On singular perturbations of quantum dynamical semigroups

A. S. Holevo
Steklov Mathematical Institute
of Russian Academy of Sciences, Moscow

Abstract
We consider two examples of dynamical semigroups obtained by singular perturbations of a standard generator which are special case of unbounded completely positive perturbations studied in detail in [10]. In the section 2 we propose a generalization of an example from [1] aimed to give a positive answer to a conjecture of Arveson. In the section 3 we consider in greater detail an improved and simplified construction of a nonstandard dynamical semigroup outlined in our short communication [13].

1 Introduction. Standard dynamical semigroups
Let $\mathcal{H}$ be a separable Hilbert space, $\mathcal{L}(\mathcal{H})$ the algebra of all bounded operators and $\mathcal{T}(\mathcal{H}) = \mathcal{L}(\mathcal{H})^*$, the Banach space of trace-class operators in $\mathcal{H}$. Quantum dynamical semigroup in $\mathcal{L}(\mathcal{H})$ is a one-parameter semigroup $T_t$, $t \geq 0$, of normal completely positive (CP) maps of $\mathcal{L}(\mathcal{H})$ such that $T_0 = \text{Id}$ (the identity map), and $T_t[X]$ is continuous in $t$ for any fixed $X \in \mathcal{L}(\mathcal{H})$ in the weak operator topology. There is a unique prediagonal semigroup $S_t = (T_t)^*$ in $\mathcal{T}(\mathcal{H})$. It was shown in the seminal paper [14] that $S_t$ is norm continuous semigroup if and only if its generator is bounded and has the representation

$$K[\omega] = \sum_j L_j^* \omega L_j - \omega K^* - K \omega, \quad \omega \in \mathcal{T}(\mathcal{H}),$$

where the series $\sum_j L_j^* L_j$ strongly converges (in the finite dimensional case the characterization of the generator was obtained in [9]). In this case the conservativity condition $\sum_j L_j^* L_j = K + K^*$ implies that the semigroup $S_t$ is trace-preserving while $T_t$ is unital. In the case of non-norm continuous semigroups, corresponding to unbounded generators, this is no longer the case, and additional conditions are required to ensure the trace preservation. This is a quantum analog of the exposure or extinction (absorption) phenomena for classical Markov processes, see e.g. [8], [5]. Also a question of universality of
a representation of the type \( \{1\} \) arizes which will be the main concern of the present note, see also \( \{14\} \).

Quantum dynamical semigroups with unbounded generators were considered in \( \{7, 4, 5, 6, 15, 3, 11, 10, 13\} \), see also references therein. We will refer in particular to the Appendix in \( \{12\} \) where the backward and forward quantum Markovian master equations (MME) with unbounded generators are described. Let \( K, L_j \) be linear operators defined on a dense domain \( D \) of a Hilbert space \( H \), satisfying the dissipativity condition

\[
\sum_j \|L_j\psi\|^2 \leq 2\text{Re} \langle \psi|K|\psi \rangle, \quad \psi \in D, \tag{2}
\]

in particular, \( K \) is accretive, \( \text{Re} \langle \psi|K|\psi \rangle \geq 0 \). In case of equality in (2) it is called the conservativity condition. We assume that \( K \) is maximal accretive (\( m \)-accretive) operator and \( D \) is invariant subspace for the contraction semigroup \( \exp(-Kt) \), \( t \geq 0 \), hence a core for \( K \) (Theorem X.49 of \( \{17\} \)) (when it is convenient, we can take \( D = \text{dom} \, K \)). Then there exists the unique minimal solution \( T_t \), \( t \geq 0 \), of the Cauchy problem for the backward MME

\[
\frac{d}{dt} \langle \phi|T_t[X]|\psi \rangle = \sum_j \langle L_j\phi|T_t[X]|L_j\psi \rangle - \langle K\phi|T_t[X]|\psi \rangle - \langle \phi|T_t[X]|K\psi \rangle - \langle \phi|T_t[X]|\psi \rangle = 0, \tag{3}
\]

\( \phi, \psi \in D, \quad X \in \mathcal{L}(H) \),

satisfying the condition \( T_0[X] = X \), which is a dynamical semigroup on the algebra \( \mathcal{L}(H) \) of all bounded operators in \( H \) (see \( \{5\} \), cf. also Theorem A.1 in \( \{12\} \)).

