-1}(\Phi_t - \mathrm{id}_A) = L,$$

where the limits are norm limits. □

The condition that a QMS commutes with the modular automorphism group may be viewed as a quantum analog of *time-translation invariance* or *stationarity.*

The class of *ergodic* quantum Markov semigroups also plays a main role and an important property of such a semigroup is that it has a unique invariant density matrix for its Hilbert-Schmidt adjoint. This is shown in the next proposition.

Definition 4.3.10. A quantum Markov semigroup $(\Phi_t)_{t \geq 0}$ on A is called *ergodic* if the identity operator spans the eigenspace of Φ_t for the eigenvalue 1 for all $t > 0$.

Proposition 4.3.11. *Let $(\Phi_t)_{t \geq 0}$ be an ergodic QMS on $M_n(\mathbb{C})$. Then there exists a unique density matrix $\tilde{\rho} \in M_n(\mathbb{C})$ such that $\tilde{\rho}$ is invariant under $\Phi_t^\dagger$ ($\Phi_t^\dagger(\tilde{\rho}) = \tilde{\rho}$ for all $t \geq 0$), where $\dagger$ is the adjoint with respect to the Hilbert-Schmidt inner product $\langle \cdot, \cdot \rangle_{\mathrm{HS}}$.*

Proof. Since $\Phi_t(1) = 1$, we see that $\mathrm{Tr}(\Phi_t^\dagger(x)) = \mathrm{Tr}(\Phi_t^\dagger(x)1) = \mathrm{Tr}(x\Phi_t(1)) = \mathrm{Tr}(x)$ for all $x \in M_n(\mathbb{C})$ so that $\Phi_t^\dagger$ is trace-preserving for all $t \geq 0$. Moreover, $\Phi_t^\dagger$ is also (completely) positive for all $t \geq 0$. To see this, let $x \in M_n(\mathbb{C})$ and $\xi \in \mathbb{C}^n$. Note that $|\xi\rangle\langle\xi| \in B(\mathbb{C}^n)$ is a positive operator so that $\Phi_t(|\xi\rangle\langle\xi|) \geq 0$. It follows that

$$\begin{aligned}
\langle \Phi_t^\dagger(x^*x)\xi, \xi \rangle &= \mathrm{Tr}((|\xi\rangle\langle\xi|)\Phi_t^\dagger(x^*x)) = \langle \Phi_t^\dagger(x^*x), |\xi\rangle\langle\xi| \rangle_{\mathrm{HS}} = \langle x^*x, \Phi_t(|\xi\rangle\langle\xi|) \rangle_{\mathrm{HS}} = \mathrm{Tr}(\Phi_t(|\xi\rangle\langle\xi|)x^*x) \\
&= \mathrm{Tr}(\Phi_t(|\xi\rangle\langle\xi|)^{\frac{1}{2}} x^*x \Phi_t(|\xi\rangle\langle\xi|)^{\frac{1}{2}}) = \mathrm{Tr}((x\Phi_t(|\xi\rangle\langle\xi|)^{\frac{1}{2}})^*(x\Phi_t(|\xi\rangle\langle\xi|)^{\frac{1}{2}})) \geq 0,
\end{aligned}$$

and this implies that $\Phi_t^\dagger$ is indeed positive for all $t \geq 0$. (Repeat this argument for the extensions $(\Phi_t^\dagger)^{(n)}$ and $\Phi_t^{(n)}$ to conclude that $\Phi_t^\dagger$ is completely positive.) So in particular, $\Phi_t(\rho)$ is a density matrix whenever $\rho \in M_n(\mathbb{C})$ is a density matrix. Now, as the set of density matrices form a compact convex set and the fact that $\Phi_1^\dagger$ is continuous, Schauder fixed-point theorem[2] implies that there exists a density matrix $\tilde{\rho} \in M_n(\mathbb{C})$ such that $\Phi_1^\dagger(\tilde{\rho}) = \tilde{\rho}$. Note that $\Phi_s^\dagger \Phi_t^\dagger = \Phi_{s+t}^\dagger$ for all $s, t \geq 0$. But then, using this semigroup property, we have $\lim_{t \to \infty} \Phi_t^\dagger(\tilde{\rho}) = \lim_{n \to \infty} (\Phi_1^\dagger)^n(\tilde{\rho}) = \lim_{n \to \infty} \tilde{\rho} = \tilde{\rho}$ where $(\Phi_1^\dagger)^n$ is $\Phi_1^\dagger$ applied n times. Consequently,

$$\Phi_s^\dagger(\tilde{\rho}) = \lim_{t \to \infty} \Phi_s^\dagger \Phi_t^\dagger(\tilde{\rho}) = \lim_{t \to \infty} \Phi_{s+t}^\dagger(\tilde{\rho}) = \lim_{t \to \infty} \Phi_t^\dagger(\tilde{\rho}) = \tilde{\rho} \quad \text{for all } s \geq 0.$$

To prove uniqueness, we note that $\dim \mathrm{Im}(\Phi_t - 1) = \dim M_n(\mathbb{C}) - \dim \ker(\Phi_t - 1) = n^2 - 1$ by the dimension theorem and ergodicity. Therefore,

$$\dim \ker(\Phi_t^\dagger - 1) = \dim \mathrm{Im}(\Phi_t - 1)^\perp = \dim M_n(\mathbb{C}) - \dim \mathrm{Im}(\Phi_t - 1) = 1.$$

So if $\tilde{\rho}_1$ is another density matrix invariant under $\Phi_t^\dagger$, then $\tilde{\rho} = \alpha\tilde{\rho}_1$ for some $\alpha \in \mathbb{C}$. However, $\alpha = \mathrm{Tr}(\alpha\tilde{\rho}_1) = \mathrm{Tr}(\rho) = 1$ so that $\tilde{\rho}$ is the unique density matrix invariant under $\Phi_t^\dagger$. □

[2]Theorem (Schauder). *Every continuous function from a nonempty convex compact subset K of a Banach space to K itself has a fixed point.*

Remark 4.3.12. Let $\rho \in \mathfrak{S}_+(A)$. For each $s \in \mathbb{R}$ the inner product $\langle \cdot, \cdot \rangle_{\rho,s}$ is compatible with ρ. From now on a dagger † will be used to denote the adjoint with respect to the Hilbert-Schmidt inner product $\langle \cdot, \cdot \rangle_{\mathrm{HS}}$. Now, if a QMS $(\Phi_t)_{t \geq 0}$ on A is self-adjoint with respect to an inner product $\langle \cdot, \cdot \rangle$ that is compatible with $\rho \in \mathfrak{S}_+(A)$, then for all $a \in A$ and $t \geq 0$ we have

$$\langle a, \Phi_t^\dagger(\rho) \rangle_{\mathrm{HS}} = \langle \Phi_t(a), \rho \rangle_{\mathrm{HS}} = \mathrm{Tr}(\rho \Phi_t(a)) = \langle \Phi_t(a), 1 \rangle = \langle a, \Phi_t(1) \rangle = \langle a, 1 \rangle = \mathrm{Tr}(\rho a) = \langle a, \rho \rangle_{\mathrm{HS}},$$

or equivalently, $\Phi_t^\dagger(\rho) = \rho$ for all $t \geq 0$ and thus ρ is invariant under $\Phi_t^\dagger$. In particular, ρ is invariant under $\Phi_t^\dagger$ if $(\Phi_t)_{t \geq 0}$ satisfies the ρ-DBC because then, for all $t \geq 0$, Φ_t is self-adjoint with respect to $\langle \cdot, \cdot \rangle_{\rho,1}$ which is compatible with ρ. If, moreover $(\Phi_t)_{t \geq 0}$ is ergodic and can be extended to $M_n(\mathbb{C})$, then ρ is the unique density matrix invariant under $\Phi_t^\dagger$ by Proposition 4.3.11.

Proposition 4.3.13. *Let $\Phi_t = e^{tL}$ be an ergodic QMS on $M_n(\mathbb{C})$ satisfying the ρ-DBC for its unique invariant density matrix $\rho \in \mathfrak{S}_+$. Then $\lim_{t \to \infty} \Phi_t^\dagger(h) = \rho$ for all density matrices $h \in M_n(\mathbb{C})$.*

Proof. Let L' be the adjoint of L with respect to $\langle \cdot, \cdot \rangle_{\rho,1}$. Then, using the fact that L is $*$-preserving, we have for all $a, b \in M_n(\mathbb{C})$ that

$$\begin{aligned}
\langle L^\dagger(a), b \rangle_{\rho,1} &= \mathrm{Tr}(\rho b^* L^\dagger(a)) = \langle L^\dagger(a), b\rho \rangle_{\mathrm{HS}} = \langle a, L(b\rho) \rangle_{\mathrm{HS}} = \mathrm{Tr}(L(\rho b^*)a) = \mathrm{Tr}(\rho^{-1}\rho L(\rho b^*)a) \\
&= \mathrm{Tr}(\rho L(\rho b^*)a\rho^{-1}) = \langle a\rho^{-1}, L(b\rho) \rangle_{\rho,1} = \langle L'(a\rho^{-1}), b\rho \rangle_{\rho,1} = \mathrm{Tr}(\rho^2 b^* L'(a\rho^{-1})) \\
&= \mathrm{Tr}(\rho b^* L'(a\rho^{-1})\rho) = \langle L'(a\rho^{-1})\rho, b \rangle_{\rho,1}.
\end{aligned}$$

This implies that $L^\dagger(a) = L'(a\rho^{-1})\rho$ for all $a \in M_n(\mathbb{C})$. Note that $L = L'$ by Corollary 4.3.9, so in this case we have $L^\dagger(a) = L(a\rho^{-1})\rho$ for all $a \in M_n(\mathbb{C})$. Using induction one can show that

$$(L^\dagger)^k(a) = L^k(a\rho^{-1})\rho \quad \text{for all } a \in M_n(\mathbb{C}) \text{ and } k \in \mathbb{N}.$$

Moreover, L has spectral decomposition $L = \sum_{k=0}^r \mu_k P_k$ where $\mu_k \in \mathbb{R}$ are eigenvalues of L and P_k are the corresponding projections onto the μ_k-eigenspace. Note that $\ker(L) = \mathrm{span}(\mathrm{id}_{\mathbb{C}^n})$ by ergodicity of $(\Phi_t)_{t \geq 0}$. Hence, we may assume that $\mu_k = 0$ and P_0 is the projection onto $\mathrm{span}(\mathrm{id}_{\mathbb{C}^n})$. Furthermore, $\mu_k \leq 0$ for $k = 0, ..., r$. Otherwise, if $\mu = \mu_k > 0$ for some $k \in \{1, ..., r\}$ with eigenvector $x \in M_n(\mathbb{C})$, then

$$\lim_{t \to \infty} \|\Phi_t(x)\| = \lim_{t \to \infty} \|e^{tL}(x)\| = \lim_{t \to \infty} \left\|e^{t\mu} x\right\| = \lim_{t \to \infty} e^{t\mu}\|x\| = \infty,$$

contradicting the contractivity of $(\Phi_t)_{t \geq 0}$. So, indeed, $\mu_k \leq 0$ for $k = 0, ..., r$ and in particular $\mu_k < 0$ for $k = 1, ..., r$. But then, for any density matrix $h \in M_n(\mathbb{C})$ we obtain

$$\begin{aligned}
\lim_{t \to \infty} \Phi_t^\dagger(h) &= \lim_{t \to \infty} \sum_{k=0}^\infty \frac{(tL^\dagger)^k(h)}{k!} = \lim_{t \to \infty} \sum_{k=0}^\infty \frac{(tL)^k(h\rho^{-1})\rho}{k!} = \lim_{t \to \infty} e^{tL}(h\rho^{-1})\rho \\
&= \lim_{t \to \infty} \sum_{k=0}^r e^{t\mu_k} P_k(h\rho^{-1})\rho = \lim_{t \to \infty} e^{t \cdot 0} P_0(h\rho^{-1})\rho + \sum_{k=1}^r \lim_{t \to \infty} e^{t\mu_k} P_k(h\rho^{-1})\rho \\
&= P_0(h\rho^{-1})\rho = \alpha\rho,
\end{aligned}$$

for some $\alpha \in \mathbb{C}$. Since $\Phi_t^\dagger$ maps density matrices to density matrices for all $t \geq 0$, we necessarily have $\alpha = 1$ and this finishes the proof. □

4.4 Generators of quantum Markov semigroups on $M_n(\mathbb{C})$ with detailed balance

This subsection focuses on the generators of quantum Markov semigroups defined on matrix algebras satisfying detailed balance. Obviously, Corollary 4.2.10 also applies to these quantum Markov semigroups since we are working finite dimensional and thus the generators are bounded. However, it turns out that another expression for generators of quantum Markov semigroups with detailed balance is also helpful.

Theorem 4.4.1. *Let $\Phi_t = e^{tL}$ be a QMS on a C^*-subalgebra $A \subseteq M_n(\mathbb{C})$. Suppose that $(\Phi_t)_{t\geq 0}$ satisfies the ρ-DBC for $\rho \in \mathfrak{S}_+(A)$ and that Φ_t has an extension $\widetilde{\Phi_t}$ to a QMS on $M_n(\mathbb{C})$. Regard the modular operator Δ_ρ built from $\mathrm{Tr}(\cdot\rho)$ as an operator on $M_n(\mathbb{C})$. Then the generator $L : A \to A$ of Φ_t has the form*

$$L(a) = \sum_{j\in\mathcal{J}} \left(e^{-\omega_j/2} v_j^*[a, v_j] + e^{\omega_j/2}[v_j, a]v_j^*\right) \tag{4.1}$$

$$= \sum_{j\in\mathcal{J}} e^{-\omega_j/2} \left(v_j^*[a, v_j] + [v_j^*, a]v_j\right), \tag{4.2}$$

where $\mathcal{J}$ is a finite index set such that $\omega_j \in \mathbb{R}$ for all $j \in \mathcal{J}$, and $\{v_j\}_{j\in\mathcal{J}}$ is a set in $M_n(\mathbb{C})$ with the properties:

(1) $\mathrm{Tr}(v_j^* v_k) = c_j\delta_{j,k}$ *for all $j, k \in \mathcal{J}$ and some constant $c_j \geq 0$;*

(2) $\mathrm{Tr}(v_j) = 0$ *for all $j \in \mathcal{J}$;*

(3) $\{v_j\}_{j\in\mathcal{J}} = \{v_j^*\}_{j\in\mathcal{J}}$*;*

(4) $\{v_j\}_{j\in\mathcal{J}}$ *consist of eigenvectors of the modular operator Δ_ρ with $\Delta_\rho v_j = e^{-\omega_j} v_j$.*

Conversely, given any $\rho \in \mathfrak{S}_+(A)$ and any set $\{v_j\}_{j\in\mathcal{J}} \subseteq M_n(\mathbb{C})$ satisfying (3) and (4) for some $\{\omega_j\}_{j\in\mathcal{J}} \subseteq \mathbb{R}$, the operator L given by (4.1)/(4.2) *is the generator of a QMS $(\Phi_t)_{t\geq 0}$ that satisfies the ρ-DBC.*

A couple remarks will be made before a proof will be given.

Remark 4.4.2. Note that the eigenvectors $\{v_j\}_{j\in\mathcal{J}}$ of Δ_ρ are not necessarily self-adjoint. Nevertheless, if $\rho = \frac{1}{n}1$, then Δ_ρ is the identity so that each v_j is an eigenvector of Δ_ρ with eigenvalue 1. So in this case we have $\omega_j = 0$ for all $j \in \mathcal{J}$ and it is then possible to take each v_j to be self-adjoint. It follows that (4.2) reduces to

$$L(a) = -\sum_{j\in\mathcal{J}} [v_j, [v_j, a]] \quad \text{for } a \in A.$$

This is verified by a straightforward computation:

$$\begin{aligned} L(a) &= \sum_{j\in\mathcal{J}} (v_j[a, v_j] + [v_j, a]v_j) = \sum_{j\in\mathcal{J}} (v_j a v_j - v_j v_j a + v_j a v_j - a v_j v_j) \\ &= -\sum_{j\in J} (v_j v_j a - v_j a v_j - v_j a v_j + a v_j v_j) = -\sum_{j\in J} (v_j[v_j, a] - [v_j, a]v_j) = -\sum_{j\in J} [v_j, [v_j, a]]. \end{aligned}$$

Remark 4.4.3. By Theorem 4.4.1, the Hilbert-Schmidt adjoint of L is given by

$$L^\dagger(b) = \sum_{j\in J} \left(e^{-\omega_j/2}[v_j b, v_j^*] + e^{\omega_j/2}[v_j^*, b v_j]\right) \quad \text{for } b \in A.$$

To see this, let $a, b \in A$. Then, using (4.1),

$$\begin{aligned}
\langle L(a), b\rangle_{\mathrm{HS}} &= \sum_{j\in J} \Big(e^{-\omega_j/2} \left(\langle v_j^* a v_j, b\rangle_{\mathrm{HS}} - \langle v_j^* v_j a, b\rangle_{\mathrm{HS}} \right) + e^{\omega_j/2} \left(\langle v_j a v_j^*, b\rangle_{\mathrm{HS}} - \langle a v_j v_j^*, b\rangle_{\mathrm{HS}} \right) \Big) \\
&= \sum_{j\in J} \Big(e^{-\omega_j/2} \left(\mathrm{Tr}(b^* v_j^* a v_j) - \mathrm{Tr}(b^* v_j^* v_j a) \right) + e^{\omega_j/2} \left(\mathrm{Tr}(b^* v_j a v_j^*) - \mathrm{Tr}(b^* a v_j v_j^*) \right) \Big) \\
&= \sum_{j\in J} \Big(e^{-\omega_j/2} \left(\langle a, v_j b v_j^*\rangle_{\mathrm{HS}} - \langle a, v_j^* v_j b\rangle_{\mathrm{HS}} \right) + e^{\omega_j/2} \left(\langle a, v_j^* b v_j\rangle_{\mathrm{HS}} - \langle a, b v_j v_j^*\rangle_{\mathrm{HS}} \right) \Big) \\
&= \sum_{j\in J} \Big(e^{-\omega_j/2} \left\langle a, [v_j b, v_j^*]\right\rangle_{\mathrm{HS}} + e^{\omega_j/2} \left\langle a, [v_j^*, b v_j]\right\rangle_{\mathrm{HS}} \Big) \\
&= \left\langle a, \sum_{j\in J} \Big(e^{-\omega_j/2} [v_j b, v_j^*] + e^{\omega_j/2} [v_j^*, b v_j] \Big) \right\rangle_{\mathrm{HS}},
\end{aligned}$$

and this exactly implies that $L^\dagger(b) = \sum_{j\in J} \Big(e^{-\omega_j/2}[v_j b, v_j^*] + e^{\omega_j/2}[v_j^*, b v_j] \Big)$.

The proof of Theorem 4.4.1 relies on few other results and it starts with an isometry property that is crucial to the characterization of generators of quantum Markov semigroups given by Gorini, Kossakowski and Sudarshan [10].

For any Hilbert space H, let $L^2(H)$ denote the Hilbert space consisting of Hilbert-Schmidt operators from $H \to H$ equipped with the Hilbert-Schmidt inner product $\langle a, b\rangle_{L^2(H)} := \mathrm{Tr}(b^* a)$ for $a, b \in L^2(H)$. We may also just write $\langle \cdot, \cdot\rangle_{\mathrm{HS}}$ for $\langle \cdot, \cdot\rangle_{L^2(H)}$ as before and both these notations will be used interchangeably. The dagger $\dagger$ denotes the adjoint with respect to $\langle \cdot, \cdot\rangle_{L^2(H)}$ as usual. We also set $H_n := (M_n(\mathbb{C}), \langle \cdot, \cdot\rangle_{\mathrm{HS}})$ for convenience.

