Quantum Dynamical Semigroups

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An Open Quantum System is a quantum system that is interacting with another system. It is generally understood that that one of the systems is rather small (the "free system") and the other one is huge (the "reservoir"). We would describe a closed system using Hamiltonian dynamics, where time evolution is determined by the Schrödinger equation and described by unitary transformations, which are generated by the Hamiltonian.

In the Markovian approach, we want to describe the two systems as one large system. Hence we need a new formalism to describe the dynamics of the system, generalizing the Hamiltonian approach.

More concretely, we will strive to replace the Schrödinger equation by the so-called *master equation in Open Quantum Systems*, where the role of the Hamiltonian will be replaced by the *Lindbladian*. Time evolution will be described by *Quantum Markov Semigroups*, replacing the group of Unitary Transformations. We will study them first.

Definition 1. *A* **Quantum Dynamical Semigroup (QDS)** *of a von Neumann algebra μ is a weakly*-continuous one-parameter semigroup $(\mathcal{T}_t)_{t\geq 0}$ of completely positive linear normal maps of μ into itself such that $\mathcal{T}_t(\mathbb{1}) \leq \mathbb{1}$ and $\mathcal{T}_0 = \mathbb{1}$.*

Definition 2. *If $\mathcal{T}_t(\mathbb{1}) = \mathbb{1}$ holds in the above definition, the semigroup is called a* **Quantum Markov Semigroup (QMS)**.

We shall work with the von Neumann algebra $\mu = \mathcal{B}(\mathcal{H})$ of all bounded operators over a given complex separable Hilbert space $\mathcal{H}$. We denote $\mathcal{L}$ the **infinitesimal generator** of the semigroup $\mathcal{T}$, whose domain is given by the set of all $X \in \mathcal{B}(\mathcal{H})$ for which the w*-limit of $\frac{1}{t}(\mathcal{T}(X) - X)$ exists when $t \to 0$, and we define $\mathcal{L}(X)$ as such a limit, i.e.

$$\mathcal{L}(X) := \lim_{t\to 0} \frac{1}{t}(\mathcal{T}(X) - X) \tag{1}$$

Definition 3. *A QDS $\mathcal{T}$ is called* **uniformly continuous** *if*

$$\lim_{t\to 0} \|\mathcal{T}_t - \mathcal{T}_0\| = 0.$$

Remark. *From the general theory of semigroup it follows that a QDS is uniformly continuous if and only if its generator $\mathcal{L}$ is a bounded operator.*

Definition 4. *Let $\mathcal{A}$ denote a C^*-subalgebra of $\mathcal{B}(\mathcal{H})$ which contains a unit. A bounded linear map $\mathcal{L}(\cdot)$ on $\mathcal{A}$ is* **conditionally completely positive** *if for any collection $a_1, ..., a_n \in \mathcal{A}$ and $u_1, ..., u_n \in \mathcal{H}$ such that $\sum_i a_i u_i = 0$, it holds that*

$$\sum_{i,j} \langle u_i, \mathcal{L}(a_i^* a_j) u_j \rangle \geq 0.$$

Theorem 1 (Christensen and Evans). *A bounded linear map $\mathcal{L}(\cdot)$ on the C^*-algebra given before such that $\mathcal{L}(a^*) = \mathcal{L}(a)^*$ holds for all $a \in \mathcal{A}$ is conditionally completely positive if and only if there exists a completely positive map Φ into its weak closure $\bar{\mathcal{A}}$ and an element $G \in \bar{\mathcal{A}}$ such that*

$$\mathcal{L}(a) = G^* a + \Phi(a) + aG \tag{2}$$

for all $a \in \mathcal{A}$.
Moreover, the operator G satisfies the inequality $G + G^* \leq \mathcal{L}(\mathbb{1})$.

Proof. We restrict the proof to the case $\mathcal{A} = \mathcal{B}(\mathcal{H})$ for simplicity.

Let us first assume that $\mathcal{L}(\cdot)$ is given by 2 and prove conditional complete positivity.