Denoting by \( K \) the generator of the preadjoint semigroup \( S_t = (T_t)_* \) in \( \mathcal{T}(H) \), the MME (3) can be rewritten in the form

\[
\frac{d}{dt} \langle \phi|T_t[X]|\psi \rangle = \text{Tr} \, K \langle \psi|T_t[X]|\phi \rangle, \quad \phi, \psi \in D, \tag{4}
\]

where

\[
K \langle \psi|\phi \rangle = \sum_j \langle L_j\phi|L_j\psi \rangle - \langle K\phi|\psi \rangle - \langle \phi|K\psi \rangle. \tag{5}
\]

The dissipativity (2) amounts to the inequality \( \text{Tr} \, K \langle \psi|\psi \rangle \leq 0 \) and conservativity \( \text{to the equality} \text{Tr} \, K \langle \psi|\psi \rangle = 0 \), \( \psi \in D \).

The dynamical semigroups \( T_t \) and \( S_t \) will be called \( \text{standard} \) if they can be obtained with the procedure described above.

In this paper we consider two examples of dynamical semigroups obtained by singular perturbations of a standard generator which are special case of unbounded completely positive perturbations studied in detail in \( \{10\} \). In the section \( \{2\} \) we propose a generalization of an example in \( \{1\} \) aimed to give a positive answer to a conjecture of Arveson. It is itself standard in the sense defined above although involves nonclosable operators \( L_j \) (cf. \( \{2\} \)). In the section \( \{8\} \)
we consider in greater detail a construction of a nonstandard dynamical semi-
group outlined in the short communication [13] following Example 3 in [10]. We
provide an improvement and simplification of the argument in [13], including a
minor correction.

The singular perturbations of the generator \( \mathcal{K} \) we consider are rank one
perturbations of the form

\[
\Lambda[\omega] = -\Omega \text{Tr} \mathcal{K}[\omega], \quad \omega \in \text{dom} \mathcal{K},
\]

where \( \Omega \) is a fixed density operator in \( \mathcal{H} \). In such case the perturbed generator
is conservative in the sense that

\[
\text{Tr} (\mathcal{K}[\omega] + \Lambda[\omega]) = 0, \quad \omega \in \text{dom} \mathcal{K},
\]

moreover \( \text{dom} (\mathcal{K} + \Lambda) = \text{dom} \mathcal{K} \), as shown in [10]. It follows that the perturbed
dynamical semigroup \( S_t \) is trace-preserving, resp. \( T_t \) is unital.

2 A generalization of Arveson’s example

In this example \( \mathcal{H} = L^2(\mathbb{R}^+) \), \( K = -\frac{d}{dx}, D = AC^1(\mathbb{R}^+) \) is the subspace of abso-
lutely continuous functions \( \varphi(x) \) on \( \mathbb{R}^+ \) such that \( \varphi'(x) \in L^2(\mathbb{R}^+) \). Thus \( W_t = \exp(-Kt), t \geq 0 \), is the semigroup of left shifts in \( \mathcal{H} \), \( W_t \varphi(x) = \varphi(x+t) \).
Then \( W_t^*W_t \) is a projector on the subspace of functions vanishing on \([0,t]\) and
\( W_t^* = I \).

In what follows we identify trace-class operators \( \omega \) in \( \mathcal{H} \) with their kernels
\( \omega(x,y), x, y \in \mathbb{R}^+ \). Consider the quantum dynamical semigroup

\[
S_t^0[\omega] = W_t\omega W_t^*; \quad S_t^0[\omega](x,y) = \omega(x+t,y+t)
\]

acting on operators \( \omega \in \mathcal{S}(\mathcal{H}) \), with the generator

\[
\mathcal{K}_0 \omega = \omega'_x(x,y) + \omega'_y(x,y) = \frac{d}{dt}\omega(x+t,y+t)|_{t=0},
\]

defined initially on the domain

\[
\mathcal{D}_0 = \text{lin} \{ \omega : \omega = |\varphi\rangle\langle\psi| ; \varphi,\psi \in D \} \subset \mathcal{S}(\mathcal{H}).
\]

A closed description of \( \mathcal{K}_0 \) is given by the following Proposition the proof of
which is postponed until the end of this Section.

**Proposition 1** The domain \( \text{dom} \mathcal{K}_0 \) consists of trace-class operators \( \omega \) with
kernels \( \omega(x,y) \) such that for almost all \( (x,y) \) the function \( \omega(x+t,y+t) \) as a
function of \( t \) is absolutely continuous and its derivative \( \sigma(x,y) = \frac{d}{dt}\omega(x+t,y+t)|_{t=0} \) is a kernel of a trace-class operator in \( \mathcal{H} \).