There is a natural identification $H_n \otimes H_n \cong L^2(H_n)$ using the following multiplication on H_n: For $a, b \in H_n$, define

$$\#(a \otimes b) : H_n \to H_n, \quad \#(a \otimes b)x = axb.$$

Lemma 4.4.4. *Let $\{f_\alpha\}$ and $\{g_\beta\}$ be two orthonormal bases of H_n, so that $\{f_\alpha \otimes g_\beta\}$ is an orthonormal basis of $H_n \otimes H_n$. Then $\{\#(f_\alpha \otimes g_\beta)\}$ is orthonormal in $L^2(H_n)$. In particular, the map $\#$ is unitary from $H_n \otimes H_n$ onto $L^2(H_n)$.*

Proof. Let $\{e_{i,j}\}_{1\le i,j\le n}$ be the matrix units of H_n and note that $\{e_{i,j}\}_{1\le i,j\le n}$ is an orthonormal basis for H_n. It follows that

$$\begin{aligned}
\langle \#(f_\alpha \otimes g_\beta), \#(f_\mu \otimes g_\nu)\rangle_{\mathrm{HS}} &= \mathrm{Tr}\left(\#(f_\mu \otimes g_\nu)^\dagger \#(f_\alpha \otimes g_\beta) \right) = \sum_{i,j=1}^n \langle f_\alpha e_{i,j} g_\beta, f_\mu e_{i,j} g_\nu\rangle_{\mathrm{HS}} \\
&= \sum_{i,j=1}^n \mathrm{Tr}\left((f_\mu e_{i,j} g_\nu)^* f_\alpha e_{i,j} g_\beta \right) = \sum_{i,j=1}^n \mathrm{Tr}(g_\nu^* e_{j,i} f_\mu^* f_\alpha e_{i,j} g_\beta) \\
&= \sum_{i,j=1}^n \left(g_\nu g_\beta^* \right)_{j,j} \left(f_\alpha^* f_\mu \right)_{i,i} = \mathrm{Tr}(g_\nu g_\beta^*)\mathrm{Tr}(f_\alpha^* f_\mu) \\
&= \delta_{\beta,\nu}\delta_{\mu,\alpha}.
\end{aligned}$$

Hence, $\{\#(f_\alpha \otimes g_\beta)\}$ is orthonormal in $L^2(H_n)$ and since $\dim(H_n \otimes H_n) = \dim(L^2(H_n))$ we conclude that $\# : H_n \otimes H_n \to L^2(H_n)$ is unitary. □

Consider any linear transformation K on H_n. Let $\{f_\beta\}$ be any orthonormal basis for H_n. Then $\{f_\alpha^*\}$ is also an orthonormal basis for H_n and by Lemma 4.4.4, $\{\#(f_\alpha^* \otimes f_\beta)\}$ is an orthonormal basis for $L^2(H_n)$. Thus K can be written as

$$K = \sum_{\alpha,\beta} c_{\alpha,\beta}\#(f_\alpha^* \otimes f_\beta), \text{ or equivalently, } K(a) = \sum_{\alpha,\beta} c_{\alpha,\beta} f_\alpha^* a f_\beta \text{ for all } a \in H_n,$$

where the coefficients $c_{\alpha,\beta}$ are uniquely determined by

$$c_{\alpha,\beta} = \langle K, \#(f_\alpha^* \otimes f_\beta)\rangle_{L^2(H_n)}.$$

Definition 4.4.5. Let K be a linear operator on H_n. The $n^2 \times n^2$ matrix $(c_{\alpha,\beta})_{\alpha,\beta}$ with entries $c_{\alpha,\beta} = \langle K, \#(f_\alpha^* \otimes f_\beta)\rangle_{L^2(H_n)}$ is called the *GKS (Gorini-Kossakowski-Sudarshan) matrix for the operator K with respect to the orthonormal basis* $\{f_\alpha\}$ for H_n. When we wish to emphasize the dependence on K, we write $c_{\alpha,\beta}(K)$ for $c_{\alpha,\beta}$.

Remark 4.4.6. Let $a, b \in M_n(\mathbb{C})$, consider the case $K = \#(a \otimes b)$. Since $\#$ is unitary (by Lemma 4.4.4), the GKS matrix of K with respect to an orthonormal basis $\{f_\alpha\}$ is given by

$$c_{\alpha,\beta} = \langle \#(a \otimes b), \#(f_\alpha^* \otimes f_\beta)\rangle_{L^2(H_n)} = \langle a \otimes b, f_\alpha^* \otimes f_\beta\rangle_{H_n \otimes H_n} = \langle a, f_\alpha^*\rangle_{\mathrm{HS}}\langle b, f_\beta\rangle_{\mathrm{HS}} = \mathrm{Tr}(f_\alpha a)\mathrm{Tr}(f_\beta^* b).$$

In particular, taking $a = b = 1$ gives $K = \mathrm{id}_{M_n(\mathbb{C})}$ so that the GKS matrix of the identity with respect to $\{f_\alpha\}$ is given by

$$c_{\alpha,\beta}\left(\mathrm{id}_{M_n(\mathbb{C})}\right) = \mathrm{Tr}(f_\alpha)\mathrm{Tr}(f_\beta^*).$$

Lemma 4.4.7. *Let K be a linear operator on $M_n(\mathbb{C})$ and let $\{f_\alpha\}$ be an orthonormal basis of H_n. Then the GKS matrix of K with respect to $\{f_\alpha\}$ is self-adjoint if and only if $K(a)^* = K(a^*)$ for all $a \in M_n(\mathbb{C})$.*

Proof. We have the GKS expansion $K = \sum_{\alpha,\beta} c_{\alpha,\beta}\#(f_\alpha^* \otimes f_\beta)$. Let $a \in M_n(\mathbb{C})$, then

$$K(a^*)^* = \left(\sum_{\alpha,\beta} c_{\alpha,\beta} f_\alpha^* a^* f_\beta\right)^* = \sum_{\alpha,\beta} \overline{c_{\alpha,\beta}} f_\beta^* a f_\alpha = \sum_{\alpha,\beta} \overline{c_{\beta,\alpha}} f_\alpha^* a f_\beta = \sum_{\alpha,\beta} \overline{c_{\beta,\alpha}}\#(f_\alpha^* \otimes f_\beta)a.$$

By the uniqueness of the GKS-expansion, we have $K(a)^* = K(a^*)$ for all $a \in M_n(\mathbb{C})$ if and only if $c_{\alpha,\beta} = \overline{c_{\beta,\alpha}}$ for all α, β. ☐

For all $a, b \in M_n(\mathbb{C})$, one can consider their tensor product $a \otimes b \in M_n(\mathbb{C}) \otimes M_n(\mathbb{C})$, which sends $\xi \otimes \eta \in \mathbb{C}^n \otimes \mathbb{C}^n$ to $a\xi \otimes b\eta \in \mathbb{C}^n \otimes \mathbb{C}^n$. If $\mathbb{C}^n \otimes \mathbb{C}^n$ is identified with $M_n(\mathbb{C})$ through $\xi \otimes \eta \mapsto \sum_{i,j=1}^n \xi_i \eta_j e_{i,j}$ ($e_{i,j}$'s are matrix units), then $a \otimes b$ becomes an operator on $M_n(\mathbb{C})$. This identification will be used in the next lemma.

Lemma 4.4.8. *Let K be a linear operator on $M_n(\mathbb{C})$ and $\{e_{i,j}\}_{1 \le i,j \le n}$ be the matrix units of $M_n(\mathbb{C})$. Then $C(K) := \sum_{i,j=1}^n K(e_{i,j}) \otimes e_{i,j} \in M_n(\mathbb{C}) \otimes M_n(\mathbb{C})$ viewed as an operator on H_n satisfies*

$$\langle C(K)f, g\rangle_{\mathrm{HS}} = \langle K, \#(g \otimes f^*)\rangle_{L^2(H_n)} \quad \textit{for all } f, g \in H_n,$$

where $\sum_{i,j=1}^n K(e_{i,j}) \otimes e_{i,j}$ may also be viewed as an element of $M_n(M_n(\mathbb{C}))$ whose i, j entry is $K(e_{i,j})$.

Proof. By a direct computation we obtain

$$\begin{aligned}\langle C(K)f,g\rangle_{\mathrm{HS}} &= \sum_{k,m=1}^{n} \overline{g_{k,m}}(C(K)f)_{k,m} = \sum_{i,j,k,l,m,p=1}^{n} \overline{g_{k,m}}[K(e_{i,j})]_{k,l}[e_{i,j}]_{m,p}f_{l,p} \\ &= \sum_{i,j,k,l.m,p=1}^{n} f_{l,p}[e_{j,i}]_{p,m}\overline{g_{k,m}}[K(e_{i,j})]_{k,l} = \sum_{i,j,k,l=1}^{n} (fe_{j,i}g^*)_{l,k}[K(e_{i,j})]_{k,l} \\ &= \sum_{i,j,k,l=1}^{n} (ge_{i,j}f^*)^*_{l,k}[K(e_{i,j})]_{k,l} = \sum_{i,j=1}^{n} \langle K(e_{i,j}), ge_{i,j}f^*\rangle_{\mathrm{HS}} = \langle K, \#(g\otimes f^*)\rangle_{L^2(H_n)}. \quad \square\end{aligned}$$

Remark 4.4.9. The matrix $C(K)$ in Lemma 4.4.8 is called the *Choi matrix of* K and a fundamental theorem of Choi states that $C(K)$ is positive on H_n if and only if K is completely positive [6]. Let $\{f_\alpha\}$ be any orthonormal basis for H_n. Then, by Lemma 4.4.8,

$$\begin{aligned}\left\langle (c_{\alpha,\beta})_{\alpha,\beta}\vec{\lambda}, \vec{\lambda}\right\rangle_{\mathbb{C}^{n^2}} &= \sum_{\alpha,\beta} c_{\alpha,\beta}\lambda_\alpha\overline{\lambda_\beta} = \sum_{\alpha,\beta}\langle K, \#(f^*_\alpha\otimes f_\beta)\rangle_{L^2(H_n)}\lambda_\alpha\overline{\lambda_\beta} \\ &= \sum_{\alpha,\beta}\langle K, \#((\lambda_\alpha f_\alpha)^*\otimes \lambda_\beta f_\beta)\rangle_{L^2(H_n)} = \sum_{\alpha,\beta}\langle C(K)(\lambda_\beta f_\beta)^*, (\lambda_\alpha f_\alpha)^*\rangle_{\mathrm{HS}} \\ &= \left\langle C(K)\sum_\beta \overline{\lambda_\beta} f^*_\beta, \sum_\alpha \overline{\lambda_\alpha} f^*_\alpha\right\rangle_{\mathrm{HS}},\end{aligned}$$

for all $\vec{\lambda}\in\mathbb{C}^{n^2}$. It follows that the GKS matrix $(c_{\alpha,\beta})$ is positive if and only if K is completely positive by Choi's theorem and the fact that $\{f^*_\alpha\}$ is also an orthonormal basis for H_n.

Going forward, it will be convenient to assume that the orthonormal bases $\{f_\alpha\}$ for H_n are indexed by $\alpha \in \{1,...,n\}\times\{1,...,n\}$, and for such bases we make the following definition:

Definition 4.4.10. Let L be a linear operator on $M_n(\mathbb{C})$ such that $L(1) = 0$ and $L(a)^* = L(a^*)$ for all $a\in M_n(\mathbb{C})$. Let $\{f_\alpha\}$ be any orthonormal basis of H_n such that $f_{(1,1)} = 1$. Let $(c_{\alpha,\beta})$ be the GKS matrix of L with respect to $\{f_\alpha\}$. The $(n^2-1)\times(n^2-1)$ matrix with entries $c_{\alpha,\beta}$ where α and β range over the set $\{(i,j) : 1\le i,j\le n \text{ and } (i,j)\ne(1,1)\}$ is called the *reduced GKS matrix of L for the basis* $\{f_\alpha\}$.

Lemma 4.4.11. *Let L be a linear operator on $M_n(\mathbb{C})$ and let $\Phi_t = e^{tL}$ be $*$-preserving. Let $\{f_\alpha\}$ be an orthonormal basis for H_n with $f_{(1,1)} = 1$. Then Φ_t is completely positive for all $t\ge 0$ if and only if the reduced GKS matrix of L for the basis $\{f_\alpha\}$ is positive.*

Proof. Suppose that Φ_t is completely positive for all $t\ge0$. By Remark 4.4.6 and orthogonality we obtain $c_{\alpha,\beta}(1) = \mathrm{Tr}(f_\alpha)\mathrm{Tr}(f^*_\beta) = \delta_{\alpha,(1,1)}\delta_{\beta,(1,1)}$. In particular, we see that the reduced GKS matrix of the identity is zero. Now since $c_{\alpha,\beta}(t^{-1}(\Phi_t - 1)) = t^{-1}c_{\alpha,\beta}(\Phi_t) - t^{-1}c_{\alpha,\beta}(1)$, it follows that the reduced GKS matrix of $t^{-1}(\Phi_t-1)$ is equal to the reduced GKS matrix of $t^{-1}\Phi_t$. Moreover, the GKS matrix of $t^{-1}\Phi_t$ is positive by Remark 4.4.9 and the reduced GKS matrix of $t^{-1}\Phi_t$ is thus also positive. Now taking the limit $t\to0$ we conclude that the reduced GKS matrix of L is positive

Conversely, suppose that the reduced GKS matrix of L is positive. First note that the GKS matrix of Φ_t is self-adjoint for all $t\ge0$ by Lemma 4.4.7. And for small enough $t>0$, we have $c_{\alpha,\beta}(\Phi_t) = c_{\alpha,\beta}(1) + tc_{\alpha,\beta}(L) + o(t)$ using the series expansion of $\Phi_t = e^{tL}$. Now since the reduced GKS matrix of L is positive and $c_{\alpha,\beta}(1) = \delta_{\alpha,(1,1)}\delta_{\beta,(1,1)}$, the GKS matrix of Φ_t is positive for sufficiently small $t > 0$. It follows that Φ_t is completely positive for sufficiently small $t > 0$ by Remark 4.4.9. Consequently, Φ_t is completely positive for all $t > 0$ by the semigroup property. $\square$

Proposition 4.4.12. *Let L be a linear operator on $M_n(\mathbb{C})$ such that $L(1) = 0$ and $L(a)^* = L(a^*)$ for all $a \in M_n(\mathbb{C})$. Let $\{f_\alpha\}$ be any orthonormal basis for H_n such that $f_{(1,1)} = 1$. Let $(c_{\alpha,\beta})$ be the GKS matrix of L with respect to $\{f_\alpha\}$. Then L has the form*

$$L(a) = -i[h, a] + \frac{1}{2} \sum_{\alpha,\beta \neq (1,1)} c_{\alpha,\beta} \left(f_\alpha^*[a, f_\beta] + [f_\alpha^*, a] f_\beta \right) \qquad (a \in M_n(\mathbb{C})),$$

where h is the traceless self-adjoint matrix given by

$$h = \frac{1}{2i} \sum_{\beta \neq (1,1)} \left(c_{(1,1),\beta} f_\beta - c_{\beta,(1,1)} f_\beta^* \right).$$

Proof. Using the facts that $c_{\alpha,\beta} = \overline{c_{\beta,\alpha}}$ for all α, β by Lemma 4.4.7 and $f_{(1,1)} = 1$, L has the GKS-expansion

$$L(a) = \sum_{\alpha,\beta} c_{\alpha,\beta} f_\alpha^* a f_\beta = g^* a + a g + \sum_{\alpha,\beta \neq (1,1)} c_{\alpha,\beta} f_\alpha^* a f_\beta,$$

where $g := \frac{c_{(1,1),(1,1)}}{2} 1 + \sum_{\beta \neq (1,1)} c_{(1,1),\beta} f_\beta$. Let $k = \frac{1}{2}(g + g^*)$ and $h = \frac{1}{2i}(g - g^*)$ be self-adjoint such that $g = k + ih$, then we have

$$L(a) = g^* a + a g + \sum_{\alpha,\beta \neq (1,1)} c_{\alpha,\beta} f_\alpha^* a f_\beta = -i[h, a] + ka + ak + \sum_{\alpha,\beta \neq (1,1)} c_{\alpha,\beta} f_\alpha^* a f_\beta,$$

for all $a \in M_n(\mathbb{C})$. Using this and the fact that $L(1) = 0$, we obtain $k = -\frac{1}{2} \sum_{\alpha,\beta \neq (1,1)} c_{\alpha,\beta} f_\alpha^* f_\beta$ and therefore

$$\begin{aligned} L(a) &= -i[h, a] + ka + ak + \sum_{\alpha,\beta \neq (1,1)} c_{\alpha,\beta} f_\alpha^* a f_\beta = -i[h, a] + \sum_{\alpha,\beta \neq (1,1)} \left(f_\alpha^* a f_\beta - \frac{1}{2} f_\alpha^* f_\beta a - \frac{1}{2} a f_\alpha^* f_\beta \right) \\ &= -i[h, a] + \frac{1}{2} \sum_{\alpha,\beta \neq (1,1)} c_{\alpha,\beta} \left(f_\alpha^*[a, f_\beta] + [f_\alpha^*, a] f_\beta \right). \end{aligned}$$

Furthermore, $\mathrm{Tr}(g) = \frac{1}{2} c_{(1,1),(1,1)} \mathrm{Tr}(1) + \sum_{\beta \neq (1,1)} c_{(1,1),\beta} \mathrm{Tr}(f_\beta) = \frac{n}{2} c_{(1,1),(1,1)} \in \mathbb{R}$ by orthogonality, so this implies that $\mathrm{Tr}(h) = 0$ as $\mathrm{Tr}(h)$ is the imaginary part of $\mathrm{Tr}(g)$. And,

$$h = \frac{1}{2i}(g - g^*) = \frac{1}{2i} \left(\sum_{\beta \neq (1,1)} c_{(1,1),\beta} f_\beta - \sum_{\beta \neq (1,1)} \overline{c_{(1,1),\beta}} f_\beta^* \right) = \frac{1}{2i} \sum_{\beta \neq (1,1)} \left(c_{(1,1),\beta} f_\beta - c_{\beta,(1,1)} f_\beta^* \right),$$

as $(c_{\alpha,\beta})$ is a self-adjoint matrix. $\square$

Next, we give the definition of a *modular basis*. Let $\rho \in \mathfrak{S}_+$. Then we first note that the modular operator Δ_ρ is also positive with respect to the Hilbert-Schmidt inner product: $\langle \Delta_\rho(x), x \rangle_{\mathrm{HS}} = \mathrm{Tr}(x^* \Delta_\rho(x)) = \mathrm{Tr}(x^* \rho x \rho^{-1}) = \mathrm{Tr}(\rho^{-1/2} x^* \rho^{1/2} \rho^{1/2} x \rho^{-1/2}) = \mathrm{Tr}(|\rho^{1/2} x \rho^{-1/2}|^2) \geq 0$ for all $x \in M_n(\mathbb{C})$. So there exists an orthonormal basis $\{x_1, ..., x_{n^2}\}$ for H_n consisting of eigenvectors of Δ_ρ and all eigenvalues of Δ_ρ are non-negative. Since $\Delta_\rho(1) = 1$, we may assume that $x_1 = 1$. In this case, we have $\text{Tr}(x_\gamma) = 0$ for $\gamma = 2, ..., n^2$ by orthogonality. Moreover, since Δ_ρ is invertible, all eigenvalues of Δ_ρ are strictly positive and we can write them in the form $e^{-\omega_\gamma}$ for some $\omega_\gamma \in \mathbb{R}$. Now since $(\Delta_\rho(x))^* = \Delta_\rho^{-1}(x^*)$ for all $x \in A$, we have

$$\Delta_\rho(x) = e^{-\omega} x \iff \Delta_\rho(x^*) = e^{\omega} x^* \quad \text{for } x \in A \text{ and } \omega \in \mathbb{R}.$$

This important equivalence will be used tacitly. In particular, $e^{-\omega}$ is an eigenvalue of Δ_ρ if and only if e^{ω} is an eigenvalue of Δ_ρ, and the set of eigenvectors of Δ_ρ is self-adjoint. Hence, it follows that there exists an eigenbasis for H_n with the following properties that are stated in the next definition:

Definition 4.4.13. Let $\rho \in \mathfrak{S}_+$. The *modular basis of* Δ_ρ is an orthonormal basis $\{x_1, ..., x_{n^2}\}$ for H_n with the following properties:

(1) $\{x_1, .., x_{n^2}\}$ consists of eigenvectors of Δ_ρ ;

(2) $x_1 = 1$;

(3) $\{x_1, ..., x_{n^2}\} = \{x_1^*, ..., x_{n^2}^*\}$, i.e. the set $\{x_1, ..., x_{n^2}\}$ of eigenvectors is self-adjoint.