Take $a_1, ..., a_n \in \mathcal{A}$ and $u_1, ..., u_n \in \mathcal{H}$ such that $\sum_i a_i u_i = 0$. Then

$$\begin{aligned}
\sum_{i,j} \langle u_i, \mathcal{L}(a_i^* a_j) u_j \rangle &= \sum_{i,j} \langle u_i, (G^*(a_i^* a_j) + \Phi(a_i^* a_j) + (a_i^* a_j) G) u_j \rangle \\
&= \sum_{i,j} \langle a_i G u_i, a_j u_j \rangle + \sum_{i,j} \langle u_i, \Phi(a_i^* a_j) u_j \rangle + \sum_{i,j} \langle a_i u_i, a_j G u_j \rangle \\
&= \langle \sum_i a_i G u_i, \underbrace{\sum_j a_j u_j}_{=0} \rangle + \sum_{i,j} \langle u_i, \Phi(a_i^* a_j) u_j \rangle + \langle \underbrace{\sum_i a_i u_i}_{=0}, \sum_j a_j G u_j \rangle \\
&= \sum_{i,j} \langle u_i, \Phi(a_i^* a_j) u_j \rangle \\
&\geq 0,
\end{aligned}$$

where the last inequality is implied by the complete positivity of Φ, cf. Remark 2.2 in [1].

For the converse direction, fix a unit vector $e \in \mathcal{H}$ and define

$$G^* u = \mathcal{L}(|u\rangle \langle e|) e - \frac{1}{2} \langle e, \mathcal{L}(|e\rangle \langle e|) e \rangle u,$$

for all $u \in \mathcal{H}$. Given $a_1, ..., a_n \in \mathcal{B}(\mathcal{H})$ and $u_1, ..., u_n \in \mathcal{H}$, let

$$u_{n+1} = e, \tag{3}$$

$$v = -\sum_{j=1}^{n} a_j u_j, \tag{4}$$

$$a_{n+1} = |v\rangle \langle e| \,. \tag{5}$$

Then,

$$\begin{aligned}
\sum_{j=1}^{n+1} a_j u_j &= \sum_{j=1}^{n} a_j u_j + |-\sum_{j=1}^{n} a_j u_j\rangle \langle e| \, e \\
&= \sum_{j=1}^{n} a_j u_j - \sum_{j=1}^{n} a_j \, |u_j\rangle \langle e| \, e \\
&= -v + |v\rangle \langle e| \, e \\
&= -v + \langle e|e\rangle \, |v\rangle \\
&= -v + |v\rangle \\
&= 0.
\end{aligned}$$

Since $\mathcal{L}(\cdot)$ is conditionally completely positive:

$$\begin{aligned}
0 \leq \sum_{i,j}^{n+1} &\langle u_i, \mathcal{L}(a_i^* a_j) u_j\rangle \\
&= \sum_{i,j}^{n} \langle u_i, \mathcal{L}(a_i^* a_j) u_j\rangle + \sum_{i=1}^{n} \langle u_i, \mathcal{L}(|a_i^* v\rangle \langle e| \, e\rangle \\
&+ \sum_{j=1}^{n} \langle e, \mathcal{L}(|e\rangle \langle a_j^* v| \, u_j\rangle + \langle e, \mathcal{L}(|e\rangle \langle e|) e\rangle \|v\|^2.
\end{aligned}$$

Using the definition of G^* and $\mathcal{L}(a^*) = \mathcal{L}(a)^*$, the sum of the last three terms becomes

$$\sum_{i=1}^{n} \langle u_i, G^* a_i^* v\rangle + \sum_{j=1}^{n} \langle G^* a_j^* v, u_j\rangle = -\sum_{i,j=1}^{n} \langle u_i, G^* a_i^* a_j u_j\rangle - \sum_{i,j=1}^{n} \langle u_i, a_i^* a_j G u_j\rangle.$$

If we define $\Phi(a) = \mathcal{L}(a) - G^* a - aG$, the inequality becomes

$$\sum_{i,j=1}^{n} \langle u_i, \Phi(A_i^* a_j) u_j\rangle \geq 0,$$

which means that Φ is completely positive and the Theorem is proved. □

Now we want to get a characterization of the generator on the whole of $\mathcal{B}(\mathcal{H})$. We obtain it as follows. First, recall the **Schwartz-type inequalities**:

Theorem 2 (Theorem 4.7 in [1]). *Let $\mathfrak{A}$ and $\mathfrak{D}$ be two C^*-algebras with unit, $\mathfrak{B} \subseteq \mathcal{B}(\mathcal{H})$, and let $\Phi : \mathfrak{A} \to \mathfrak{B}$ be a linear completely positive map such that $\Phi(\mathbb{1}) = \mathbb{1}$. Then, for all $a_1, ..., a_n \in \mathfrak{A}, u_1, ..., u_n \in \mathcal{H}$:*

$$\sum_{i,j} \langle u_i, [\Phi(a_i^* a_j) - \Phi(a_i)^* \Phi(a_j)] u_j \rangle \geq 0.$$