Now consider the perturbed generator

\[
\mathcal{K}[\omega] = \mathcal{K}_0[\omega] + \Lambda[\omega], \quad \omega \in \text{dom} \mathcal{K}_0,
\]
where
\[ \Lambda[\omega] = -\Omega \text{Tr} K_0[\omega] = \Omega \omega(0,0), \]
\( \Omega \) is a density operator. Here the second equality follows from
\[ \int_0^\infty \frac{d}{dx} \omega(x,x)dx = -\omega(0,0). \]

Since the perturbation has rank one, \( \text{dom} K = \text{dom} K_0 \) [10]. The perturbed (minimal) dynamical semigroup \( S_t \) constructed as in [10] is standard and trace preserving. Indeed, the dual semigroup \( T_t = (S_t)^\ast \) is unital and is the minimal solution of the backward MME [4], which in our case reads
\[ \frac{d}{dt} \langle \varphi | T_t[X] | \psi \rangle = \text{Tr} \left( K_0 + \Lambda \right) \langle |\psi\rangle | T_t[X], \quad \varphi, \psi \in \mathcal{D}, \tag{8} \]
where
\[ K_0[|\psi\rangle \langle \varphi|] = |\psi\rangle \langle \varphi| + |\psi\rangle \langle \varphi| = -|K\psi\rangle \langle \varphi| - |\psi\rangle \langle K\varphi|; \]
\[ \Lambda[|\psi\rangle \langle \varphi|] = \Omega \psi(0) \varphi(0) = \sum_j |L_j\psi\rangle \langle L_j\varphi|. \tag{9} \]

Here \( L_j \) are nonclosable operators (cf. [2])
\[ L_j |\psi\rangle = |l_j\rangle \psi(0), \quad \psi \in \mathcal{D} = AC^1(\mathbb{R}+), \]
and the vectors \( |l_j\rangle \) are such that \( \Omega = \sum_j |l_j\rangle \langle l_j| \).

In Arveson’s example [1] \( \Omega = |f\rangle \langle f| \), where \( f(x) = c \exp(-\alpha x) \). In that case the perturbed semigroups are constructed explicitly as
\[ S_t[\omega] = W_t \omega W_t^* + \Omega \text{Tr} (I - W_t^* W_t) \omega, \]
\[ T_t[X] = W_t^* X W_t + (I - W_t^* W_t) \text{Tr} \Omega X. \tag{10} \]

Arveson introduces a general notion of the domain algebra of a quantum dynamical semigroup with generator \( L \) as
\( \mathcal{A} = \{ X \in \text{dom} L : X^* X \in \text{dom} L, X X^* \in \text{dom} L \} \)
and shows that the strong closure of the domain algebra for the semigroup [10] consists of all operators commuting with \( \Omega = |f\rangle \langle f| \). He also asks if there exist dynamical semigroups whose domain algebra is as small as \( C \cdot I \). Our generalization allows to give a positive answer to this question.

**Theorem 2** Let \( \Omega \) be an arbitrary density operator, \( T_t \) – the dynamical semigroup solving [8] and \( L \) – its generator. If \( X \in \mathcal{A} \), the domain algebra of \( T_t \), then
\[ [X - (\text{Tr} \Omega X) I] \Omega = \Omega [X - (\text{Tr} \Omega X) I] = 0. \]
In particular, if \( \Omega \) is nondegenerate, then \( X \) is a multiple of identity, so that \( \mathcal{A} = C \cdot I \).
We use the criterion (iii) of Lemma 1 in [1] for an arbitrary quantum dynamical semigroup $T_t$ which says that $X \in \text{dom } L$ iff
\[ \sup_{t>0} t^{-1} \|T_t[X] - X\| \leq M < \infty. \] (11)

**Lemma 3** Let $L_0$ be the generator of the semigroup $T_t^0 = (S_t^0)^*$, $T_t^0[X] = W_t^*XW_t$. Then dom $L_0$ is $*$-algebra and $I \notin \text{dom } L_0$.

**Proof.** $W_t^*W_t$ is a projector, hence $\|T_t^0[I] - I\| = \|W_t^*W_t - I\| = 1$, hence $I \notin \text{dom } L_0$.

The first assertion holds for any semigroup of endomorphisms, but we include the proof for completeness. Apparently dom $L_0$ is selfadjoint.