Theorem 4.4.14. *Let L be the generator of a QMS that satisfies the ρ-DBC for some $\rho \in \mathfrak{S}_+$. Let $(c_{\alpha,\beta})$ be the GKS matrix of L with respect to a modular orthonormal basis $\{f_\alpha\}$ for H_n. Then for all α, β we have*

$$e^{\omega_\alpha} c_{\alpha,\beta} = c_{\alpha,\beta} e^{\omega_\beta} \quad \textit{and} \quad c_{\alpha,\beta} = e^{-\omega_\alpha} c_{\beta',\alpha'},$$

where for each α, ω_α is the real number satisfying $\Delta_\rho(f_\alpha) = e^{-\omega_\alpha} f_\alpha$ and α', β' are defined by $f_{\alpha'} = f_\alpha^*$ and $f_{\beta'} = f_\beta^*$. In particular, the GKS matrix of L commutes with the diagonal matrix $(\delta_{\alpha,\beta} e^{\omega_\alpha})_{\alpha,\beta}$

Proof. By Corollary 4.3.9, L and Δ_ρ commute and it follows that for all $a \in M_n(\mathbb{C})$,

$$\rho^{-1} L(\rho a \rho^{-1})\rho = \rho^{-1} L(\Delta_\rho(a))\rho = \rho^{-1} \Delta_\rho(L(a))\rho = \rho^{-1}\rho L(a)\rho^{-1}\rho = L(a).$$

From $\Delta_\rho(f_\alpha) = e^{-\omega_\alpha} f_\alpha$, it follows that $\rho^{-1} f_\alpha^* \rho = \Delta_\rho(f_\alpha)^* = e^{-\omega_\alpha} f_\alpha^*$ and $\rho^{-1} f_\beta \rho = \Delta_\rho(f_\beta^*)^* = e^{\omega_\beta} f_\beta$. Consequently, using the GKS-expansion of L, we see that

$$\sum_{\alpha,\beta} c_{\alpha,\beta} f_\alpha^* a f_\beta = L(a) = \rho^{-1} L(\rho a \rho^{-1})\rho = \sum_{\alpha,\beta} c_{\alpha,\beta} \rho^{-1} f_\alpha^* \rho a \rho^{-1} f_\beta \rho = \sum_{\alpha,\beta} e^{\omega_\beta - \omega_\alpha} f_\alpha^* a f_\beta,$$

and we obtain $e^{\omega_\alpha} c_{\alpha,\beta} = c_{\alpha,\beta} e^{\omega_\beta}$ by the uniqueness of the coefficients. And in particular, the GKS-matrix of L commutes with the diagonal matrix $(\delta_{\alpha,\beta} e^{\omega_\alpha})_{\alpha,\beta}$

Now note that for all $a, b \in M_n(\mathbb{C})$ we have

$$\begin{aligned} \langle L(a), b\rangle_{\text{HS}} &= \text{Tr}(b^* L(a)) = \sum_{\alpha,\beta} \text{Tr}(b^* c_{\alpha,\beta} f_\alpha^* a f_\beta) = \sum_{\alpha,\beta} \text{Tr}(c_{\alpha,\beta} f_\beta b^* f_\alpha^* a) \\ &= \sum_{\alpha,\beta} \text{Tr}((\overline{c_{\alpha,\beta}} f_\alpha b f_\beta^*)^* a) = \left\langle a, \sum_{\alpha,\beta} \overline{c_{\alpha,\beta}} f_\alpha b f_\beta^* \right\rangle_{\text{HS}}, \end{aligned}$$

which implies $L^\dagger(b) = \sum_{\alpha,\beta} \overline{c_{\alpha,\beta}} f_\alpha b f_\beta^* = \sum_{\alpha,\beta} c_{\beta,\alpha} f_\alpha b f_\beta^*$, where the last equality follows from Lemma 4.4.7. In the proof of Proposition 4.3.13 we have shown that $L^\dagger(b) = L'(b\rho^{-1})\rho$ for all $b \in M_n(\mathbb{C})$, where L' is the adjoint of L with respect to $\langle \cdot, \cdot \rangle_{\rho,1}$. And since $L' = L$, we obtain $L^\dagger(b) = L(b\rho^{-1})\rho$, or equivalently, $L(b) = L^\dagger(b\rho)\rho^{-1}$ for all $b \in M_n(\mathbb{C})$. Using the GKS-expansion of L,

$$\sum_{\alpha,\beta} c_{\alpha,\beta} f_\alpha^* b f_\beta = L(b) = L^\dagger(b\rho)\rho^{-1} = \sum_{\alpha,\beta} c_{\beta,\alpha} f_\alpha b \rho f_\beta^* \rho^{-1} = \sum_{\alpha,\beta} c_{\beta,\alpha} e^{\omega_\beta} f_\alpha b f_\beta^*,$$

where the last equality uses $\rho f_\beta^* \rho^{-1} = \Delta_\rho(f_\beta^*) = e^{\omega_\beta} f_\beta^*$. Since $f_{\gamma'} = f_\gamma^*$, we have $\omega_{\gamma'} = -\omega_\gamma$ for all γ. Continuing with the last floating equation, we then have

$$\sum_{\alpha,\beta} c_{\alpha,\beta} f_\alpha^* b f_\beta = \sum_{\alpha,\beta} c_{\beta,\alpha} e^{\omega_\beta} f_\alpha b f_\beta^* = \sum_{\alpha,\beta} c_{\beta',\alpha'} e^{\omega_{\beta'}} f_{\alpha'} b f_{\beta'}^* = \sum_{\alpha,\beta} c_{\beta',\alpha'} e^{-\omega_\beta} f_\alpha^* b f_\beta.$$

Using the the uniqueness of the coefficients again, we obtain $c_{\alpha,\beta} = c_{\beta',\alpha'} e^{-\omega_\beta}$ for all α, β. Therefore, $c_{\beta',\alpha'} = c_{\alpha,\beta} e^{\omega_\beta} = e^{\omega_\alpha} c_{\alpha,\beta}$ and this is obviously equivalent to $c_{\alpha,\beta} = e^{-\omega_\alpha} c_{\beta',\alpha'}$ for all α, β. □

Remark 4.4.15. An important observation is that the condition $e^{\omega_\alpha} c_{\alpha,\beta} = c_{\alpha,\beta} e^{\omega_\beta}$ implies that

$$\omega_\alpha \neq \omega_\beta \implies c_{\alpha,\beta} = 0.$$

*Proof of **Theorem 4.4.1**.* By assumption Φ_t has an extension $\widetilde{\Phi_t}$ to a QMS on $M_n(\mathbb{C})$. It suffices to consider $(\widetilde{\Phi_t})_{t\geq 0}$ and for convenience we suppose that the extension is done and Φ_t is a QMS on $M_n(\mathbb{C})$ satisfying the ρ-DBC.

To this end, let $\{f_\alpha\}$ be a modular basis of Δ_ρ for H_n and for each α, ω_α is the real number satisfying $\Delta_\rho(f_\alpha) = e^{-\omega_\alpha} f_\alpha$, and α' is defined by $f_{\alpha'} = f_\alpha^*$. Let $c_{\alpha,\beta}$ be the GKS matrix of L with respect to $\{f_\alpha\}$.

By applying Proposition 4.4.12, we have

$$L(a) = -i[h,a] + \frac{1}{2} \sum_{\alpha,\beta \neq (1,1)} c_{\alpha,\beta} \left(f_\alpha^*[a, f_\beta] + [f_\alpha^*, a] f_\beta\right) \quad \text{for all } a \in M_n(\mathbb{C}),$$

where h is the traceless self-adjoint matrix given by

$$h = \frac{1}{2i} \sum_{\beta \neq (1,1)} \left(c_{(1,1),\beta} f_\beta - c_{\beta,(1,1)} f_\beta^*\right).$$

Since $\omega_{(1,1)} = 0$, it follows that $c_{(1,1),\beta} = c_{\beta,(1,1)} = 0$ whenever $\omega_\beta \neq 0$ by Remark 4.4.15. Moreover, the modular basis $\{f_\alpha\}$ may be chosen such that $f_\beta^* = f_\beta$ if $\omega_\beta = 0$ (by considering their real and imaginary parts and noticing that the real and imaginary parts are eigenvectors of Δ_ρ again with eigenvalue 1) and in this case $\beta = \beta'$. Thus,

$$h = \frac{1}{2i} \sum_{\beta \neq (1,1)} \left(c_{(1,1),\beta} f_\beta - c_{\beta,(1,1)} f_\beta^*\right) = \frac{1}{2i} \sum_{\beta \neq (1,1),\ \omega_\beta = 0} \left(c_{(1,1),\beta} - c_{\beta',(1,1)}\right) f_\beta.$$

However, $c_{\beta',(1,1)} = e^{\omega_{(1,1)'}} c_{\beta',(1,1)} = c_{(1,1),\beta}$ for all β by Theorem 4.4.14 as $(1,1)' = (1,1)$ and $\omega_{(1,1)'} = \omega_{(1,1)} = 0$. Hence, $h = 0$.
Since L has GKS-expansion $L(a) = \sum_{\alpha,\beta} c_{\alpha,\beta} f_\alpha^* a f_\beta$, we can replace α with β' and β with α' to obtain

$$L(a) = \sum_{\alpha,\beta} c_{\alpha,\beta} f_\alpha^* a f_\beta = \sum_{\alpha,\beta} c_{\beta',\alpha'} f_{\beta'}^* a f_{\alpha'} = \sum_{\alpha,\beta} c_{\beta',\alpha'} f_\beta a f_\alpha^* = \sum_{\alpha,\beta} c_{\alpha,\beta} e^{\omega_\alpha} f_\beta a f_\alpha^*,$$

where we used $f^*_\gamma = f_{\gamma'}$ for all γ and Theorem 4.4.14. Applying Proposition 4.4.12 to this GKS-expansion for L, we can rewrite it as

$$L(a) = -i[\hat{h}, a] + \frac{1}{2} \sum_{\alpha,\beta \neq (1,1)} c_{\alpha,\beta} e^{\omega_\alpha} \left(f_\beta [a, f^*_\alpha] + [f_\beta, a] f^*_\alpha \right),$$

for some self adjoint matrix $\hat{h} \in M_n(\mathbb{C})$ and by the same argument as before we also have $\hat{h} = 0$. At this point we have two expressions for L, namely

$$L(a) = \frac{1}{2} \sum_{\alpha,\beta \neq (1,1)} c_{\alpha,\beta} \left(f^*_\alpha [a, f_\beta] + [f^*_\alpha, a] f_\beta \right) \quad \text{and} \quad L(a) = \frac{1}{2} \sum_{\alpha,\beta \neq (1,1)} c_{\alpha,\beta} e^{\omega_\alpha} \left(f_\beta [a, f^*_\alpha] + [f_\beta, a] f^*_\alpha \right).$$

We can average these two to get

$$L(a) = \frac{1}{4} \sum_{\alpha,\beta \neq (1,1)} c_{\alpha,\beta} \left(f^*_\alpha [a, f_\beta] + [f^*_\alpha, a] f_\beta + e^{\omega_\alpha} \left(f_\beta [a, f^*_\alpha] + [f_\beta, a] f^*_\alpha \right) \right).$$

Since the reduced GKS matrix of L is self-adjoint by Lemma 4.4.7 and commutes with the diagonal matrix $(\delta_{\alpha,\beta} e^{\omega_\alpha})_{\alpha,\beta \neq (1,1)}$ by Theorem 4.4.14, there exists a $(n^2-1) \times (n^2-1)$ unitary matrix u that diagonalizes the reduced GKS matrix of L and commutes with $(\delta_{\alpha,\beta} e^{\omega_\alpha})_{\alpha,\beta \neq (1,1)}$. By the same argument as in Remark 4.4.15, we have $u_{\alpha,\gamma} = 0$ if $\omega_\alpha \neq \omega_\gamma$. We may then write each $c_{\alpha,\beta}$ in the form

$$c_{\alpha,\beta} = \frac{1}{2} \sum_{\gamma \neq (1,1)} \overline{u_{\gamma,\alpha}} e^{-\omega_\gamma/2} c_\gamma u_{\gamma,\beta}$$

for some constants c_γ such that $\{\frac{1}{2} e^{-\omega_\gamma/2} c_\gamma\}_{\gamma \neq (1,1)}$ are eigenvalues of the reduced GKS matrix of L. Each c_γ is non-negative since the reduced GKS matrix of L is positive by Lemma 4.4.11. Now since $u_{\alpha,\gamma} = 0$ if $\omega_\alpha \neq \omega_\gamma$, we also have

$$e^{\omega_\alpha} c_{\alpha,\beta} = \frac{1}{2} \sum_{\gamma \neq (1,1)} \overline{u_{\gamma,\alpha}} e^{\omega_\gamma/2} c_\gamma u_{\gamma,\beta}.$$

Define $v_\gamma := \sum_{\beta \neq (1,1)} u_{\gamma,\beta} f_\beta \in M_n(\mathbb{C})$ for $\gamma \neq (1,1)$. Then, for all $a \in M_n(\mathbb{C})$,

$$\begin{aligned}
\sum_{\alpha,\beta \neq (1,1)} c_{\alpha,\beta} f^*_\alpha [a, f_\beta] &= \sum_{\alpha,\beta \neq (1,1)} \left(\frac{1}{2} \sum_{\gamma \neq (1,1)} \overline{u_{\gamma,\alpha}} e^{-\omega_\gamma/2} c_\gamma u_{\gamma,\beta} \right) \left(f^*_\alpha a f_\beta - f^*_\alpha f_\beta a \right) \\
&= \frac{1}{2} \sum_{\alpha,\beta \neq (1,1)} \sum_{\gamma \neq (1,1)} c_\gamma e^{-\omega_\gamma/2} \left(\overline{u_{\gamma,\alpha}} u_{\gamma,\beta} f^*_\alpha a f_\beta - \overline{u_{\gamma,\alpha}} u_{\gamma,\beta} f^*_\alpha f_\beta a \right) \\
&= \frac{1}{2} \sum_{\gamma \neq (1,1)} c_\gamma e^{-\omega_\gamma/2} \sum_{\alpha,\beta \neq (1,1)} \left(\overline{u_{\gamma,\alpha}} u_{\gamma,\beta} f^*_\alpha a f_\beta - \overline{u_{\gamma,\alpha}} u_{\gamma,\beta} f^*_\alpha f_\beta a \right) \\
&= \frac{1}{2} \sum_{\gamma \neq (1,1)} c_\gamma e^{-\omega_\gamma/2} \left(v^*_\gamma a v_\gamma - v^*_\gamma v_\gamma a \right) = \frac{1}{2} \sum_{\gamma \neq (1,1)} c_\gamma e^{-\omega_\gamma/2} v^*_\gamma [a, v_\gamma],
\end{aligned}$$

and similarly,

$$\sum_{\alpha,\beta\neq(1,1)} c_{\alpha,\beta}[f_\alpha^*,a]f_\beta = \frac{1}{2}\sum_{\gamma\neq(1,1)} c_\gamma e^{-\omega_\gamma/2}[v_\gamma^*,a]v_\gamma \ ;$$
$$\sum_{\alpha,\beta\neq(1,1)} c_{\alpha,\beta}e^{\omega_\alpha} f_\beta[a,f_\alpha^*] = \frac{1}{2}\sum_{\gamma\neq(1,1)} c_\gamma e^{\omega_\gamma/2}v_\gamma[a,v_\gamma^*] \ ;$$
$$\sum_{\alpha,\beta\neq(1,1)} c_{\alpha,\beta}e^{\omega_\alpha}[f_\beta,a]f_\alpha^* = \frac{1}{2}\sum_{\gamma\neq(1,1)} c_\gamma e^{\omega_\gamma/2}[v_\gamma,a]v_\gamma^*,$$

so that

$$\begin{aligned} L(a) &= \frac{1}{4}\sum_{\alpha,\beta\neq(1,1)} c_{\alpha,\beta}\left(f_\alpha^*[a,f_\beta]+[f_\alpha^*,a]f_\beta + e^{\omega_\alpha}\left(f_\beta[a,f_\alpha^*]+[f_\beta,a]f_\alpha^*\right)\right) \\ &= \frac{1}{2}\sum_{\gamma\neq(1,1)} c_\gamma\left(e^{-\omega_\gamma/2}\left(v_\gamma^*[a,v_\gamma]+[v_\gamma^*,a]v_\gamma\right)+e^{\omega_\gamma/2}\left(v_\gamma[a,v_\gamma^*]+[v_\gamma,a]v_\gamma^*\right)\right). \end{aligned}$$

By symmetry, we may assume without loss of generality that $c_\gamma = c_{\gamma'}$, so that $v_{\gamma'} = v_\gamma^*$ for all $\gamma \neq (1,1)$. But then,

$$\sum_{\gamma\neq(1,1)} c_\gamma e^{-\omega_\gamma/2}[v_\gamma^*,a]v_\gamma = \sum_{\gamma\neq(1,1)} c_{\gamma'}e^{-\omega_{\gamma'}/2}[v_{\gamma'}^*,a]v_{\gamma'} = \sum_{\gamma\neq(1,1)} c_\gamma e^{\omega_\gamma/2}[v_\gamma,a]v_\gamma^*, \quad \text{and}$$
$$\sum_{\gamma\neq(1,1)} c_\gamma e^{\omega_\gamma/2}v_\gamma[a,v_\gamma^*] = \sum_{\gamma\neq(1,1)} c_{\gamma'}e^{\omega_{\gamma'}/2}v_{\gamma'}[a,v_{\gamma'}^*] = \sum_{\gamma\neq(1,1)} c_\gamma e^{-\omega_\gamma/2}v_\gamma^*[a,v_\gamma],$$

so that the expression for $L(a)$ reduces to

$$L(a) = \sum_{\gamma\neq(1,1)} c_\gamma\left(e^{-\omega_\gamma/2}v_\gamma^*[a,v_\gamma]+e^{\omega_\gamma/2}[v_\gamma,a]v_\gamma^*\right).$$

This is (4.1) up to some constants. On the other hand, using the expression $L(a) = \frac{1}{2}\sum_{\alpha,\beta\neq(1,1)} c_{\alpha,\beta}\left(f_\alpha^*[a,f_\beta]+[f_\alpha^*,a]f_\beta\right)$ (that was shown in the beginning), we also have

$$\begin{aligned} L(a) &= \frac{1}{2}\sum_{\alpha,\beta\neq(1,1)} c_{\alpha,\beta}\left(f_\alpha^*[a,f_\beta]+[f_\alpha^*,a]f_\beta\right) \\ &= \sum_{\gamma\neq(1,1)} c_\gamma e^{-\omega_\gamma/2}\left(v_\gamma^*[a,v_\gamma]+[v_\gamma^*,a]v_\gamma\right). \end{aligned}$$

which is (4.2) up to some constants.
Now since u has orthonormal rows, we have

$$\mathrm{Tr}(v_\mu^* v_\gamma) = \sum_{\alpha,\beta\neq(1,1)} \overline{u_{\mu,\alpha}}u_{\gamma,\beta}\mathrm{Tr}(f_\alpha^* f_\beta) = \sum_{\alpha\neq(1,1)} \overline{u_{\mu,\alpha}}u_{\gamma,\alpha} = \delta_{\mu,\gamma}.$$

For all $\gamma \neq (1,1)$, we also have $\mathrm{Tr}(v_\gamma) = \sum_{\beta\neq(1,1)} u_{\gamma,\beta}\mathrm{Tr}(f_\beta) = 0$ as $\{f_\alpha\}$ is an orthonormal basis for H_n and $f_{(1,1)} = 1$. And $\{v_\gamma^*\}_{\gamma\neq(1,1)} = \{v_\gamma\}_{\gamma\neq(1,1)}$ since $v_\gamma^* = v_{\gamma'}$. Moreover, using the fact that

$u_{\gamma,\beta} = 0$ if $\omega_\gamma \neq \omega_\beta$,

$$\Delta_\rho(v_\gamma) = \rho v_\gamma \rho^{-1} = \sum_{\beta\neq(1,1)} u_{\gamma,\beta}\rho f_\beta \rho^{-1} = \sum_{\beta\neq(1,1)} u_{\gamma,\beta}\Delta_\rho(f_\beta)$$
$$= \sum_{\beta\neq(1,1)} u_{\gamma,\beta} e^{-\omega_\beta} f_\beta = e^{-\omega_\gamma} \sum_{\beta\neq(1,1)} u_{\gamma,\beta} f_\beta = e^{-\omega_\gamma} v_\gamma$$

for all $\gamma \neq (1,1)$.