When we assume $\mathcal{T}$ to be a norm continuous QMS on $\mathcal{B}(\mathcal{H})$, we then obtain that for any $a_1, ..., a_n \in \mathcal{B}(\mathcal{H}), u_1, ..., u_n \in \mathcal{H}$ and any $t \geq 0$:

$$\sum_{i,j} \langle u_i, [\mathcal{T}_t(a_i^* a_j) - \mathcal{T}_t(a_i)^* \mathcal{T}_t(a_j)] u_j \rangle \geq 0$$

The norm continuity of $\mathcal{T}$ implies that $\mathcal{L}(\cdot)$ is defined as a bounded operator on the whole algebra $\mathcal{B}(\mathcal{H})$. So (1) and the above inequality implies

$$\sum_{i,j} \langle u_i, [\mathcal{L}(a_i^* a_j) - \mathcal{L}(a_i^*) a_j - a_i^* \mathcal{L}(a_i)] u_j \rangle \geq 0. \tag{6}$$

If $\sum_i a_i u_i = 0$, then it follows

$$\sum_{i,j} \langle u_i, \mathcal{L}(a_i^* a_j) u_j \rangle \geq 0. \tag{7}$$

So that $\mathcal{L}(\cdot)$ is conditionally completely positive. We can conclude the desired characterization:

Theorem 3. *Given a norm continuous QDS $\mathcal{T}$ on $\mathcal{B}(\mathcal{H})$, there exists an operator G and a completely positive map Φ such that its generator is represented as*

$$\mathcal{L}(x) = G^* x + \Phi(x) + xG, x \in \mathcal{B}(\mathcal{H}). \tag{8}$$

Finally, since $\mathcal{B}(\mathcal{H})$ is a von Neumann algebra, we can improve this representation using Kraus' Theorem (Theorem 4.3 in [1]).

Theorem 4 (Lindblad). *Let be given a uniformly continuous QDS on the algebra $\mathcal{B}(\mathcal{H})$ of a complex separable Hilbert space $\mathcal{H}$. Let ρ be any state in $\mathcal{H}$. Then there exists a bounded self-adjoint operator H and a sequence $(L_k)_{k \in \mathbb{N}}$ of elements in $\mathcal{B}(\mathcal{H})$ which satisfy:*

1. *$tr \rho L_k = 0$ for each k,*
2. *$\sum_k L_k^* L_k$ is a strongly convergent sum,*
3. *If $\sum_k |c_k|^2 < \infty$ and $c_0 + \sum_k c_k L_k = 0$ for scalars c_k, then $c_k = 0$ for all k,*

4. The generator $\mathcal{L}$ of the semigroup admits the representation

$$\mathcal{L}(X) = i[H, X] - \frac{1}{2} \sum_k (L_k^* L_k X - 2L_k^* X L_k + X L_k^* L_k), \tag{9}$$

for all $X \in \mathcal{B}(\mathcal{H})$.

Consider once more $\mathcal{A} = \mathcal{B}(\mathcal{H})$. $\mathcal{A}$ is a von Neumann algebra and thus the dual of a Banach space (Theorem 1 (Sakai Theorem) covered on October 20). Its predual consists of $\mathcal{A}_* = B^1(\mathcal{H})$ the Banach space of trace-class operators. Then a QDS induces a predual semigroup $\mathcal{T}_*$ on $\mathcal{A}_*$ given through the relation

$$tr(\mathcal{T}_{*t}(Y)X) = tr(Y\mathcal{T}_t(X)),$$

for any $Y \in \mathcal{A}_*$ and $X \in \mathcal{A}$.

The generator of the predual semigroup is denoted $\mathcal{L}_*$. We can relate the predual semigroup and its generator through the so-called *master equation* in Open Quantum Systems:

$$\frac{d}{dt}\rho_t = \mathcal{L}_*(\rho_t),$$

where $\rho_t = \mathcal{T}_{*t}(\rho)$ for any $t \geq 0$ and ρ being a state, that is, an element $\rho \in \mathcal{A}_*$ with unit trace.

References

[1] Ronaldo Rebolledo: *Complete Positivity and the Markov structure of Open Quantum Systems.* In: S. Attal, A. Joye, C.-A. Pillet (Eds.): *Open Quantum Systems II.* Springer-Verlag, Berlin, Heidelberg 2006.