Using the identity $W_tW_t^* = I$,
\[ t^{-1}(T_t^0[XY] - XY) = t^{-1}(T_t^0[X] - X)T_t^0[Y] + t^{-1}X(T_t^0[Y] - Y), \]
hence
\[ t^{-1}\|T_t^0[XY] - XY\| \leq t^{-1} \|T_t^0[X] - X\| \|T_t^0[Y]\| + t^{-1}\|X\| \|T_t^0[Y] - Y\|. \]

Let $X, Y \in \text{dom } L_0$. Then by (11) $XY \in \text{dom } L_0$.

The perturbed backward Markovian master equation [8] is equivalent to the integral equation
\[ \langle \varphi|T_t[X]|\psi \rangle = \langle \varphi|T_t^0[X]|\psi \rangle + \int_0^t \text{Tr } \Lambda[S_s^0][\varphi]|\psi\rangle|\psi\rangle]T_{t-s}[X] ds, \quad \varphi, \psi \in \mathcal{D}, \] (12)
see [6], [12] (Appendix). Taking into account [6], [9], we have $\Lambda[S_s^0][\varphi]|\psi\rangle = \Omega[\psi(s)\varphi(s)]$, so that the integral term becomes $\int_0^t \psi(s)\varphi(s)\text{Tr} \Omega T_{t-s}[X] ds$. It follows
\[ \langle \varphi|t^{-1}(T_t[X] - X)|\psi \rangle = \langle \varphi|t^{-1}(T_t^0[X] - X)|\psi \rangle \]
\[ + t^{-1} \int_0^t \psi(s)\varphi(s)\text{Tr} \Omega T_{t-s}[X] ds, \quad \varphi, \psi \in \mathcal{D}. \] (13)

**Lemma 4** If $X \in \text{dom } L$ then $X_0 = X - (\text{Tr } \Omega X)I \in \text{dom } L_0$ and $\text{L}[X] = L_0[X_0]$.

**Proof.** Since $I \in \text{dom } L$ and $\text{L}[I] = 0$, then $X_0 \in \text{dom } L$ and (13) implies
\[ \langle \varphi|t^{-1}(T_t[X_0] - X_0)|\psi \rangle = \langle \varphi|t^{-1}(T_t[X_0] - X_0)|\psi \rangle \]
\[ - t^{-1} \int_0^t \psi(s)\varphi(s)\text{Tr} \Omega t^{-1}(T_{t-s}[X_0] - X_0) ds, \quad \varphi, \psi \in \mathcal{D}, \]
From the criterion (11),
\[ \langle \varphi|t^{-1}(T_t[X_0] - X_0)|\psi \rangle \]
\[ \leq M \| \varphi \| \| \psi \| + \left| \int_0^t \psi(s) \varphi(s) M t^{-1} (t-s) \, ds \right| \leq 2M \| \varphi \| \| \psi \|. \]

By the same criterion \( X_0 \in \text{dom} \mathcal{L}_0 \). □

**Proof of Theorem 2**

Let \( X \in \text{dom} \mathcal{L}, X^* X \in \text{dom} \mathcal{L}, X X^* \in \text{dom} \mathcal{L} \), then

\[
X = [X - (\text{Tr} \Omega X) I] + (\text{Tr} \Omega X) I = X_0 + (\text{Tr} \Omega X) I, \\
X^* X = [X^* X - (\text{Tr} \Omega X^* X) I] + (\text{Tr} \Omega X^* X) I = Y_0 + (\text{Tr} \Omega X^* X) I,
\]

where \( X_0, Y_0 \in \text{dom} \mathcal{L}_0 \) by Lemma 4. Then

\[
Y_0 + (\text{Tr} \Omega X^* X) I = [X_0 + (\text{Tr} \Omega X) I]^* [X_0 + (\text{Tr} \Omega X) I],
\]

whence

\[
(\text{Tr} \Omega X^* X - |\text{Tr} \Omega X|^2) I = X_0^* X_0 + X_0^* (\text{Tr} \Omega X) + (\text{Tr} \Omega X^* X) X_0 - Y_0.
\]

By Lemma 3, the term in righthand side belongs to \( \text{dom} \mathcal{L}_0 \). Since \( I \notin \text{dom} \mathcal{L}_0 \), this is possible iff \( \text{Tr} \Omega X^* X = |\text{Tr} \Omega X|^2 \), i.e. the equality holds in the noncommutative Cauchy-Schwarz inequality \( \text{Tr} \Omega X^* X \geq |\text{Tr} \Omega X|^2 \). But this holds iff \( [X - (\text{Tr} \Omega X) I] \Omega = 0 \).