The final step is to absorb all the constants c_γ into v_γ: Since $c_\gamma \geq 0$ for all $\gamma \neq (1,1)$, we can make the substitution $v_\gamma \to \sqrt{c_\gamma} v_\gamma$. It is readily verified that properties (2), (3) and (4) of Theorem 4.4.1 still hold for the new v_γ. For property (1) we have $\mathrm{Tr}(v_\mu^* v_\gamma) = c_\gamma \delta_{\mu,\gamma}$. Letting $\mathcal{J} = \{(i,j) : 1 \leq i,j \leq n \text{ and } (i,j) \neq (1,1)\}$, we see that the generator L has the specified form as in (4.1) and (4.2).

For the converse, if L has the form (4.1)/(4.2) then it is clear that $L(1) = 0$ and

$$\begin{aligned}
L(a)^* &= \sum_{j\in\mathcal{J}} e^{-\omega_j/2} \left(v_j^*[a,v_j] + [v_j^*,a]v_j\right)^* = \sum_{j\in\mathcal{J}} e^{-\omega_j/2} \left(v_j^* a v_j - v_j^* v_j a + v_j^* a v_j - a v_j^* v_j\right)^* \\
&= \sum_{j\in\mathcal{J}} e^{-\omega_j/2} \left(v_j^* a^* v_j - a^* v_j^* v_j + v_j^* a^* v_j - v_j^* v_j a^*\right) = \sum_{j\in\mathcal{J}} e^{-\omega_j/2} \left(v_j^*[a^*,v_j] + [v_j^*,a^*]v_j\right) \\
&= L(a^*).
\end{aligned}$$

One can restore the c_j's by normalizing the v_j's. Then the set $\{v_j\}_{j\in\mathcal{J}}$ together with 1 and any v_k's with $c_k = 0$ form an orthonormal basis for H_n. The reduced GKS matrix of L for this basis is positive as the argument starting from Proposition 4.4.12 shows, which implies that L generates a QMS Φ_t by Lemma 4.4.11. Furthermore, we have

$$\langle a, [v_j, b]\rangle_{\rho,1} = \langle v_j^* a - e^{\omega_j} a v_j^*, b\rangle_{\rho,1} \quad \text{and} \quad \langle [v_j,b], a\rangle_{\rho,1} = \langle a, v_j^* b - e^{\omega_j} b v_j^*\rangle_{\rho,1} \quad \text{for all } j \in \mathcal{J},$$

using the fact that $\Delta_\rho(v_j) = e^{-\omega_j} v_j$ (compare with Lemma 6.1.6 as a similar computation is done there in detail). But then from this we obtain

$$\begin{aligned}
e^{-\omega_j/2}\langle [v_j,a],[v_j,b]\rangle_{\rho,1} &= e^{-\omega_j/2}\langle v_j^*[v_j,a] - e^{\omega_j}[v_j,a]v_j^*, b\rangle_{\rho,1} \\
&= \langle e^{-\omega_j/2} v_j^*[v_j,a] - e^{\omega_j/2}[v_j,a]v_j^*, b\rangle_{\rho,1} \\
&= -\langle e^{-\omega_j/2} v_j^*[a,v_j] + e^{\omega_j/2}[v_j,a]v_j^*, b\rangle_{\rho,1},
\end{aligned}$$

and similarly,

$$e^{-\omega_j/2}\langle [v_j,a],[v_j,b]\rangle_{\rho,1} = -\langle a, e^{-\omega_j/2} v_j^*[b,v_j] + e^{\omega_j/2}[v_j,b]v_j^*\rangle_{\rho,1}.$$

Consequently,

$$\begin{aligned}
\langle L(a), b\rangle_{\rho,1} &= \sum_{j\in\mathcal{J}} \langle e^{-\omega_j/2} v_j^*[a,v_j] + e^{\omega_j/2}[v_j,a]v_j^*, b\rangle_{\rho,1} \\
&= -\sum_{j\in\mathcal{J}} e^{-\omega_j/2}\langle [v_j,a],[v_j,b]\rangle_{\rho,1} \\
&= \sum_{j\in\mathcal{J}} \langle a, e^{-\omega_j/2} v_j^*[b,v_j] + e^{\omega_j/2}[v_j,b]v_j^*\rangle_{\rho,1} \\
&= \langle a, L(b)\rangle_{\rho,1},
\end{aligned}$$

so that $\Phi_t = e^{tL}$ satisfies the ρ-DBC. □

5 Classical detailed balance vs. quantum detailed balance

The main result (Theorem 5.0.2) of this section shows that ergodic quantum Markov semigroups satisfying detailed balance induce a continuous-time Markov chain that satisfies the classical detailed balance condition when a restriction of the QMS to a commutative subalgebra is possible.

Lemma 5.0.1. *Let $A \subseteq M_n(\mathbb{C})$ be a unital commutative C^*-subalgebra. Then A has a basis $\{e_1, ..., e_m\}$ consisting of mutually orthogonal projections in A with $\sum_{k=1}^m e_k = 1$. Consequently,*

$$a = \sum_{k=1}^{m} \frac{\mathrm{Tr}(e_k a)}{\mathrm{Tr}(e_k)} e_k \quad \textit{for all } a \in A.$$

Proof. Since A is a unital abelian C^*-algebra, there exists a compact Hausdorff space X such that the Gelfand representation $\pi : A \xrightarrow{\sim} C(X)$ is an isometric $*$-isomorphism. Now note that $C(X)$ is finite dimensional if and only if X is finite. Thus, X is necessarily finite, say $X = \{x_1, ..., x_m\}$ since A is finite dimensional. Now define for $i = 1, ..., m$ the functions $f_i \in C(X)$ by $f_i(x) = \begin{cases} 1, & x = x_i \\ 0, & x \neq x_i \end{cases}$. Set $e_i := \pi^{-1}(f_i) \in A$ for $i = 1, ..., m$. Then for all $i = 1, ..., m$, we have

$$e_i^2 = \pi^{-1}(f_i)^2 = \pi^{-1}(f_i^2) = \pi^{-1}(f_i) = e_i \quad \text{and} \quad e_i^* = \pi^{-1}(f_i)^* = \pi^{-1}(\overline{f_i}) = \pi^{-1}(f_i) = e_i,$$

so that $\{e_1, ..., e_m\} \subseteq A$ are projections. Moreover, if $i \neq j$ then

$$e_i e_j = \pi^{-1}(f_i)\pi^{-1}(f_j) = \pi^{-1}(f_i f_j) = \pi^{-1}(0) = 0 \quad \text{and,}$$
$$\sum_{k=1}^{m} e_k = \sum_{k=1}^{m} \pi^{-1}(f_i) = \pi^{-1}\left(\sum_{k=1}^{m} f_i\right) = \pi^{-1}(1) = 1.$$

This implies that $\{e_1, ..., e_m\}$ is a set of mutually orthogonal projections in A summing to 1. It is clear that $\{f_1, ..., f_m\}$ is a basis for $C(X)$, but then it follows almost immediately that $\{e_1, ..., e_m\}$ is a basis for A using π^{-1} once again.

Equip A with the Hilbert-Schmidt inner product $\langle \cdot, \cdot \rangle_{\mathrm{HS}}$. Then for all $a \in A$, we can write

$$a = \sum_{k=1}^{m} \frac{\langle a, e_k \rangle_{\mathrm{HS}}}{\langle e_k, e_k \rangle_{\mathrm{HS}}} e_k = \sum_{k=1}^{m} \frac{\mathrm{Tr}(e_k a)}{\mathrm{Tr}(e_k)} e_k.$$

□

A vector $\lambda = (\lambda_1, ..., \lambda_m) \in \mathbb{R}^m$ is called a *distribution* or *probability vector* if $\lambda_k \geq 0$ for all $k = 1, ..., m$ and $\sum_{k=1}^m \lambda_k = 1$.

Theorem 5.0.2. *Let $\Phi_t = e^{tL}$ be an ergodic QMS on $M_n(\mathbb{C})$ that satisfies the ρ-DBC for its unique invariant density matrix $\rho \in \mathfrak{S}_+$. Let $A \subseteq M_n(\mathbb{C})$ be a unital commutative C^*-subalgebra that is invariant under $\Phi_t^\dagger$ ($\Phi_t^\dagger(A) \subseteq A$ for all $t \geq 0$). Let $\{e_1, ..., e_m\} \subseteq A$ be a basis for A consisting of mutually orthogonal projections such that $\sum_{k=1}^m e_k = 1$. Then the following statements hold:*

(a) The $m \times m$ matrix $Q = (Q_{k,l})_{1 \leq k,l \leq m}$ defined by

$$Q_{k,l} := \frac{\mathrm{Tr}(e_k L(e_l))}{\mathrm{Tr}(e_k)} \quad (1 \leq k, l \leq m)$$

specifies a continuous-time Markov chain with state space $\{1, ..., m\}$ and jump rates $Q_{k,l}$ from k to l.

(b) The corresponding forward equation, governing the evolution of site occupation probabilities is

$$\frac{d}{dt}\lambda_l(t) = \sum_{k=1}^{m} \lambda_k(t) Q_{k,l} = \sum_{k=1}^{m} \left(\lambda_k(t) Q_{k,l} - \lambda_l(t) Q_{l,k}\right).$$

where $\vec{\lambda(t)} = (\lambda_1(t), ..., \lambda_m(t)) \in \mathbb{R}^m$ is a probability vector.

(c) A time-dependent probability vector $\vec{\lambda}(t) = (\lambda_1(t), ..., \lambda_m(t)) \in \mathbb{R}^m$ satisfies the equation in (b) if and only if the time-dependent density matrix $\lambda(t) \in A$ given by

$$\lambda(t) = \sum_{k=1}^{m} \frac{\lambda_k(t)}{\mathrm{Tr}(e_k)} e_k$$

satisfies $\frac{d}{dt}\lambda(t) = L^\dagger(\lambda(t))$.

(d) The probability vector $\vec{\rho} = (\rho_1, ..., \rho_m)$ given by $\rho_k = \mathrm{Tr}(\rho e_k)$ for $k = 1, ..., m$ is the unique invariant distribution for the Markov chain, and the classical detailed balance equations

$$\rho_k Q_{k,l} = \rho_l Q_{l,k} \quad (1 \le k, l \le m)$$

are satisfied.

Proof. We first show that the matrix Q satisfies $\sum_{l=1}^{m} Q_{k,l} = 0$ for all $k \in \{1, ..., m\}$ and that $Q_{k,l} \ge 0$ for all $k \ne l$, which makes it a transition rate matrix. First note that $\Phi_t(1) = 1$ for all $t \ge 0$ so that $0 = L(1) = \sum_{l=1}^{m} L(e_l)$ which implies that $\sum_{l=1}^{m} Q_{k,l} = \sum_{l=1}^{m} \frac{\mathrm{Tr}(e_k L(e_l))}{\mathrm{Tr}(e_k)} = 0$ for all $k = 1, ..., m$. Let L be given in the form (4.2) of Theorem 4.4.1. Then for $k \ne l$, we have

$$\begin{aligned}
\mathrm{Tr}(e_k L(e_l)) &= \sum_{j \in J} e^{-\omega_j/2} \mathrm{Tr}\left(e_k \left(v_j^*[e_l, v_j] + [v_j^*, e_l] v_j\right)\right) \\
&= \sum_{j \in \mathcal{J}} e^{-\omega_j/2} \left(\mathrm{Tr}\left(e_k v_j^* e_l v_j\right) - \mathrm{Tr}\left(e_k v_j^* v_j e_l\right) + \mathrm{Tr}\left(e_k v_j^* e_l v_j\right) - \mathrm{Tr}\left(e_k e_l v_j^* v_j\right)\right) \\
&= \sum_{j \in \mathcal{J}} e^{-\omega_j/2} \left(\mathrm{Tr}\left(e_k v_j^* e_l v_j\right) - 0 + \mathrm{Tr}\left(e_k v_j^* e_l v_j\right) - 0\right) \\
&= 2 \sum_{j \in \mathcal{J}} e^{-\omega_j/2} \mathrm{Tr}\left(e_k v_j^* e_l v_j\right) \ge 0,
\end{aligned}$$

where in the third equality we used the pairwise orthogonality of $\{e_1, ..., e_m\}$ and the last expression is positive since $e_k \ge 0$ and $v_j^* e_l v_j \ge 0$ and that implies that $\mathrm{Tr}(e_k v_j^* e_l v_j) \ge 0$ (take square roots). Further, $\mathrm{Tr}(e_k) \ge 0$ for all k. Thus, $Q_{k,l} \ge 0$ for all $k \ne l$ and therefore Q is a transition rate matrix. It is now possible to construct a continuous-time Markov chain with state space $\{1, ..., m\}$ and jump rates $Q_{k,l}$ from k to l, see section 2.6 in [17]. This proves (a).

The *forward equation* in (row) vector form is given by $\frac{d}{dt}\vec{\lambda}(t) = \vec{\lambda}(t) Q$ where $\vec{\lambda}(t) = (\lambda_1(t), ..., \lambda_m(t)) \in \mathbb{R}^m$ is a probability vector. For $l = 1, ..., m$ this can be written as

$$\frac{d}{dt}\lambda_l(t) = \sum_{k=1}^{m} \lambda_k(t) Q_{k,l} = \sum_{k=1}^{m} \left(\lambda_k(t) Q_{k,l} - \lambda_l(t) Q_{l,k}\right),$$

and the last equality follows from $Q_{l,l} = -\sum_{k \ne l} Q_{l,k}$. This proves (b).

Let $\vec{\lambda}(t) = (\lambda_1(t), ..., \lambda_m(t)) \in \mathbb{R}^m$ be a time-dependent probability vector. Define the time-dependent density matrix $\lambda(t) \in A$ by $\lambda(t) := \sum_{k=1}^m \frac{\lambda_k(t)}{\mathrm{Tr}(e_k)} e_k$. Since A is invariant under $\Phi_t^\dagger$, it is also invariant under $L^\dagger$. In particular, we can write $L^\dagger(\lambda(t)) = \sum_{k=1}^m \frac{\mathrm{Tr}(e_k L^\dagger(\lambda(t)))}{\mathrm{Tr}(e_k)} e_k = \sum_{k=1}^m \frac{\mathrm{Tr}(L(e_k)\lambda(t))}{\mathrm{Tr}(e_k)} e_k$ by Lemma 5.0.1. On the other hand, we have $\frac{d}{dt}\lambda(t) = \sum_{k=1}^m \frac{d}{dt}\lambda_k(t)\mathrm{Tr}(e_k)^{-1} e_k$. Now since $\{e_1, ..., e_m\}$ is a basis for A, we see that

$$\frac{d}{dt}\lambda(t) = L^\dagger(\lambda(t)) \iff \frac{d}{dt}\lambda_l(t) = \mathrm{Tr}(L(e_l)\lambda(t)) \text{ for all } l = 1, ...m.$$

Now note that for each $l = 1, ..., m$ we have

$$\mathrm{Tr}(L(e_l)\lambda(t)) = \mathrm{Tr}\left(L(e_l) \sum_{k=1}^m \frac{\lambda_k(t)}{\mathrm{Tr}(e_k)} e_k \right) = \sum_{k=1}^m \lambda_k(t) \frac{\mathrm{Tr}(e_k L(e_l))}{\mathrm{Tr}(e_k)} = \sum_{k=1}^m \lambda_k(t) Q_{k,l}.$$

From this and the 'iff' statement above, it follows that $\vec{\lambda}(t)$ satisfies the equation in (b) if and only if $\frac{d}{dt}\lambda(t) = L^\dagger(\lambda(t))$ and this proves (c).

Note that $\rho = \lim_{t\to\infty} \Phi_t^\dagger(h)$ for any density matrix $h \in M_n(\mathbb{C})$ by Proposition 4.3.13. But since A is invariant under $\Phi_t^\dagger$, we see that $\rho = \lim_{t\to\infty} \Phi_t^\dagger(h) \in A$ for any density matrix $h \in A$ as A is closed. Thus we can write $\rho = \sum_{k=1}^m \frac{\mathrm{Tr}(e_k\rho)}{\mathrm{Tr}(e_k)} e_k = \sum_{k=1}^m \frac{\rho_k}{\mathrm{Tr}(e_k)} e_k$ by Lemma 5.0.1. In particular, $\rho e_k = \frac{\rho_k}{\mathrm{Tr}(e_k)} e_k = e_k \rho$ for all $k = 1, .., m$ by orthogonality. It follows for $1 \le k, l \le m$ that

$$\begin{aligned} \rho_k Q_{k,l} &= \frac{\rho_k}{\mathrm{Tr}(e_k)} \mathrm{Tr}(e_k L(e_l)) = \mathrm{Tr}(\rho e_k L(e_l)) = \mathrm{Tr}(\rho L(e_k) e_l) \\ &= \mathrm{Tr}(e_l \rho L(e_l)) = \frac{\rho_l}{\mathrm{Tr}(e_l)} \mathrm{Tr}(e_l L(e_k)) = \rho_l Q_{l,k}, \end{aligned}$$

where in the third equality we used the self-adjointness of L with respect to $\langle \cdot, \cdot \rangle_{\rho,1}$. Hence, Q satisfies the classical detailed balance conditions with respect to $\vec{\rho}$. Furthermore, for $l = 1, ..., m$ we have $\sum_{k=1}^m \rho_k Q_{k,l} = \sum_{k=1}^m \rho_l Q_{l,k} = \rho_l \sum_{k=1}^m Q_{l,k} = 0$ since Q has rows that sum to 0. Therefore $\vec{\rho}Q = 0$ and this implies that $\vec{\rho}$ is the unique invariant distribution for the Markov chain with semigroup $P_t = e^{tQ}$. This proves statement (d). □

Example 5.0.3. Let $A \subseteq M_n(\mathbb{C})$ be unital C^*-algebra, and let $\rho \in \mathfrak{S}_+(A)$. Since ρ is self-adjoint, the commutant of $\{\rho\}$ is a C^*-subalgebra of $M_n(\mathbb{C})$ and we set $A_\rho := \{\rho\}' \cap A$. Then A_ρ is a C^*-subalgebra of A and we call it the *ρ-modular subalgebra of A*. It consist exactly of those element in A that commute with ρ and it also readily verified that A_ρ equals the eigenspace of Δ_ρ with eigenvalue 1.

Now let $(\Phi_t)_{t\ge0}$ be an ergodic QMS on $M_n(\mathbb{C})$ satisfying the ρ-DBC for its unique invariant density matrix $\rho \in \mathfrak{S}_+$. Moreover, assume that $\Phi_t(A) \subseteq A$ for all $t \ge 0$. Since Φ_t and Δ_ρ commute for all $t \ge 0$ by Corollary 4.3.9, we have for all $a \in A_\rho$ and $t \ge 0$ that

$$\Delta_\rho(\Phi_t(a)) = \Phi_t(\Delta_\rho(a)) = \Phi_t(a).$$

Therefore, $\Phi_t(a)$ commutes with ρ and $\Phi_t(A_\rho) \subseteq A_\rho$ for all $t \ge 0$. Moreover, for all $a \in A_\rho$ and $b \in A$,

$$\langle \Delta_\rho(\Phi_t^\dagger(a)), b \rangle_{\mathrm{HS}} = \langle a, \Phi_t(\Delta_\rho(b)) \rangle_{\mathrm{HS}} = \langle a, \Delta_\rho(\Phi_t(b)) \rangle_{\mathrm{HS}} = \langle \Phi_t^\dagger(\Delta_\rho(a)), b \rangle_{\mathrm{HS}} = \langle \Phi_t^\dagger(a), b \rangle_{\mathrm{HS}},$$

where we also used that Δ_ρ is self-adjoint with respect to the Hilbert-Schmidt inner product. Thus, $\Delta_\rho(\Phi_t^\dagger(a)) = \Phi_t^\dagger(a)$ and this means that A_ρ is invariant under $\Phi_t^\dagger$ as well. Now let $\{\eta_1, ..., \eta_n\}$ be an orthonormal basis of $\mathbb{C}^n$ consisting of eigenvectors of ρ with $\rho\eta_j = e^{-\lambda_j}\eta_j$ for $j = 1, ..., n$ and $\lambda_j \in \mathbb{R}$. If the numbers $\lambda_1, ..., \lambda_n$ are all distinct, then the eigenspace of Δ_ρ for the eigenvalue 1 is exactly the span of the set $\{|\eta_j\rangle\langle\eta_j|\}_{j=1}^n$ [1]. So in this case A_ρ is an n-dimensional abelian C^*-subalgebra of A and Theorem 5.0.2 applies.

6 Riemannian metrics and gradient flow

The notion of non-commutative differential operators associated to a quantum Markov generator will be introduced. By means of these operators, it is possible to consider *forms* associated to a quantum Markov generator.

One of the important results (Theorem 6.2.8) shows that associated to any QMS $\Phi_t = e^{tL}$ with detailed balance, the flow induced by the dual generator $L^\dagger$ is *gradient flow* with respect to some Riemannian metric g_L for the *relative entropy.*

In this section A will be a fixed unital C^*-subalgebra of some matrix algebra $M_n(\mathbb{C})$.

6.1 Forms associated to generators of quantum Markov semigroups

Let $\Phi_t = e^{tL}$ be a QMS on A that satisfies the ρ-DBC for some $\rho \in \mathfrak{S}_+(A)$ and assume that $(\Phi_t)_{t\geq 0}$ has an extension to a QMS on $M_n(\mathbb{C})$. Then we know that the generator L can be written in the form given in (4.2) of Theorem 4.4.1. Throughout the rest of this subsection we fix such a generator L, and the sets $\{v_j\}_{j\in\mathcal{J}} \subseteq M_n(\mathbb{C})$ and $\{\omega_j\}_{j\in\mathcal{J}} \subseteq \mathbb{R}$ that specify L according to Theorem 4.4.1.

Definition 6.1.1. The *(non-commutative) partial derivatives associated to* L are the operators $\partial_j : A \to A$ defined by

$$\partial_j(a) := [v_j, a] \quad \text{for } a \in A \text{ and } j \in \mathcal{J}.$$

An immediate consequence is that for all $a, b \in A$ we have

$$\langle \partial_j(a), b\rangle_{\mathrm{HS}} = \mathrm{Tr}(b^* v_j a) - \mathrm{Tr}(b^* a v_j) = \mathrm{Tr}(b^* v_j a) - \mathrm{Tr}(v_j b^* a) = \langle a, v_j^* b\rangle_{\mathrm{HS}} - \langle a, b v_j^*\rangle_{\mathrm{HS}} = \langle a, [v_j^*, b]\rangle_{\mathrm{HS}},$$

so that

$$\partial_j^\dagger b = [v_j^*, b] \quad \text{for all } b \in A \text{ and } j \in \mathcal{J}.$$

Having a notion of 'non-commutative partial derivatives' available, allows us to introduce non-commutative analogs of the Laplace operator, gradient and divergence associated to L.

Definition 6.1.2. The *(non-commutative) Laplace operator associated to* L is the operator $L_0 : A \to A$ defined by

$$L_0(a) := -\sum_{j\in\mathcal{J}} \partial_j^\dagger \partial_j(a) = -\sum_{j\in\mathcal{J}} [v_j^*, [v_j, a]].$$

Clearly, $L^\dagger = L$ and we also have

$$\begin{aligned} L_0(a) &= -\sum_{j\in\mathcal{J}} [v_j^*, [v_j, a]] = -\sum_{j\in\mathcal{J}} \left(v_j^*[v_j, a] - [v_j, a]v_j^*\right) = -\sum_{j\in\mathcal{J}} \left(v_j^* v_j a - v_j^* a v_j - v_j a v_j^* + a v_j v_j^*\right) \\ &= \sum_{j\in\mathcal{J}} \left(v_j^* a v_j - v_j^* v_j a + v_j a v_j^* - a v_j v_j^*\right) = \sum_{j\in\mathcal{J}} \left(v_j^*[a, v_j] + [v_j, a]v_j^*\right) \quad \text{for all } a \in A. \end{aligned}$$

Thus, by Theorem 4.4.1, L_0 is the generator of a quantum Markov semigroup $\Phi_{0,t} = e^{tL_0}$ satisfying the h-DBC where $h = \frac{1}{n}\mathbb{1}$ because in this case Δ_h is the identity and $\omega_j = 0$ for all $j \in \mathcal{J}$. We call $\Phi_{0,t} = e^{tL_0}$ the *heat semigroup* associated to $\Phi_t = e^{tL}$.

Define the C^*-algebra

$$A^{\oplus\mathcal{J}} := \bigoplus_{j\in\mathcal{J}} A^{(j)},$$

where each $A^{(j)}$ is a copy of A. In other words, $A^{\oplus \mathcal{J}}$ is the direct sum of $|\mathcal{J}|$ copies of A. For $\mathbf{a} \in A^{\oplus \mathcal{J}}$ and $j \in \mathcal{J}$, let a_j denote the component of $\mathbf{a}$ in $A^{(j)}$. Thus, by picking some linear ordering of $\mathcal{J}$, we may suggestively write

$$\mathbf{a} = \left(a_1, ..., a_{|\mathcal{J}|}\right).$$

We equip $A^{\oplus \mathcal{J}}$ with the inner product $\langle \mathbf{a}, \mathbf{b} \rangle_{\mathrm{HS}} := \sum_{j \in \mathcal{J}} \langle a_j, b_j \rangle_{\mathrm{HS}}$ for $\mathbf{a}, \mathbf{b} \in A^{\oplus \mathcal{J}}$.

Definition 6.1.3. The *(non-commutative) gradient associated to* L is the operator $\nabla : A \to A^{\oplus \mathcal{J}}$ defined by

$$\nabla(a) := \left(\partial_1(a), ..., \partial_{|\mathcal{J}|}(a)\right).$$

Definition 6.1.4. The *(non-commutative) divergence associated to* L is the operator $\mathrm{div} : A^{\oplus \mathcal{J}} \to A$ defined by

$$\mathrm{div}(\mathbf{a}) := -\sum_{j \in \mathcal{J}} \partial_j^\dagger(a_j) = \sum_{j \in \mathcal{J}} [a_j, v_j^*].$$

Remark 6.1.5. We have $\mathrm{div}^\dagger = -\nabla$ since

$$\langle \mathrm{div}^\dagger(\mathbf{a}), b \rangle_{\mathrm{HS}} = -\sum_{j \in \mathcal{J}} \langle \partial_j^\dagger(a_j), b \rangle_{\mathrm{HS}} = -\sum_{j \in \mathcal{J}} \langle a_j, \partial_j(b) \rangle_{\mathrm{HS}} = \langle \mathbf{a}, -\nabla(b) \rangle_{\mathrm{HS}}$$

for all $\mathbf{a} \in A^{\oplus \mathcal{J}}$ and $b \in A$. Consequently, in our finite-dimensional setting,

$$\ker(\mathrm{div})^\perp = \mathrm{Im}(\mathrm{div}^\dagger) = \mathrm{Im}(-\nabla) = \mathrm{Im}(\nabla).$$

Lemma 6.1.6. *Let $s \in [0, 1]$, $j \in \mathcal{J}$ and $a, b \in A$. Then*

$$\langle a, \partial_j(b) \rangle_{\rho,s} = e^{s\omega_j} \langle e^{-\omega_j} v_j^* a - a v_j^*, b \rangle_{\rho,s}.$$

Proof. We first note that $(\Delta_\rho(x))^* = \Delta_\rho^{-1}(x^*)$ for all $x \in A$. This implies that

$$\Delta_\rho(x) = e^{-\omega_j} x \iff \Delta_\rho x^* = e^{\omega_j} x^* \quad \text{for } x \in A.$$

In particular, we have $\Delta_\rho^{s-1}(v_j^*) = e^{(s-1)\omega_j} v_j^*$ and $\Delta_\rho^s(v_j^*) = e^{s\omega_j} v_j^*$ since $\Delta_\rho(v_j) = e^{-\omega_j} v_j$ by Theorem 4.4.1 and functional calculus. Using this, we obtain for all $a, b \in A$,

$$\begin{aligned}
\langle a, \partial_j(b) \rangle_{\rho,s} &= \mathrm{Tr}(\rho^s (\partial_j(b))^* \rho^{1-s} a) = \mathrm{Tr}(\rho^s (v_j b - b v_j)^* \rho^{1-s} a) \\
&= \mathrm{Tr}(\rho^s b^* v_j^* \rho^{1-s} a) - \mathrm{Tr}(\rho^s v_j^* b^* \rho^{1-s} a) \\
&= \mathrm{Tr}(\rho^s b^* \rho^{1-s} \Delta_\rho^{s-1}(v_j^*) a) - \mathrm{Tr}(\Delta_\rho^s(v_j^*) \rho^s b^* \rho^{1-s} a) \\
&= e^{(s-1)\omega_j} \mathrm{Tr}(\rho^s b^* \rho^{1-s} v_j^* a) - e^{s\omega_j} \mathrm{Tr}(v_j^* \rho^s b^* \rho^{1-s} a) \\
&= e^{s\omega_j} \left(\mathrm{Tr}(\rho^s b^* \rho^{1-s} e^{-\omega_j} v_j^* a) - \mathrm{Tr}(\rho^s b^* \rho^{1-s} a v_j^*) \right) \\
&= e^{s\omega_j} \mathrm{Tr}(\rho^s b^* \rho^{1-s} (e^{-\omega_j} v_j^* a - a v_j^*)) = e^{s\omega_j} \langle e^{-\omega_j} v_j^* a - a v_j^*, b \rangle_{\rho,s}.
\end{aligned}$$

This is exactly what we needed to show. □

Using Lemma 6.1.6, it follows that

$$\begin{aligned}
e^{(1/2-s)\omega_j} \langle \partial_j(a), \partial_j(b) \rangle_{\rho,s} &= e^{(1/2-s)\omega_j} e^{s\omega_j} \langle e^{-\omega_j} v_j^* [v_j, a] - [v_j, a] v_j^*, b \rangle_{\rho,s} \\
&= e^{\omega_j/2} \langle e^{-\omega_j} v_j^* [v_j, a] - [v_j, a] v_j^*, b \rangle_{\rho,s} \\
&= \langle e^{-\omega_j/2} v_j^* [v_j, a] - e^{\omega_j/2} [v_j, a] v_j^*, b \rangle_{\rho,s} \\
&= -\langle e^{-\omega_j/2} v_j^* [a, v_j] + e^{\omega_j/2} [v_j, a] v_j^*, b \rangle_{\rho,s}.
\end{aligned}$$

For each $s \in [0,1]$ define

$$\mathcal{E}_s : A \times A \to \mathbb{C}, \quad \mathcal{E}_s(a,b) = \sum_{j \in \mathcal{J}} e^{(1/2-s)\omega_j} \langle \partial_j(a), \partial_j(b) \rangle_{\rho,s}.$$

Then $\mathcal{E}_s$ is called a *form associated to* L and by (4.1) of Theorem 4.4.1 we obtain

$$\mathcal{E}_s(a,b) = -\langle L(a), b \rangle_{\rho,s}.$$

In particular, taking $s = \frac{1}{2}$, we see that

$$\mathcal{E}_{1/2}(a,b) = \sum_{j \in \mathcal{J}} \langle \partial_j(a), \partial_j(b) \rangle_{\rho,1/2} = -\langle L(a), b \rangle_{\rho,1/2},$$

for $a, b \in A$ and $\mathcal{E}_{1/2}$ is called the *Dirichlet form associated to* L.

A simple consequence of the Dirichlet form is an ergodicity result:

Theorem 6.1.7. *Let $\Phi_t = e^{tL}$ be a QMS on A that satisfies the ρ-DBC for $\rho \in \mathfrak{S}_+(A)$. Then the commutant of $\{v_j\}_{j \in \mathcal{J}}$ equals the kernel of L. In particular, $(\Phi_t)_{t \geq 0}$ is ergodic if and only if the commutant of $\{v_j\}_{j \in \mathcal{J}}$ is spanned by the identity.*

Proof. We may assume that L is in the form (4.1) of Theorem 4.4.1. Let a be in the commutant of $\{v_j\}_{j \in \mathcal{J}}$. By definition, this means that $[v_j, a] = [a, v_j] = 0$ for all $j \in \mathcal{J}$. Therefore, $L(a) = 0$ as L has the form (4.1).

Conversely, let $a \in \ker(L)$. Then, using the Dirichlet form of L, we see that

$$\sum_{j \in \mathcal{J}} \langle \partial_j(a), \partial_j(a) \rangle_{\rho,1/2} = \mathcal{E}_{1/2}(a,a) = -\langle L(a), a \rangle_{\rho,1/2} = 0.$$

Consequently, $[v_j, a] = \partial_j(a) = 0$ for all $j \in \mathcal{J}$, that is, a belongs to the commutant of $\{v_j\}_{j \in \mathcal{J}}$. Thus, the commutant of $\{v_j\}_{j \in \mathcal{J}}$ coincides with the kernel of L.

Note that $(\Phi_t)_{t \geq 0}$ is ergodic if and only if $\ker(L) = \operatorname{span}(\mathrm{id}_{\mathbb{C}^n})$ which follows almost immediately from the definition of ergodicity. Hence, $(\Phi_t)_{t \geq 0}$ is ergodic if and only if the commutant of $\{v_j\}_{j \in \mathcal{J}}$ is spanned by the identity. ☐

Remark 6.1.8. For all $x \in A$, we have

$$\langle L_0(x), x \rangle_{\mathrm{HS}} = -\sum_{j \in \mathcal{J}} \langle \partial_j^\dagger \partial_j(x), x \rangle_{\mathrm{HS}} = -\sum_{j \in \mathcal{J}} \langle \partial_j(x), \partial_j(x) \rangle_{\mathrm{HS}} = -\langle \nabla(x), \nabla(x) \rangle_{\mathrm{HS}}.$$

We claim that $\{v_j : j \in \mathcal{J}\}' = \ker(L_0) = \ker(\nabla)$. Indeed, if $x \in \ker(L_0)$, then $[v_j, x] = \partial_j(x) = 0$ for all $j \in \mathcal{J}$ by the above relation. In other words, x belongs to the commutant of $\{v_j\}_{j \in \mathcal{J}}$. Conversely, if x belongs to the commutant of $\{v_j\}_{j \in \mathcal{J}}$, then $L_0(x) = -\sum_{j \in \mathcal{J}} [v_j^*, [v_j, x]] = 0$ by definition of L_0. Therefore, $\{v_j : j \in \mathcal{J}\}' = \ker(L_0)$. Further, $\ker(L_0) \subseteq \ker(\nabla)$ is clear from the relation above. And $\ker(\nabla) \subseteq \ker(L_0)$ follows from the fact that $L_0 = \operatorname{div} \circ \nabla$.

Theorem 6.1.9. *Let $\Phi_t = e^{tL}$ be an ergodic QMS on A that satisfies the ρ-DBC for $\rho \in \mathfrak{S}_+(A)$. Let L_0 be the associated Laplacian operator. Then for given $b \in A$, there exists an $x \in A$ such that $L_0(x) = b$ if and only $\operatorname{Tr}(b) = 0$. Consequently, if $\operatorname{Tr}(b) = 0$, then there exists a non-trivial affine subspace of $A^{\oplus \mathcal{J}}$ consisting of elements $\mathbf{a}$ for which $\operatorname{div}(\mathbf{a}) = b$.*

Proof. Since $(\Phi_t)_{t\geq 0}$ is ergodic, it follows that $\ker(L_0)$ is spanned by the identity according to Theorem 6.1.7 and remark 6.1.8. Let $b \in A$ given. Then there exists an $x \in A$ such that $L_0(x) = b$ if and only if $b \in \ker(L_0^\dagger)^\perp = \ker(L_0)^\perp = (\mathbb{C}1)^\perp$ by the Fredholm alternative, where $\perp$ denotes the orthogonal complement with respect to $\langle \cdot, \cdot \rangle_{\mathrm{HS}}$. But $b \in (\mathbb{C}1)^\perp$ if and only if $\mathrm{Tr}(b) = 0$, so that $L_0^{-1}(\{b\})$ is non-empty if and only if $\mathrm{Tr}(b) = 0$. In particular, when $\mathrm{Tr}(b) = 0$ then the solution space $L_0^{-1}(\{b\})$ defines a non-trivial affine subspace. Using the fact that $L_0 = \mathrm{div} \circ \nabla$, we see that there exists a non-trivial affine subspace of $A^{\oplus \mathcal{J}}$ consisting of elements $\mathbf{a}$ for which $\mathrm{div}(\mathbf{a}) = b$. □

Going forward, $R_a : M_n(\mathbb{C}) \to M_n(\mathbb{C})$ denotes the right multiplication by $a \in A$.