Applying similar argument to \( XX^* \), we obtain

\[ \Omega [X - (\text{Tr} \Omega X) I] = 0. \] □

**Proof of Proposition 1**

Denote by \( \tilde{K}_0 \) the operator acting as

\[ \tilde{K}_0 \omega(x, y) = \frac{d}{dt} \omega(x + t, y + t)|_{t=0}, \]

with the domain \( \text{dom} \tilde{K}_0 \) described in the Proposition 4. We will check that \( \tilde{K}_0 \) satisfies

\[ \left( \lambda I - \tilde{K}_0 \right) \mathcal{R}_\lambda \omega = \omega, \quad \omega \in \mathfrak{I}(\mathcal{H}); \quad \mathcal{R}_\lambda \left( \lambda I - \tilde{K}_0 \right) \omega = \omega, \quad \omega \in \text{dom} \tilde{K}_0, \]

where \( \mathcal{R}_\lambda \) is the resolvent of the semigroup \( S^0 \). Then the first equality implies that \( \tilde{K}_0 \supseteq K_0 \), while the second – that \( \text{dom} \tilde{K}_0 \subseteq \text{dom} K_0 \), because then \( \omega = \mathcal{R}_\lambda \left( \lambda \omega - \tilde{K}_0 \omega \right) \in \text{dom} K_0 \). Thus \( \tilde{K}_0 = K_0 \).

Let \( \omega \in \mathfrak{I}(\mathcal{H}) \), then \( \mathcal{R}_\lambda [\omega] \in \text{dom} K_0 \), and

\[ \mathcal{R}_\lambda [\omega](x, y) = \int_0^\infty e^{-\lambda t} \omega(x + t, y + t) \, dt. \]

Notice that for any \( \omega \in \mathfrak{I}(\mathcal{H}) \) the function \( \omega(x + t, y + t) \) is integrable in \( t \) for almost all \( (x, y) \). This follows from the fact that this function is the diagonal value of the kernel of the trace-class operator \( W^*_x \omega W^*_y \). For the same reason, \( \mathcal{R}_\lambda [\omega](x + t, y + t) \) is integrable in \( t \) for almost all \( (x, y) \).
To prove the first equality we compute the generalized derivative of $R_\lambda[\omega](x + t, y + t)$ with respect to $t$. For any smooth function $f(t)$ with compact support

$$\begin{align*}
&-\int_0^\infty R_\lambda[\omega](x + s, y + s)f'(s)ds \\
&= -\int_0^\infty \int_0^\infty e^{-\lambda t}\omega(x + t + s, y + t + s)f'(s)dsdt \\
&= -\int_0^\infty e^{\lambda s}\int_s^\infty e^{-\lambda \xi}\omega(x + \xi, y + \xi)d\xi f'(s)ds \\
&= \int_0^\infty \left[-\omega(x + s, y + s) + \lambda \int_0^\infty e^{-\lambda t}\omega(x + t + s, y + t + s)dt\right]f(s)ds,
\end{align*}$$

where the last equality is obtained by integration by parts. It follows that

$$[16]$$

the expression in the squared brackets

$$[16]$$

hence

$$\begin{align*}
&\mathcal{K}_0R_\lambda[\omega](x, y) = \frac{d}{dt}R_\lambda[\omega](x + t, y + t)|_{t=0} = \lambda R_\lambda[\omega](x, y) - \omega(x, y),
\end{align*}$$

and the function on the left is kernel of a trace class operator, which proves the first equality. The second equality follows similarly from integration by parts:

$$\begin{align*}
R_\lambda\mathcal{K}_0\omega(x, y) = \int_0^\infty e^{-\lambda t}\frac{d}{dt}\omega(x + t, y + t)dt = \lambda R_\lambda[\omega](x, y) - \omega(x, y).
\end{align*}$$