Lemma 6.1.10. *For all $v \in M_n(\mathbb{C})$, $h \in \mathfrak{S}_+$ and $\omega \in \mathbb{R}$, we have*

$$\int_0^1 e^{\omega(s-1/2)} R_h \Delta_h^s \left(v \log(e^{-\omega/2}\rho) - \log(e^{\omega/2}h)v \right) \, ds = e^{-\omega/2} vh - e^{\omega/2} hv,$$

where the integral is a Banach-valued Riemann integral.

Proof. This is a consequence of the calculus rules. Define $f(s) = e^{\omega(1/2-s)} h^{1-s} v h^s$, then f is continuously differentiable on $[0, 1]$ with

$$\begin{aligned} f'(s) &= -\omega e^{\omega(1/2-s)} h^{1-s} v \rho^s + e^{\omega(1/2-s)} \left(-\rho^{1-s} \log(h) v h^s + \rho^{1-s} v h^s \log(h) \right) \\ &= -\omega e^{\omega(1/2-s)} h^{1-s} v \rho^s - e^{\omega(1/2-s)} h^{1-s} \log(\rho) v h^s + e^{\omega(1/2-s)} h^{1-s} v \log(h) h^s \\ &= e^{\omega(1/2-s)} h^{1-s} \left(-\omega v - \log(h) v + v \log(h) \right) h^s \\ &= e^{\omega(1/2-s)} h^{1-s} \left(\log(e^{-\omega/2}) v - \log(e^{\omega/2}) v - \log(h) v + v \log(\rho) \right) h^s \\ &= e^{\omega(1/2-s)} h^{1-s} \left(v \log(e^{-\omega/2} h) - \log(e^{\omega/2} h) v \right) h^s. \end{aligned}$$

Consequently,

$$\begin{aligned} &\int_0^1 e^{\omega(s-1/2)} R_h \Delta_h^s (v \log(e^{-\omega/2} h) - \log(e^{\omega/2} h) v) \, ds = \\ &\qquad \int_0^1 e^{\omega(s-1/2)} h^s \left(v \log(e^{-\omega/2} h) - \log(e^{\omega/2} h) v \right) h^{1-s} \, ds = \int_0^1 f'(1-s) \, ds \\ &\qquad = \int_0^1 f'(t) \, dt = f(1) - f(0) = e^{-\omega/2} vh - e^{\omega/2} hv, \end{aligned}$$

which is the desired identity. □

Remark 6.1.11. For each $\omega \in \mathbb{R}$, define the function $f_\omega : (0, \infty) \to \mathbb{R}$ by

$$f_\omega(t) := \int_0^1 e^{\omega(s-1/2)} t^s ds.$$

Then the identity in Lemma 6.1.10 can be reformulated as

$$R_h f_\omega(\Delta_h) \left(v \log(e^{-\omega/2} h) - \log(e^{\omega/2} h) v \right) = e^{-\omega/2} vh - e^{\omega/2} hv,$$

and for $\omega = 0$ it reduces to $R_h f_0(\Delta_h)([v, \log(h)]) = [v, h]$. Take $v = v_j$ and then from the latter identity we obtain $R_h f_0(\Delta_h)(\partial_j(\log h)) = \partial_j(h)$ and this can be seen as the non-commutative

analog of $g(x)\nabla \log(g(x)) = \nabla g(x)$, which holds for all smooth, strictly positive probability density functions $g : \mathbb{R}^n \to \mathbb{R}$.
Moreover, if $a \in A$ commutes with $h \in \mathfrak{S}_+$, then $f_0(\Delta_h)(a) = a$ by definition of f_0. So for each $\omega \in \mathbb{R}$, the operation $a \mapsto R_h f_\omega(\Delta_h)(a)$ can be viewed as one of the non-commutative interpretations of multiplication of a by h.

The previous remark motivates the following definition:

Definition 6.1.12. For $\omega \in \mathbb{R}$ and $h \in \mathfrak{S}_+$, define the operator $[h]_\omega : M_n(\mathbb{C}) \to M_n(\mathbb{C})$ by

$$[h]_\omega = R_h \circ f_\omega(\Delta_h),$$

where f_ω is defined as in Remark 6.1.11.

Note that $[h]_\omega$ is invertible for all $h \in \mathfrak{S}_+$ and $w \in \mathbb{R}$ with $[h]_\omega^{-1} = (1/f_\omega)(\Delta_h) \circ R_{h^{-1}}$ and may be viewed as the corresponding non-commutative interpretation of division by h.

Lemma 6.1.13. *For all $\omega \in \mathbb{R}$, the maps $h \mapsto [h]_\omega$ and $h \mapsto [h]_\omega^{-1}$ are C^∞ on $\mathfrak{S}_+$. Furthermore, for all $a \in M_n(\mathbb{C})$ we have*

$$[h]_\omega(a)^* = [h]_{-\omega}(a^*) \quad \text{and} \quad [h]_\omega^{-1}(a)^* = [h]_{-\omega}^{-1}(a^*).$$

Proof. First note that the following identities hold for $\lambda, \mu > 0$:

$$\int_0^1 \lambda^s \mu^{1-s}\, ds = \frac{\lambda - \mu}{\log\lambda - \log\mu} \quad \text{and} \quad \int_0^\infty \frac{1}{(t+\lambda)(t+\mu)}\, dt = \frac{\log\lambda - \log\mu}{\lambda - \mu},$$

so that $\left(\int_0^1 \lambda^s \mu^{1-s}\, ds\right)\left(\int_0^\infty \frac{1}{(t+\lambda)(t+\mu)}\, dt\right) = 1$ for all $\lambda, \mu > 0$. Using the definitions we obtain for all $h \in \mathfrak{S}_+$,

$$[h]_\omega = R_h f_\omega(\Delta_h) = \int_0^1 e^{\omega(s-1/2)} L_h^s R_h^{1-s}\, ds = \int_0^1 \left(e^{\omega/2} L_h\right)^s \left(e^{-\omega/2} R_h\right)^{1-s}\, ds,$$

where L_h is the left multiplication by h. Note that $t + e^{\omega/2} L_h$ and $t + e^{-\omega/2} R_h$ are invertible for all $t \geq 0$ (where $(t + e^{\omega/2} L_h)^{-1}$ is the left multiplication by $(t1 + e^{\omega/2} h)^{-1}$ and $(t + e^{-\omega/2} R_h)^{-1}$ is the right multiplication by $(t1 + e^{-\omega/2} h)^{-1}$). But then,

$$[h]_\omega^{-1} = \left(\int_0^1 \left(e^{\omega/2} L_h\right)^s \left(e^{-\omega/2} R_h\right)^{1-s}\right)^{-1} ds = \int_0^\infty (t + e^{\omega/2} L_h)^{-1} (t + e^{-\omega/2} R_h)^{-1}\, dt.$$

Now using the fact that taking inverses is C^∞ ([16], Theorem 1.2.3), we see that the map $h \mapsto (t + e^{\omega/2} L_h)^{-1}(t + e^{-\omega/2} R_h)^{-1}$ is C^∞ on $\mathfrak{S}_+$ for all $t \geq 0$. It follows that $h \mapsto [h]_\omega^{-1}$ is C^∞ on $\mathfrak{S}_+$ and C^∞ of the map $h \mapsto [h]_\omega$ follows immediately since taking inverses is C^∞. Furthermore,

$$\begin{aligned}[h]_\omega(a)^* = (R_h f_\omega(\Delta_h)(a))^* &= \int_0^1 \left(e^{\omega(s-1/2)} h^s a h^{1-s}\right)^* ds = \int_0^1 e^{\omega(s-1/2)} h^{1-s} a^* h^s\, ds \\ &= -\int_1^0 e^{\omega(1/2-t)} h^t a^* h^{1-t}\, dt = \int_0^1 e^{-\omega(t-1/2)} h^t a^* h^{1-t}\, dt = [h]_{-\omega}(a^*),\end{aligned}$$

for all $a \in M_n(\mathbb{C})$. Consequently,

$$[h]_{-\omega}^{-1}(a^*) = [h]_{-\omega}^{-1}\left([h]_\omega\left([h]_\omega^{-1}(a)\right)^*\right) = [h]_{-\omega}^{-1}\left([h]_{-\omega}\left([h]_\omega^{-1}(a)^*\right)\right) = [h]_\omega^{-1}(a)^*. \qquad \square$$

Lemma 6.1.14. *Let $\Phi_t = e^{tL}$ be a QMS on A that satisfies the ρ-DBC for some $\rho \in \mathfrak{S}_+(A)$, and let L be given in the form* (4.1) *or* (4.2) *. Then for all $h \in \mathfrak{S}_+(A)$ and all $j \in \mathcal{J}$, we have*

$$\partial_j(\log h - \log \rho) = v_j \log(e^{-\omega_j/2}h) - \log(e^{\omega_j/2}h)v_j.$$

Proof. Note that $\Delta_\rho^s v_j = e^{-s\omega_j} v_j$ by Theorem 4.4.1 and functional calculus, so that

$$\partial_s(\Delta_\rho^s v_j) = \partial_s(e^{-s\omega_j} v_j) = -\omega_j e^{-s\omega_j} v_j.$$

On the other hand, we have

$$\partial_s(\Delta_\rho^s v_j) = \partial_s(\rho^s v_j \rho^{-s}) = \rho^s \log(\rho) v_j \rho^{-s} - \rho^s v_j \rho^{-s} \log(\rho).$$

Evaluating at $s = 0$ with a minus yields $[v_j, \log(\rho)] = -\partial_s|_{s=0}(\Delta_\rho^s v_j) = \omega_j v_j$. Consequently, for all $h \in \mathfrak{S}_+(A)$,

$$\begin{aligned}
\partial_j(\log h - \log \rho) &= [v_j, \log(h)] - [v_j, \log(\rho)] = v_j \log(h) - \log(h)v_j - \omega_j v_j \\
&= v_j \log(h) - \log(h)v_j - \log(e^{\omega_j/2})v_j + \log(e^{-\omega_j/2})v_j \\
&= v_j \log(e^{-\omega_j/2}h) - \log(e^{\omega_j/2}h)v_j,
\end{aligned}$$

which is the desired identity. □

Theorem 6.1.15. *Let $\Phi_t = e^{tL}$ be a QMS on A that satisfies the ρ-DBC for some $\rho \in \mathfrak{S}_+(A)$, and let L be given in the form* (4.1) *or* (4.2)*. Then for all $h \in \mathfrak{S}_+(A)$ we have*

$$-L^\dagger(h) = \sum_{j \in \mathcal{J}} \partial_j^\dagger \left([h]_{\omega_j} \partial_j(\log h - \log \rho)\right).$$

Proof. Let $h \in \mathfrak{S}_+(A)$, then

$$\begin{aligned}
\sum_{j \in \mathcal{J}} \partial_j^\dagger \left([h]_{\omega_j} \partial_j(\log h - \log \rho)\right) &= \sum_{j \in \mathcal{J}} \partial_j^\dagger \left([h]_{\omega_j} \left(v_j \log(e^{-\omega_j/2}h) - \log(e^{\omega_j/2}h)v_j\right)\right) \\
&= \sum_{j \in \mathcal{J}} \partial_j^\dagger \left(e^{-\omega_j/2} v_j h - e^{\omega_j/2} h v_j\right) \\
&= -\sum_{j \in \mathcal{J}} \left(e^{-\omega_j/2}[v_j h, v_j^*] + e^{\omega_j/2}[v_j^*, h v_j]\right) \\
&= -L^\dagger(h),
\end{aligned}$$

where the first equality follows from Lemma 6.1.14, the second equality follows from Lemma 6.1.10 and/or Remark 6.1.11 and the last equality follows from Remark 4.4.3. □

6.2 Riemannian metrics and gradient flow for the relative entropy

As in the preceding subsection, we let $\Phi_t = e^{tL}$ be a QMS on A that satisfies the ρ-DBC for some $\rho \in \mathfrak{S}_+(A)$ and assume that $(\Phi_t)_{t \geq 0}$ has an extension to a QMS on $M_n(\mathbb{C})$. But now we also assume that $(\Phi_t)_{t \geq 0}$ is ergodic. As before, L can be written in the form (4.1) and (4.2) by Theorem 4.4.1. Throughout this subsection we fix such a generator L and the sets $\{v_j\}_{j \in \mathcal{J}} \subseteq M_n(\mathbb{C})$ and $\{\omega_j\}_{j \in \mathcal{J}} \subseteq \mathbb{R}$ that specify L according to Theorem 4.4.1.

Let $I \subseteq \mathbb{R}$ be an open interval containing $0 \in \mathbb{R}$ and let $h : I \to \mathfrak{S}_+(A)$ be a differentiable path in $\mathfrak{S}_+(A)$. We denote $\dot{h}(t) \in A$ for the derivative of h in $t \in I$. Since $\mathrm{Tr}(\dot{h}(0)) = \lim_{t\to 0} \frac{\mathrm{Tr}(h(t))-\mathrm{Tr}(h(0))}{t} = \lim_{t\to 0} \frac{1-1}{h} = 0$, there exists by Theorem 6.1.9 an affine subspace of $A^{\oplus \mathcal{J}}$ consisting of elements $\mathbf{a} \in A^{\oplus \mathcal{J}}$ such that

$$\dot{h}(0) = \mathrm{div}(\mathbf{a}).$$

We wish to rewrite this as an analog of the classical continuity equation which arises in the study of fluid dynamics:

$$\frac{\partial h}{\partial t}(x,t) + \mathrm{div}(h(x,t)\mathbf{y}(x,t)) = 0,$$

(where in this case $h(x,t)$ is a fluid density and $\mathbf{y}(x,t)$ is a flow velocity vector field). To achieve this, we first extend Definition 6.1.12:

Definition 6.2.1. Let $\vec{\lambda} \in \mathbb{R}^{|\mathcal{J}|}$ and $h \in \mathfrak{S}_+(A)$. Define the linear operator $[h]_{\vec{\lambda}} : A^{\oplus \mathcal{J}} \to A^{\oplus \mathcal{J}}$ by

$$[h]_{\vec{\lambda}}(a_1, ..., a_{|\mathcal{J}|}) = \left([h]_{\lambda_1}(a_1), ..., [h]_{\lambda_{|\mathcal{J}|}}(a_{|\mathcal{J}|})\right).$$

Note that $[h]_{\vec{\lambda}}$ is invertible with $[h]_{\vec{\lambda}}^{-1}(a_1, ..., a_{|\mathcal{J}|}) = \left([h]_{\lambda_1}^{-1}(a_1), ..., [h]_{\lambda_{|\mathcal{J}|}}^{-1}(a_{|\mathcal{J}|})\right)$. But now if $\mathbf{a} \in A^{\oplus \mathcal{J}}$ satisfies $\dot{h}(0) = \mathrm{div}(\mathbf{a})$ for some differentiable path $h : I \to \mathfrak{S}_+(A)$, then by setting $\mathbf{y} := -[h]_{\vec{\lambda}}^{-1}(\mathbf{a})$ we obtain

$$\dot{h}(0) + \mathrm{div}\left([h]_{\vec{\lambda}}(\mathbf{y})\right) = 0,$$

which is an analog of the classical continuity equation. Note that we abuse some notation here, since $h(t)$ is a differentiable path but h is also an invertible density matrix.

Remember that we have fixed a generator L and the sets $\{v_j\}_{j\in\mathcal{J}} \subseteq M_n(\mathbb{C})$ and $\{\omega_j\}_{j\in\mathcal{J}} \subseteq \mathbb{R}$ that specify L according to Theorem 4.4.1. We will also set $\vec{\omega} := \left(\omega_1, ..., \omega_{|\mathcal{J}|}\right) \in \mathbb{R}^{|\mathcal{J}|}$. The following inner products on $A^{\oplus \mathcal{J}}$ will be of relevance and can be seen as a non-commutative analog of weighted L^2-norms.

Definition 6.2.2. For each $h \in \mathfrak{S}_+$, define an inner product $\langle \cdot, \cdot \rangle_{L,h}$ on $A^{\oplus \mathcal{J}}$ by

$$\langle \mathbf{x}, \mathbf{y} \rangle_{L,h} := \langle \mathbf{x}, [h]_{\vec{\omega}}(\mathbf{y}) \rangle_{\mathrm{HS}} = \sum_{j\in\mathcal{J}} \langle x_j, [h]_{\omega_j}(y_j) \rangle_{\mathrm{HS}},$$

where $\mathbf{x} = \left(x_1, ..., x_{|\mathcal{J}|}\right), \mathbf{y} = \left(y_1, ..., y_{|\mathcal{J}|}\right) \in A^{\oplus \mathcal{J}}$.

Theorem 6.2.3. *Let $h(t)$ be a differentiable path in $\mathfrak{S}_+(A)$ defined on $(-\epsilon, \epsilon)$ for some $\epsilon > 0$ such that $h(0) = h_0 \in \mathfrak{S}_+(A)$. Then there exists a unique $\mathbf{x}_h \in A^{\oplus \mathcal{J}}$ of the form $\mathbf{x}_h = \nabla u$ with $u \in A$, for which the non commutative continuity equation*

$$\dot{h}(0) = -\mathrm{div}([h_0]_{\vec{\omega}}(\mathbf{x}_h)) = -\mathrm{div}([h_0]_{\vec{\omega}}(\nabla u))$$

holds and such that

$$\|\mathbf{x}_h\|_{L,h_0} \leq \|\mathbf{y}\|_{L,h_0}$$

for all $\mathbf{y} \in A^{\oplus \mathcal{J}}$ satisfying $\dot{h}(0) = -\mathrm{div}([h_0]_{\vec{\omega}}(\mathbf{y}))$. Moreover, u can be taken traceless, and is then uniquely determined and self-adjoint.

Proof. By Theorem 6.1.9, $R := \{\mathbf{a} \in A^{\oplus \mathcal{J}} : \dot{h}(0) = \mathrm{div}(\mathbf{a})\}$ is a nontrivial affine subspace of $A^{\oplus \mathcal{J}}$. In particular, R is convex and so is $-[h_0]_{\vec{\omega}}^{-1}(R)$ as $-[h_0]_{\vec{\omega}}^{-1}$ is linear. In our finite-dimensional setting, $-[h_0]_{\vec{\omega}}^{-1}(R)$ is a closed convex set consisting exactly of elements $\mathbf{y} \in A^{\oplus \mathcal{J}}$ such that $\dot{h}(0) = -\mathrm{div}([h_0]_{\vec{\omega}}\mathbf{y})$ by our previous discussion. Hence, there exists a unique $\mathbf{x}_h \in A^{\oplus \mathcal{J}}$ satisfying $\dot{h}(0) = -\mathrm{div}([h_0]_{\vec{\omega}}\mathbf{x}_h)$ and such that $\|\mathbf{x}_h\|_{L,h_0} \leq \|\mathbf{y}\|_{L,h_0}$ for all $\mathbf{y} \in A^{\oplus \mathcal{J}}$ satisfying $\dot{h}(0) = \mathrm{div}([h_0]_{\vec{\omega}}\mathbf{y})$.

We now show that $\mathbf{x}_h$ is gradient using Remark 6.1.5. Let $\mathbf{a} \in \ker(\mathrm{div})$ and set $\mathbf{w} := [h_0]_{\vec{\omega}}^{-1}(\mathbf{a})$ and $\mathbf{y}_c := \mathbf{x}_h - c\mathbf{w}$ for $c \in \mathbb{C}$. Then

$$\dot{h}(0) + \mathrm{div}([h_0]_{\vec{\omega}}(\mathbf{y}_c)) = \dot{h}(0) + \mathrm{div}([h_0]_{\vec{\omega}}(\mathbf{x}_h)) - c \cdot \mathrm{div}([h_0]_{\vec{\omega}}(\mathbf{w})) = 0$$

as $\dot{h}(0) + \mathrm{div}([h_0]_{\vec{\omega}}(\mathbf{x}_h)) = 0$ and $\mathrm{div}(\mathbf{a}) = 0$. Hence $\|\mathbf{x}_h\|_{L,h_0} \leq \|\mathbf{y}_c\|_{L,h_0}$ for all $c \in \mathbb{C}$, or equivalently,

$$2\Re[c\langle \mathbf{x}_h, \mathbf{w}\rangle_{L,h_0}] \leq |c|^2 \|\mathbf{w}\|_{L,h_0}^2$$

for all $c \in \mathbb{C}$. Taking $c = \overline{\langle \mathbf{x}_h, \mathbf{w}\rangle}_{L,h_0} / \|\mathbf{w}\|_{L,h_0}^2$, gives

$$2\frac{|\langle \mathbf{x}_h, \mathbf{w}\rangle_{L,h_0}|^2}{\|\mathbf{w}\|_{L,h_0}^2} \leq \frac{|\langle \mathbf{x}_h, \mathbf{w}\rangle_{L,h_0}|^2}{\|\mathbf{w}\|_{L,h_0}^2},$$

which is only possible if $\langle \mathbf{x}_h, \mathbf{w}\rangle_{L,h_0} = 0$, and therefore

$$\langle \mathbf{x}_h, \mathbf{a}\rangle_{\mathrm{HS}} = \langle \mathbf{x}_h, [h_0]\mathbf{w}\rangle_{\mathrm{HS}} = \langle \mathbf{x}_h, \mathbf{w}\rangle_{L,h_0} = 0.$$

It follows that $\mathbf{x}_h \in \ker(\mathrm{div})^{\perp} = \mathrm{Im}(\nabla)$ by Remark 6.1.5, i.e. there exist $u \in A$ such that $\mathbf{x}_h = \nabla u$. By subtracting a multiple of the identity from u, we may take u to be traceless. And if there exists another traceless $\tilde{u} \in A$ such that $\mathbf{x}_h = \nabla \tilde{u}$, then $\nabla(u - \tilde{u}) = 0$ so that $u - \tilde{u} = \alpha 1$ for some $\alpha \in \mathbb{C}$ by Theorem 6.1.7 and Remark 6.1.8 ($(\Phi)_{t\geq 0}$ is ergodic). But then $\alpha = \mathrm{Tr}(u) - \mathrm{Tr}(\tilde{u}) = 0$ so that u is then uniquely determined.

To show that in this case u is self-adjoint, we define the operator L_{h_0} on A by $L_{h_0}(a) = \mathrm{div}([h_0]_{\vec{\omega}}\nabla a)$. A direct computation gives

$$\begin{aligned} L_{h_0}(a) &= \mathrm{div}([h_0]_{\omega_1}\partial_1(a), ..., [h_0]_{\omega_{|\mathcal{J}|}}\partial_{|\mathcal{J}|}(a))) = \sum_{j\in\mathcal{J}} \left[[h_0]_{\omega_j}(\partial_j(a_j), v_j^*\right] \\ &= \sum_{j\in\mathcal{J}} \left[[h_0]_{\omega_j}([v_j, a_j]), v_j^*\right] = \sum_{j\in\mathcal{J}} ([h_0]_{\omega_j}(v_j a - a v_j))v_j^* - \sum_{j\in\mathcal{J}} v_j^*([h_0]_{\omega_j}(v_j a - a v_j)). \end{aligned}$$

Then using Lemma 6.1.13, we get

$$\begin{aligned} L_{h_0}(a)^* &= \sum_{j\in\mathcal{J}} v_j([h_0]_{-\omega_j}(a^* v_j^* - v_j^* a^*)) - \sum_{j\in\mathcal{J}} ([h_0]_{-\omega_j}(a^* v_j^* - v_j^* a^*))v_j \\ &= \sum_{j\in\mathcal{J}} ([h_0]_{-\omega_j}(v_j^* a^* - a^* v_j^*))v_j - \sum_{j\in\mathcal{J}} v_j([h_0]_{-\omega_j}(v_j^* a^* - a^* v_j^*)). \end{aligned}$$

By the fact that $\{v_j\}_{j\in\mathcal{J}} = \{v_j^*\}_{j\in\mathcal{J}}$ and that for all $j \in \mathcal{J}$, $\Delta_\rho(v_j) = e^{-\omega_j}v_j$ and $\Delta_\rho(v_j^*) = e^{\omega_j}v_j^*$, we may define $j' \in \mathcal{J}$ by $v_{j'} = v_j^*$ so that $\omega_{j'} = -\omega_j$. So continuing with the expression for $L_{h_0}(a)^*$,

$$\begin{aligned}
L_{h_0}(a)^* &= \sum_{j\in\mathcal{J}}([h_0]_{-\omega_j}(v_j^*a^* - a^*v_j^*))v_j - \sum_{j\in\mathcal{J}} v_j([h_0]_{-\omega_j}(v_j^*a^* - a^*v_j^*)) \\
&= \sum_{j\in\mathcal{J}}([h_0]_{-\omega_{j'}}(v_{j'}^*a^* - a^*v_{j'}^*))v_{j'} - \sum_{j\in\mathcal{J}} v_{j'}([h_0]_{-\omega_{j'}}(v_{j'}^*a^* - a^*v_{j'}^*)) \\
&= \sum_{j\in\mathcal{J}}([h_0]_{\omega_j}(v_ja^* - a^*v_j))v_j^* - \sum_{j\in\mathcal{J}} v_j^*([h_0]_{\omega_j}(v_ja^* - a^*v_j)) \\
&= L_{h_0}(a^*).
\end{aligned}$$

However, $L_{h_0}(u) = -\dot{h}(0)$ and since $\dot{h}(0)$ is self-adjoint, we obtain $\operatorname{div}([h_0]_{\vec{\omega}}\nabla u^*) = L_{h_0}(u^*) = L_{h_0}(u)^* = -\dot{h}(0)$. Now by the uniqueness of u, we see that $u = u^*$. □

Theorem 6.2.3 allows us to define a Riemannian manifold $(\mathfrak{S}_+(A), g)$ for some Riemannian metric g which we will show. Set $m := \dim(A)$. Let $a_1, ..., a_{m-1}$ be an orthonormal set of self-adjoint traceless elements in $(A, \langle\cdot,\cdot\rangle_{\text{HS}})$ such that the orthogonal complement of the identity is the span of $a_1, ..., a_{m-1}$. We can regard $\mathfrak{S}_+(A)$ as an $m-1$ dimensional manifold with one coordinate map $u : \mathfrak{S}_+(A) \to \mathbb{R}^{m-1}$ defined by

$$\phi(h) = (\operatorname{Tr}(a_1 h), ..., \operatorname{Tr}(a_{m-1}h)).$$

This map is indeed a chart, because if $\phi(h_1) = \phi(h_2)$, then $\langle h_1 - h_2, a_k\rangle_{\text{HS}}$ for all $k = 1, ..., m-1$. But $h_1 - h_2 \in \operatorname{span}(a_1, ..., a_{m-1})$ so that $\langle h_1 - h_2, h_1 - h_2\rangle_{\text{HS}} = 0$, or $h_1 = h_2$. If follows that $\phi : \mathfrak{S}_+(A) \to \phi(\mathfrak{S}_+(A)) \subseteq \mathbb{R}^{m-1}$ is a homeomorphism.

Let $h_0 \in \mathfrak{S}_+(A)$. By Theorem 6.2.3, there is a one-to-one correspondence between the tangent space $T_{h_0}\mathfrak{S}_+(A)$ and the set $G := \{\nabla u : u \in A,\ \operatorname{Tr}(u) = 0 \text{ and } u = u^*\}$. Henceforth, we will identity the tangent space $T_{h_0}\mathfrak{S}_+(A)$ with G through Theorem 6.2.3.

Definition 6.2.4. Let $h_0 \in \mathfrak{S}_+(A)$. Let $h^1(t), h^2(t)$ be two smooth paths in $\mathfrak{S}_+(A)$ defined on $(-\epsilon, \epsilon)$ for some $\epsilon > 0$ such that $h^1(0) = h^2(0) = h_0$. We define the (complex) Riemannian metric $g_{L,h_0} : T_{h_0}\mathfrak{S}_+(A) \times T_{h_0}\mathfrak{S}_+(A) \to \mathbb{C}$ by

$$g_{L,h_0}(\dot{h}^1(0), \dot{h}^2(0)) = \langle \mathbf{x}_{h^1}, \mathbf{x}_{h^2}\rangle_{L,h_0},$$

where h^i and $\mathbf{x}_{h^i}$ are uniquely related by Theorem 6.2.3 ($i = 1, 2$). We denote the norm with respect to this metric by $\|\cdot\|_{g_{L,h_0}}$.

To show that $g_{L,h}$ indeed varies smoothly with $h \in \mathfrak{S}_+(A)$, we let $\phi^k(h) = \operatorname{Tr}(a_k h)$ be the kth coordinate function. We may define $u_{k,h}$ to be the unique traceless self-adjoint matrix in A such that $a_k = -\operatorname{div}([h]_{\vec{\omega}}(\nabla u_{k,h}))$ by choosing a smooth curve $h(t) := h + ta_k$ with $h \in \mathfrak{S}_+(A)$ and without loss of generality we may assume that there exists an interval $(-\epsilon, \epsilon)$ such that $h(t) \in \mathfrak{S}_+(A)$ for all $t \in (-\epsilon, \epsilon)$. It follows that $\dot{h}(0) = -\operatorname{div}([h]_{\vec{\omega}}(\nabla u_{k,h}))$. But, by orthonormality of $\{a_1, ..., a_{m-1}\}$, the corresponding coordinate of $\dot{h}(0)$ is

$$\begin{aligned}
\lim_{t\to 0}\frac{\phi(h + ta_k) - \phi(h)}{t} &= \lim_{t\to 0}\frac{(\operatorname{Tr}(a_1(h + ta_k)), ..., \operatorname{Tr}(a_{m-1}(h + ta_k))) - (\operatorname{Tr}(a_1 h), ..., \operatorname{Tr}(a_{m-1}h))}{t} \\
&= \lim_{t\to 0}\frac{t(\operatorname{Tr}(a_1 a_k), ..., \operatorname{Tr}(a_{m-1}a_k))}{t} = e_k \in \mathbb{R}^{m-1},
\end{aligned}$$

where e_k is the kth is the standard unit vector of $\mathbb{R}^{m-1}$. Hence, the kth coordinate basis vector for $T_h\mathfrak{S}_+(A) \simeq G$ is given by $\frac{\partial}{\partial x^k} = \nabla u_{k,h}$ (where we identified $T_h\mathfrak{S}_+(A)$ with G through Theorem 6.2.3). Therefore, in this coordinate system, the k,l component of the metric tensor is given by

$$[g_{L,h}]_{k,l} = g_{L,h}(\nabla u_{k,h}, \nabla u_{l,h}) = \langle \nabla u_{k,h}, \nabla u_{l,h}\rangle_{L,h} = \sum_{j\in\mathcal{J}} \langle \partial_j(u_{k,h}), [h]_{\omega_j}\partial_j(u_{l,h})\rangle_{\mathrm{HS}}.$$

Now by Lemma 6.1.13, the map $h \to [h]_{\omega_j}$ is C^∞ for all $j \in \mathcal{J}$. Consequently, $g_{L,h}$ is a C^∞ function of $h \in \mathfrak{S}_+(A)$ which is what we needed to show.

Definition 6.2.5. Let $f : \mathfrak{S}_+(A) \to \mathbb{R}$ be differentiable. The *differential of f at $h \in \mathfrak{S}_+(A)$*, denoted by $\dfrac{\delta f}{\delta h}(h)$, is the unique traceless self-adjoint element in A satisfying

$$\lim_{t\to 0} \frac{f(h+ta) - f(h)}{t} = \left\langle a, \frac{\delta f}{\delta h}(h)\right\rangle_{\mathrm{HS}} = \left\langle \frac{\delta f}{\delta h}(h), a\right\rangle_{\mathrm{HS}}$$

for all traceless self-adjoint elements $a \in A$.

In Chapter 2 we introduced gradient flows. For the sake of completeness, we introduce it again as it will not hurt to repeat these concepts.

Definition 6.2.6. Let (M, g) be a Riemannian manifold and let $f : M \to \mathbb{R}$ be continuously differentiable. The *Riemannian gradient of f at $p \in M$*, denoted by $\mathrm{grad}_p f$, is the unique tangent vector in T_pM satisfying the equation

$$\frac{d}{dt}\Big|_{t=0} f(\gamma(t)) = g_p(\mathrm{grad}_p f, \dot\gamma(0))$$

for all smooth curves $\gamma : (-\epsilon, \epsilon) \to M$ such that $\gamma(0) = p$.

Let (M, g) be a Riemannian manifold and let $f : M \to \mathbb{R}$ continuously differentiable. Fix $p \in M$. Then one might ask for which smooth curve $\gamma : (-\epsilon, \epsilon) \to M$ with $\gamma(0) = p$ the derivative $\frac{d}{dt}\big|_{t=0} f(\gamma(t))$ is as large or as small as possible. By the definition of the Riemannian gradient, we see that we need to choose γ such that $\dot\gamma(0)$ and $\mathrm{grad}_p f$ are linearly dependent. So essentially, $\mathrm{grad}_p f$ indicates the direction in which f increases and decreases most rapidly. The corresponding *gradient flow equation for strongest ascent* associated to f is the flow induced by the differential equation

$$\dot\gamma(t) = \mathrm{grad}_{\gamma(t)} f, \quad \gamma(0) = p.$$

Similarly, the *gradient flow equation for steepest descent* associated to f is the flow induced by the differential equation

$$\dot\gamma(t) = -\mathrm{grad}_{\gamma(t)} f, \quad \gamma(0) = p.$$

Now take $f : \mathfrak{S}_+(A) \to \mathbb{R}$ continuously differentiable. Let $h \in \mathfrak{S}_+(A)$. The identification of $T_h\mathfrak{S}_+(A)$ with $G = \{\nabla u : u \in A,\ \mathrm{Tr}(u) = 0 \text{ and } u = u^*\}$ through Theorem 6.2.3 shows that we can interpret the Riemannian gradient $\mathrm{grad}_h f$ of f at $h \in \mathfrak{S}_+(A)$ with respect to the Riemannian metric g_L as the unique element in G satisfying

$$\frac{d}{dt}\Big|_{t=0} f(h(t)) = \langle \mathrm{grad}_h f, \nabla u\rangle_{L,h}$$

for all smooth curves $h(t)$ in $\mathfrak{S}_+(A)$ defined on $(-\epsilon, \epsilon)$ for some $\epsilon > 0$ with $h(0) = h$ and $\dot h(0) = -\mathrm{div}([h]_{\vec\omega}(\nabla u))$ for some self-adjoint $u \in A$.

Theorem 6.2.7. *Let $f : \mathfrak{S}_+(A) \to \mathbb{R}$ be a continuously differentiable function. The Riemannian gradient* $\operatorname{grad}_h f$ *of f at $h \in \mathfrak{S}_+(A)$ with respect to the Riemannian metric g_L is given by*

$$\operatorname{grad}_h f = \nabla \left(\frac{\delta f}{\delta h}(h) \right).$$

Furthermore, the corresponding gradient flow equation (for steepest descent) is

$$\dot{h}(t) = \operatorname{div}\left([h(t)]_{\vec{\omega}} \nabla \frac{\delta f}{\delta h}(h(t)) \right).$$

Proof. Let $h(t)$ be a smooth curve in $\mathfrak{S}_+(A)$ defined on $(-\epsilon, \epsilon)$ for some $\epsilon > 0$ with $h(0) = h$ and $\dot{h}(0) = -\operatorname{div}([h]_{\vec{\omega}}(\nabla u))$ for some self-adjoint $u \in A$. Then, using the definitions,

$$\begin{aligned}
\langle \operatorname{grad}_h f, [h]_{\vec{\omega}}(\nabla u) \rangle_{\text{HS}} &= \langle \operatorname{grad}_h f, \nabla u \rangle_{L,h} = \frac{d}{dt}\Big|_{t=0} f(h(t)) = \lim_{t \to 0} \frac{f(h(t)) - f(h(0))}{t} \\
&= \lim_{t \to 0} \frac{f(h + t\dot{h}(0)) - f(h)}{t} = \left\langle \frac{\delta f}{\delta h}(h), \dot{h}(0) \right\rangle_{\text{HS}} \\
&= -\left\langle \frac{\delta f}{\delta h}(h), \operatorname{div}([h]_{\vec{\omega}}(\nabla u)) \right\rangle_{\text{HS}} = \left\langle \nabla \left(\frac{\delta f}{\delta h}(h) \right), [h]_{\vec{\omega}}(\nabla u) \right\rangle_{\text{HS}},
\end{aligned}$$

where the last equality follows from $\nabla = -\operatorname{div}^\dagger$ (Remark 6.1.5). In particular, we see that the identity $\langle \operatorname{grad}_h f, [h]_{\vec{\omega}}(\nabla u) \rangle_{\text{HS}} = \left\langle \nabla \left(\frac{\delta f}{\delta h}(h) \right), [h]_{\vec{\omega}}(\nabla u) \right\rangle_{\text{HS}}$ is path-independent. So by Theorem 6.2.3, we obtain $\langle \operatorname{grad}_h f, [h]_{\vec{\omega}}(\mathbf{x}) \rangle_{\text{HS}} = \left\langle \nabla \left(\frac{\delta f}{\delta h}(h) \right), [h]_{\vec{\omega}}(\mathbf{x}) \right\rangle_{\text{HS}}$ for all $\mathbf{x} \in A^{\oplus \mathcal{J}}$ and since $[h]_{\vec{\omega}}$ is invertible, we obtain $\operatorname{grad}_h f = \nabla \left(\frac{\delta f}{\delta h}(h) \right)$. The identification of G with $T_p \mathfrak{S}_+(A)$ through Theorem 6.2.3 shows that the corresponding gradient flow equation (for steepest descent) is

$$\dot{h}(t) = \operatorname{div}\left([h(t)]_{\vec{\omega}} \nabla \frac{\delta f}{\delta h}(h(t)) \right).$$

□

The *relative entropy with respect to* $\rho \in \mathfrak{S}_+(A)$ is the functional $D(\cdot||\rho) : \mathfrak{S}_+(A) \to \mathbb{R}$ defined by

$$D(h||\rho) = \operatorname{Tr}(h(\log h - \log \rho)).$$

Applying Theorem 6.2.7 to $D(\cdot||\rho)$ yields:

Theorem 6.2.8. *Let $\Phi_t = e^{tL}$ be an ergodic QMS on A that satisfies the ρ-DBC for $\rho \in \mathfrak{S}_+(A)$. Then*

$$\frac{d}{dt} h(t) = L^\dagger(h(t))$$

is gradient flow for the relative entropy $D(\cdot||\rho)$ in the Riemannian metric g_L canonically associated to L through its representation in the form (4.1)/(4.2).