□

3 A nonstandard dynamical semigroup

3.1 Quantum diffusion with extinction

Let $\mathcal{H} = L^2(\mathbb{R}_+)$, and trace-class operators $\omega$ in $\mathcal{H}$ are identified with their kernels $\omega(x, y)$, $x, y \in \mathbb{R}_+$. Let $\mathcal{D} = AC^0_0(\mathbb{R}_+)$ be the subspace of differentiable functions $\varphi(x)$ on $\mathbb{R}_+$ with $\varphi(0) = 0$, and such that $\varphi'(x)$ is absolutely continuous with $\varphi'' \in L^2(\mathbb{R}_+)$. Notice that $\varphi'(0)$ exists and is finite for $\varphi \in AC^0_0(\mathbb{R}_+)$. Consider the operators $L = \sqrt{2}\frac{d}{dx}$ with $\mathcal{D}(L) = \mathcal{D}$, $L^* = -\sqrt{2}\frac{d}{dx}$, and $K = -\frac{d^2}{dx^2}$ selfadjoint with the domain $\mathcal{D}$. The condition (2) is then fulfilled with equality. The corresponding backward MME [5], in which the sum consists of one term, has the form

$$\begin{align*}
\frac{d}{dt}\langle \varphi|T_t[X]|\psi\rangle = 2\langle \varphi'|T_t[X]|\psi'\rangle + \langle \varphi''|T_t[X]|\psi''\rangle + \langle \varphi|T_t[X]|\psi''\rangle, \quad \varphi, \psi \in \mathcal{D}.
\end{align*}$$

(15)

The conditions of Theorems A.1, A.2 in [12] are fulfilled in this case ensuring existence of the minimal solution of the MME which is a standard nonunital dynamical semigroup $T_t^\lambda$, with the predual semigroup $S_t^0$ in $\mathcal{F}(\mathcal{H})$ satisfying the forward MME, which in this special case has the form similar to [15]:

$$\begin{align*}
\frac{d}{dt}\langle f|S_t^\lambda[\omega]|g\rangle = 2\langle f'|S_t^\lambda[\omega]|g'\rangle + \langle f''|S_t^\lambda[\omega]|g''\rangle + \langle f|S_t^\lambda[\omega]|g''\rangle, \quad f, g \in \mathcal{D}.
\end{align*}$$

(16)
The generator $K_0$ of $S^0_t$ is an extension of the operator

$$K_0[\omega] = \omega''_{xx}(x, y) + 2\omega''_{xy}(x, y) + \omega''_{yy}(x, y), \quad (17)$$

defined initially on the domain

$$\mathcal{D}_0 = \text{lin} \{ \omega : \omega = |\psi\rangle\langle\varphi|; \varphi, \psi \in \mathcal{D} \} \subset \mathfrak{F}(\mathcal{H}),$$

see Example 3 in [10]. A detailed description of $K_0$ and its domain is given in Proposition 9 in the subsection 3.3.

**Lemma 5** Let $\varphi, \psi \in \mathcal{H}$ be such that $|\psi\rangle\langle\varphi| \in \text{dom} K_0$, then $|\psi\rangle, |\varphi\rangle \subseteq AC^2_0(\mathbb{R}_+)$, in particular $\psi(0) = \varphi(0) = 0$, and

$$K_0[|\psi\rangle\langle\varphi|](x, y) = 2\psi'(x)\overline{\varphi'(y)} + \psi''(x)\overline{\varphi(y)} + \psi(x)\overline{\varphi''(y)}. \quad (18)$$

**Proof.** If $\omega \in \text{dom} K_0$ then taking $t = 0$ in (16) we obtain

$$\langle f|K_0[\omega]|g\rangle = 2\langle f'|\omega|g\rangle + \langle f''|\omega|g\rangle + \langle f|\omega|g''\rangle, \quad f, g \in AC^2_0(\mathbb{R}_+).$$

For $\omega = |\psi\rangle\langle\varphi|$ this amounts to

$$\langle f|K_0[|\psi\rangle\langle\varphi|]|g\rangle = 2\langle f'||\psi\rangle\langle\varphi|g\rangle + \langle f''||\psi\rangle\langle\varphi|g\rangle + \langle f|\psi\rangle\langle\varphi|g''\rangle.$$

Take $g$ such that $\langle \varphi|g'\rangle = 0$, $\langle \varphi|g\rangle = 1$ (this is possible because $g$ and $g'$ are linearly independent for $g \in AC^2_0(\mathbb{R}_+)$), then

$$\langle f''|\psi\rangle = \langle f|g_1\rangle, \quad f \in AC^2_0(\mathbb{R}_+),$$

where $|g_1\rangle = K_0[|\omega\rangle|g\rangle - |\psi\rangle\langle\varphi|g''\rangle \in L^2(\mathbb{R}_+)$. Restricting to infinite differentiable functions $f$ with compact support in $(0, \infty)$, this means that $\psi$ has generalized second derivative in $(0, \infty)$, see [10], which belongs to $L^2(\mathbb{R}_+)$. Moreover, for continuously differentiable $f$ in $\mathbb{R}_+$ one can integrate by parts, obtaining

$$f'(0)\psi(0) - \int_0^\infty f'(x)\psi'(x)dx = \int_0^\infty f(x)g_1(x)dx.$$

One can choose $f$ such that $f'(0) \neq 0$, while both integrals are arbitrarily small. Therefore $\psi(0) = 0$, hence $\psi \in AC^2_0(\mathbb{R}_+)$. Similar proof applies to $\varphi$. Relation (18) follows from (17). □