Proof. For all traceless self-adjoint $a \in A$ we have

$$\begin{aligned}
\lim_{t\to 0}\frac{D(h+ta||\rho)-D(h)}{t} &= \lim_{t\to 0}\frac{\mathrm{Tr}\left[h\log(h+ta)+ta\log(h+ta)-h\log(\rho)-ta\log(\rho)\right]}{t} \quad - \\
&\quad \lim_{t\to 0}\frac{\mathrm{Tr}(h\log(h)-h\log(\rho))}{t} \\
&= \lim_{t\to 0}\mathrm{Tr}[a(\log(h+ta)-\log(\rho))] + \lim_{t\to 0}\frac{\mathrm{Tr}[h\log(h+ta)-h\log(h)]}{t} \\
&= \mathrm{Tr}(a(\log h-\log\rho)) + \mathrm{Tr}(a) \\
&= \mathrm{Tr}(a(\log h-\log\rho)) = \langle \log h-\log\rho, a\rangle_{\mathrm{HS}},
\end{aligned}$$

as $\lim_{t\to 0}\dfrac{h\log(h+ta)-h\log(h)}{t} = \dfrac{d}{dt}\Big|_{t=0}\varphi(t) = a$ with $\varphi(t) := h\log(h+ta)$. Thus,

$$\frac{\delta}{\delta h}D(h||\rho) = \log h - \log\rho.$$

But then by Theorem 6.1.15, we obtain

$$\begin{aligned}
\dot h(t) = L^\dagger(h(t)) &\iff \dot h(t) = -\sum_{j\in\mathcal{J}}\partial_j^\dagger\left([h(t)]_{\omega_j}\partial_j(\log h(t)-\log\rho)\right) \\
&\iff \dot h(t) = \mathrm{div}\left([h(t)]_{\vec\omega}\nabla(\log h(t)-\log\rho)\right) \\
&\iff \dot h(t) = \mathrm{div}\left([h(t)]_{\vec\omega}\nabla\left(\frac{\delta}{\delta h}D(h(t)||\rho)\right)\right).
\end{aligned}$$

So indeed, $\frac{d}{dt}h(t) = L^\dagger(h(t))$ is equivalent to the gradient flow equation for the relative entropy $D(\cdot||\rho)$ by Theorem 6.2.7. □

7 Quantum Ornstein-Uhlenbeck semigroups

In this section we present some examples of quantum Markov semigroups with detailed balance. The semigroups that we will discuss are motivated by quantum theory.

7.1 The infinite-temperature Fermi Ornstein–Uhlenbeck semigroup

Definition 7.1.1. Let $n \in \mathbb{N} \cup \{\infty\}$ and let $q_1, ..., q_n$ be self adjoint operators on a finite-dimensional Hilbert space H such that $q_i q_j + q_j q_i = 2\delta_{i,j}1$ for all $1 \leq i, j \leq n$. The equations $q_i q_j + q_j q_i = 2\delta_{i,j}1$ are called the *canonical anti-commutation relations (CAR)* and the C^*-algebra generated by $q_1, ..., q_n$ is called a *CAR algebra*.

Fix $n = 2m$ for some $m \in \mathbb{N}$ and let $\mathfrak{C}^n$ be the (finite-dimensional) CAR-algebra generated by some self-adjoint operators $q_1, ..., q_n$ on a finite dimensional Hilbert space H. Define the (unique) automorphism $\Gamma : \mathfrak{C}^n \to \mathfrak{C}^n$ by $\Gamma(q_i) = -q_i$ for all $j = 1, .., n$ and define $w \in \mathfrak{C}^n$ by

$$w = i^m \prod_{j=1}^{2m} q_j.$$

Since the operators $iq_{2j-1}q_{2j}$ are self adjoint and unitary for all $j = 1, ..., m$ by the canonical anti-commutation relations and they commute with each other, it follows that w is also self-adjoint and unitary. Moreover, Γ is given by

$$\Gamma(a) = waw = w^*aw = waw^* \quad \text{for all } a \in \mathfrak{C}^n$$

as $wq_jw = -q_j$ for all $j = 1, ...n$ (use that w and q_j anti-commute and $w^2 = 1$). For a multi-index $\boldsymbol{\alpha} = (\alpha_1, ..., \alpha_n) \in \{0, 1\}^n$ (and in this context $\boldsymbol{\alpha}$ is also called a *fermion multi-index*), we define

$$q^{\boldsymbol{\alpha}} = q_1^{\alpha_1} \dots q_n^{\alpha_n} \quad \text{and} \quad |\boldsymbol{\alpha}| := \sum_{j=1}^{n} \alpha_j.$$

Now also define

$$\begin{aligned} &L : \mathfrak{C}^n \to \mathfrak{C}^n, \quad L(a) = \frac{1}{2}\sum_{j=1}^{n}(q_j\Gamma(a)q_j - a) \quad \text{and} \\ &v_j := iwq_j, \quad j = 1, ..., n. \end{aligned}$$

By a direct computation,

$$\begin{aligned} L(q^{\boldsymbol{\alpha}}) &= \frac{1}{2}\sum_{j=1}^{n}(q_j\Gamma(q_1^{\alpha_1})\cdots\Gamma(q_n^{\alpha_n})q_j - q^{\boldsymbol{\alpha}}) = \frac{1}{2}\sum_{j=1}^{n}\left((-1)^{|\boldsymbol{\alpha}|}q_jq^{\boldsymbol{\alpha}}q_j - q^{\boldsymbol{\alpha}}\right) \\ &= \frac{1}{2}\sum_{j:\alpha_j=1}(-q^{\boldsymbol{\alpha}} - q^{\boldsymbol{\alpha}}) = -|\boldsymbol{\alpha}|q^{\boldsymbol{\alpha}}. \end{aligned}$$

Hence, $-L$ is called the *fermion number operator*. Note that v_j is self-adjoint and unitary since w

and q_j anti-commute for each j. In particular, $v_j^2 = 1$ so that

$$\begin{aligned}
L(a) &= \frac{1}{2}\sum_{j=1}^{n}(q_j\Gamma(a)q_j - a) = \frac{1}{2}\sum_{j=1}^{n}(q_j wawq_j - a) = \frac{1}{2}\sum_{j=1}^{n}(v_j a v_j - a) \\
&= -\frac{1}{4}\sum_{j=1}^{n}(2a - 2v_j a v_j) = -\frac{1}{4}\sum_{j=1}^{n}(v_j^2 a - v_j a v_j - v_j a v_j + a v_j^2) \\
&= -\frac{1}{4}\sum_{j=1}^{n}(v_j[v_j, a] - [v_j, a]v_j) = -\frac{1}{4}\sum_{j=1}^{n}[v_j, [v_j, a]].
\end{aligned}$$

By making the substitution $v_j \to \frac{1}{2}v_j$, we see that L has the expression as in Remark 4.4.2. Thus, $\Phi_t = e^{tL}$ is a QMS satisfying the $\dim(H)^{-1}1$-DBC by Theorem 4.4.1 and we refer to it as the *infinite-temperature Fermi Ornstein–Uhlenbeck semigroup.*

7.2 The finite-temperature Fermi Ornstein–Uhlenbeck semigroup

Let $\{q_1, .., q_m, p_1, ..., p_m\}$ be a set of self-adjoint operators acting on some Hilbert space that satisfy CAR:

$$q_j q_k + q_k q_j = p_j p_k + p_k p_j = 2\delta_{j,k}1 \quad \text{and} \quad q_j p_k + p_k q_j = 0 \quad \text{for all } 1 \le j, k \le m.$$

Denote $\mathfrak{C}^{2m}$ as the CAR-algebra generated by $q_1, .., q_m, p_1, ..., p_m$. Define the operators

$$z_j := \frac{1}{\sqrt{2}}(q_j + ip_j) \quad \text{for } j = 1, ..., m.$$

It immediately follows that for all $1 \le j, k \le m$,

$$\begin{aligned}
z_j z_k + z_k z_j &= \frac{1}{2}\left((q_j + ip_j)(q_k + ip_k) + (q_k + ip_k)(q_j + ip_j)\right) \\
&= \frac{1}{2}(q_j q_k + iq_j p_k + ip_j q_k - p_j p_k + q_k q_j + iq_k p_j + ip_k q_j - p_k p_j) = 0, \quad \text{and} \\
z_j z_k^* + z_k^* z_j &= \frac{1}{2}\left((q_j + ip_j)(q_k - ip_k) + (q_k - ip_k)(q_j + ip_j)\right) \\
&= \frac{1}{2}(q_j q_k - iq_j p_k + ip_j q_k + p_j p_k + q_k q_j + iq_k p_j - ip_k q_j + p_k p_j) = 2\delta_{j,k}1.
\end{aligned}$$

Define

$$r_j := \frac{1}{2}z_j^* z_j \quad \text{and} \quad r_j^{\perp} := \frac{1}{2}z_j z_j^* \quad \text{for } j = 1, ..., m.$$

Then r_j is a projection since $r_j^2 = \frac{1}{4}(z_j^* z_j)(z_j^* z_j) = \frac{1}{4}(2 - z_j z_j^*)z_j^* z_j = \frac{1}{4}\left(2z_j^* z_j - z_j(z_j^*)^2 z_j\right) = \frac{1}{2}z_j^* z_j = r_j$ as $(z_j^*)^2 = 0$ and it is clear that $r_j^* = r_j$. Similarly, $r_j^{\perp}$ is a projection and r_j and $r_j^{\perp}$ are mutually orthogonal (as the notation already suggests) since $z_j^2 = (z_j^*)^2 = 0$.

Now, using $z_j z_k^* + z_k^* z_j = 2\delta_{j,k}1$ and $z_j^2 = (z_j^*)^2 = 0$, we have

$$z_j r_j = r_j^{\perp} z_j = z_j \quad \text{and} \quad r_j z_j = z_j r_j^{\perp} = 0.$$

Furthermore, for all $j \neq k$,

$$r_k z_j = \frac{1}{2}z_k^* z_k z_j = -\frac{1}{2}z_k^* z_j z_k = \frac{1}{2}z_j z_k^* z_k = z_k r_k \quad \text{and similarly} \quad z_j r_k^{\perp} = r_k^{\perp} z_j.$$

In the same vein, the set $\{r_1, ...r_m, r_1^\perp, ..., r_m^\perp\}$ is a set of commuting projections.

For any set of m real numbers $\{\mu_1, ..., \mu_m\} \subseteq \mathbb{R}$ and any $\beta > 0$ (β in interpreted as the *inverse temperature*), we define the *free Hamiltonian* h and *Gibbs state* σ_β by

$$h = \sum_{j=1}^{m} \mu_j r_j \quad \text{and} \quad \sigma_\beta = \frac{1}{\mathrm{Tr}(e^{-\beta h})} e^{-\beta h}.$$

Since $r_1, ..., r_m$ are commuting projections, we note that $e^{-\beta h} = \prod_{j=1}^m e^{-\beta \mu_j r_j} = \prod_{j=1}^m \left(e^{-\beta\mu_j} r_j + r_j^\perp\right)$ where in the last equality we used functional calculus and the fact that the spectrum of r_j is $\{0, 1\}$. Hence,

$$\begin{aligned}
\Delta_{\sigma_\beta}(z_k) &= \left[\prod_{j=1}^{m} \left(e^{-\beta\mu_j} r_j + r_j^\perp\right)\right] z_k \left[\prod_{j=1}^{m} \left(e^{\beta\mu_j} r_j + r_j^\perp\right)\right] \\
&= \left(e^{-\beta\mu_k} r_k + r_k^\perp\right) \left[\prod_{j\neq k} \left(e^{-\beta\mu_j} r_j + r_j^\perp\right)\right] z_k \left[\prod_{j\neq k} \left(e^{\beta\mu_j} r_j + r_j^\perp\right)\right] \left(e^{\beta\mu_k} r_k + r_k^\perp\right) \\
&= \left(e^{-\beta\mu_k} r_k + r_k^\perp\right) z_k \left[\prod_{j\neq k} \left(e^{-\beta\mu_j} r_j + r_j^\perp\right)\right] \left[\prod_{j\neq k} \left(e^{-\beta\mu_j} r_j + r_j^\perp\right)\right] \left(e^{\beta\mu_k} r_k + r_k^\perp\right) \\
&= \left(e^{-\beta\mu_k} r_k + r_k^\perp\right) z_k \left(e^{\beta\mu_k} r_k + r_k^\perp\right) \\
&= r_k z_k r_k + e^{-\beta\mu_k} r_k z_k r_k^\perp + e^{\beta\mu_k} r_k^\perp z_k r_k + r_k^\perp z_k r_k^\perp \\
&= e^{\beta\mu_k} z_k,
\end{aligned}$$

where we used that $r_1, ..., r_m, r_1^\perp, ..., r_m^\perp$ commute with each other, the third equality is because z_k commutes with r_j and $r_j^\perp$ for $j \neq k$, the fourth equality is the fact that $\left(e^{-\beta\mu_j} r_j + r_j^\perp\right)\left(e^{\beta\mu_j} r_j + r_j^\perp\right) = r_j + r_j^\perp = 1$ for all j and the last equality comes from $z_k r_k = r_k^\perp z_k = z_k$ and $r_k z_k = z_k r_k^\perp = 0$.

For each $j = 1, ..., m$, $q_j p_j$ commutes with both q_k and p_k for all $k \neq j$ by CAR and $i q_j p_j$ is self-adjoint and unitary also by CAR. Consequently, as in the previous subsection,

$$w := i^m \prod_{j=1}^{m} q_j p_j$$

is also self-adjoint and unitary. Note that w commutes with every even element in $\mathfrak{C}^{2m}$. In particular, w commutes with r_j and $r_j^\perp$ for all j. Therefore, $\Delta_{\sigma_\beta}(w z_k) = e^{\beta\mu_k} w z_k$ by a similar computation as before and it directly follows that $\Delta_{\sigma_\beta}(z_k^* w) = e^{-\beta\mu_k} z_k^* w$.

Define the operators

$$v_j = w z_j \quad \text{for } j = 1, ..., m.$$

Then the set $\{v_1, ..., v_m, v_1^*, ..., v_m^*\}$ satisfies properties (3) and (4) of Theorem 4.4.1 so that L_β defined by

$$L_\beta(a) = \frac{1}{4} \sum_{j=1}^{m} \left[e^{\beta\mu_j/2} \left(v_j^*[a, v_j] + [v_j^*, a] v_j\right) + e^{-\beta\mu_j/2} \left(v_j [a, v_j^*] + [v_j, a] v_j^*\right) \right]$$

is the generator of a QMS $\Phi_t = e^{tL_\beta}$ that satisfies the σ_β-DBC by Theorem 4.4.1. The QMS $\Phi_t = e^{tL_\beta}$ is called the *finite-temperature Fermi Ornstein–Uhlenbeck semigroup*. The justification of calling it the *finite*-temperature Fermi Ornstein–Uhlenbeck semigroup is because in the infinite temperature limit, that is when $\beta \to 0$, we recover the *infinite*-temperature Fermi Ornstein–Uhlenbeck semigroup:

Proposition 7.2.1. *Adopt the foregoing definitions. Then, for all $a \in \mathfrak{C}^{2m}$,*

$$\lim_{\beta\to 0} L_\beta(a) = -\frac{1}{4}\sum_{j=1}^{m}\left(\left[v_j,[v_j^*,a]\right] + \left[v_j^*,[v_j,a]\right]\right) = \frac{1}{2}\sum_{j=1}^{m}(q_j\Gamma(a)q_j + p_j\Gamma(a)p_j - 2a),$$

where $\Gamma : \mathfrak{C}^n \to \mathfrak{C}^n$ is the automorphism defined by $\Gamma(a) = waw$.

Proof. By a direct computation, we obtain

$$\begin{aligned}
\lim_{\beta\to 0} L_\beta(a) &= \frac{1}{4}\sum_{j=1}^{m}\left(v_j^*[a,v_j] + [v_j^*,a]v_j + v_j[a,v_j^*] + [v_j,a]v_j^*\right)\\
&= \frac{1}{4}\sum_{j=1}^{m}(v_j^*av_j - v_j^*v_ja + v_j^*av_j - av_j^*v_j + v_jav_j^* - v_jv_j^*a + v_jav_j^* - av_jv_j^*)\\
&= -\frac{1}{4}\sum_{j=1}^{m}(v_jv_j^*a - v_jav_j^* - v_j^*av_j + av_j^*v_j + v_j^*v_ja - v_j^*av_j - v_jav_j^* + av_jv_j^*)\\
&= -\frac{1}{4}\sum_{j=1}^{m}(v_j[v_j^*,a] - [v_j^*,a]v_j + v_j^*[v_j,a] - [v_j,a]v_j^*)\\
&= -\frac{1}{4}\sum_{j=1}^{m}\left(\left[v_j,[v_j^*,a]\right] + \left[v_j^*,[v_j,a]\right]\right).
\end{aligned}$$

Remember that $z_j = \frac{1}{\sqrt{2}}(p_j + iq_j)$, so that $\Gamma(z_j) = -z_j$. Using this and the definitions,

$$\begin{aligned}
[v_j,[v_j^*,a]] &= v_jv_j^*a - v_jav_j^* - v_j^*av_j + av_j^*v_j\\
&= wz_jz_j^*wa - wz_jaz_j^*w - z_j^*wawz_j + az_j^*w^2z_j\\
&= \Gamma(z_jz_j^*)a - \Gamma(z_jaz_j^*) - z_j^*\Gamma(a)z_j + az_j^*z_j\\
&= z_jz_j^*a - z_j\Gamma(a)z_j^* - z_j^*\Gamma(a)z_j + az_j^*z_j\\
&= 2r_j^\perp a - \frac{1}{2}\left((p_j + iq_j)\Gamma(a)(p_j - iq_j) + (p_j - iq_j)\Gamma(a)(p_j + iq_j)\right) + 2ar_j\\
&= 2r_j^\perp a + 2ar_j - \frac{1}{2}(2p_j\Gamma(a)p_j + 2q_j\Gamma(a)q_j)\\
&= 2r_j^\perp a + 2ar_j - p_j\Gamma(a)p_j - q_j\Gamma(a)q_j.
\end{aligned}$$

By a similar computation, we also have

$$[v_j^*,[v_j,a]] = 2r_ja + 2ar_j^\perp - p_j\Gamma(a)p_j - q_j\Gamma(a)q_j.$$

Hence,

$$\begin{aligned}
-\frac{1}{4}\sum_{j=1}^{m}\left(\left[v_j,[v_j^*,a]\right] + \left[v_j^*,[v_j,a]\right]\right) &= -\frac{1}{4}\sum_{j=1}^{m}\Big(2(r_j + r_j^\perp)a + 2a(r_j + r_j^\perp) - 2p_j\Gamma(a)p_j - 2q_j\Gamma(a)q_j\Big)\\
&= \frac{1}{2}\sum_{j=1}^{m}\left(q_j\Gamma(a)q_j + p_j\Gamma(a)p_j - 2a\right).
\end{aligned}$$

□

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