### 3.2 Quantum diffusion with rebound

The semigroup $S^0_t$ describes “noncommutative diffusion on $\mathbb{R}_+$ with absorption at the point 0” (with extinction of the absorbed particle). The example of the nonstandard semigroup will be obtained as a result of perturbation of the generator of this semigroup by the term $\Lambda[\omega] = \Omega \frac{d}{dx} \omega(x, x)_{x=0}$, where $\Omega$ is a fixed density operator. Consider the perturbed generator

$$K[\omega] = K_0[\omega] + \Omega \frac{d}{dx} \omega(x, x)_{x=0}. \quad (19)$$
which corresponds to “rebound from 0 to the state Ω” [10]. Since the perturbation has rank one, it follows (see [10])

$$\text{dom } \mathcal{K} = \text{dom } \mathcal{K}_0. \quad (20)$$

The semigroup $T_t$ is the minimal solution of the MME

$$\frac{d}{dt} \text{Tr}_\omega T_t[X] = \text{Tr} \mathcal{K} [\omega T_t[X]], \quad \omega \in \text{dom } \mathcal{K}_0,$$

and it is unital [10].

We will prove that $T_t$ is not standard.

Assume the contrary, i.e. that there exist some operators $K, L_j$ defined on $\text{dom } K$ (such that $K$ is $m$-accretive) and satisfying (2) such that $T_t$ is the minimal solution of the Eq. (3), or equivalently (4).

**Lemma 6**

$$K [\langle \psi | \varphi \rangle] = K_0 [\langle \psi | \varphi \rangle], \quad \varphi, \psi \in \text{dom } K. \quad (21)$$

**Proof.** If $\varphi, \psi \in \text{dom } K$, then $|\psi \rangle \langle \varphi|$ $\in \text{dom } K$ (see Example 1 in § 4 of [10]), hence by (20) $|\psi \rangle \langle \varphi| \in \text{dom } K_0$. By Lemma 3 we then have $\psi, \varphi \in AC_0^2(\mathbb{R}_+)$.

Thus

$$\text{dom } K \subseteq AC_0^2(\mathbb{R}_+). \quad (22)$$

The perturbation term in (19) vanishes for $\omega(x, x) = \psi(x)\overline{\varphi(x)}$ because

$$\frac{d}{dx} \psi(x)\overline{\varphi(x)}|_{x=0} = \psi'(0)\overline{\varphi(0)} + \psi(0)\varphi'(0) = 0$$

and $\psi(0) = \varphi(0) = 0$ due to (22). \qed

**Lemma 7** $\text{dom } K = AC_0^2(\mathbb{R}_+)$.  

**Proof.** The equation (3) is invariant under transformations

$$L_j \rightarrow L'_j = L_j + \alpha_j, \quad K \rightarrow K' = K + \sum_j \left( \alpha_j L_j + \frac{|\alpha_j|^2}{2} \right),$$

where $\sum_j |\alpha_j|^2 < \infty$. Then the $m$-accretive operator $K$ is transformed into the $m$-accretive operator $K'$ with the same domain

$$\text{dom } K' = \text{dom } K, \quad (23)$$

as it follows from the Corollary to Theorem X.50 of [17] and the following estimate

$$\left\| \sum_j \alpha_j L_j \psi \right\| \leq \frac{1}{\sqrt{2}} \left\| \left( K + \sum_j \frac{|\alpha_j|^2}{2} \right) \psi \right\| + \frac{\sum_j |\alpha_j|^2}{2\sqrt{2}} \left\| \psi \right\|, \quad \psi \in \text{dom } K. \quad (24)$$
To prove this estimate, observe that

\[
\left\| \sum_j \alpha_j L_j \psi \right\|^2 \leq \sum_j |\alpha_j|^2 \sum_j \|L_j \psi\|^2
\]

\[
\leq 2 \text{Re} \sum_j |\alpha_j|^2 \langle \psi | K \psi \rangle \leq \frac{1}{2} \left( K + \sum_j |\alpha_j|^2 \right) \|\psi\|^2,
\]

where in the second inequality we used (2), and in the last – the general relation

\[
2 \text{Re} \langle \psi | \varphi \rangle = \frac{1}{2} \|\psi + \varphi\|^2 - \frac{1}{2} \|\psi - \varphi\|^2 \leq \frac{1}{2} \|\psi + \varphi\|^2.
\]

Then (24) follows from (25) by splitting \( K + \sum_j |\alpha_j|^2 = \left( K + \sum_j |\alpha_j|^2 / 2 \right) + \sum_j |\alpha_j|^2 / 2 \) and using the triangle inequality.

By using (21) we obtain

\[
\sum_j |L_j' \psi\rangle \langle L_j' \varphi| - |K' \psi\rangle \langle \varphi| - |\psi\rangle \langle K' \varphi| = K [\|\psi\rangle \langle \varphi\|] = K_0 [\|\psi\rangle \langle \varphi\|], \quad \varphi, \psi \in \text{dom } K.
\]

Let us fix a unit vector \( \psi_0 \in \text{dom } K \) and put \( \alpha_j = - \langle \psi_0 | L_j \psi_0 \rangle \), then \( \langle \psi_0 | L_j \psi_0 \rangle = 0 \). Taking \( \varphi = \psi_0 \) and multiplying by \( |\psi_0\rangle \), we obtain

\[
K' \psi(x) = -\psi(x) \langle K' \psi_0 | \psi_0 \rangle - \int_0^\infty K_0 [\|\psi\rangle \langle \varphi\|](x, y) \psi_0(y) \, dy
\]

(26)

for \( \psi \in \text{dom } K \). Notice that \( \psi_0(0) = 0 \) since \( \psi_0 \in \text{dom } K \). By using (18), we have

\[
K_0 [\|\psi\rangle \langle \varphi\|](x, y) = \psi''(x) \overline{\psi_0(y)} + 2i \psi'(x) \overline{\psi'_0(y)} + \psi(x) \overline{\psi''_0(y)}
\]

hence

\[
\int_0^\infty K_0 [\|\psi\rangle \langle \varphi\|](x, y) \psi_0(y) \, dy = \psi''(x) + 2i c_1 \psi'(x) + c_0 \psi(x),
\]

where

\[
c_1 = -i \int_0^\infty \overline{\psi'_0(y)} \psi_0(y) \, dy \in \mathbb{R},
\]

\[
c_0 = \int_0^\infty \overline{\psi''_0(y)} \psi_0(y) \, dy = -\int_0^\infty |\psi'_0(y)|^2 \, dy \leq 0.
\]

Here in integration by parts we took into account that \( \psi_0(0) = 0 \). Therefore the righthand side of (25), up to an additive term which is a multiple of unit operator, defines an accretive operator of the form \( -\psi'' - 2ic_1 \psi' + c_2 \psi \) for \( \psi \in AC^2_0(\mathbb{R}_+) \). By the gauge transformation \( \psi(x) \to \psi(x)e^{-2ic_1 x} \), leaving \( AC^2_0(\mathbb{R}_+) \) invariant, this operator is unitarily equivalent to \( -\psi'' + c_3 \psi \), therefore it is \( m \)-accretive. Since \( K \) is \( m \)-accretive, \( \text{dom } K' = \text{dom } K = AC^2_0(\mathbb{R}_+) \) and \( K' = -\psi'' + c_3 \psi. \square \)
We have assumed that $T_t$ is standard. To obtain a contradiction, notice that Lemmas 6 and 7 imply that $K[|\psi\rangle\langle\varphi|] = K[|\psi\rangle\langle\varphi|]$ for $\varphi, \psi \in D = \text{dom } K = AC^2_0(\mathbb{R}^+).$ Thus both $T_t$ and $T^\theta_t$ are the minimal solutions of the same Eq. (4), hence $K = K_0$ which is a contradiction. □

Remark We conclude with a brief comment concerning “nonstandardness” of the perturbation term

$$\Lambda[\omega] = \Omega d\omega(x,x)|_{x=0}.$$ $\Lambda[\omega]$ Its complete positivity as a map from $\text{dom } K_0$ to $\mathcal{F}(\mathcal{H})$ amounts to the positivity of the unbounded linear functional $\omega \to d\omega(x,x)|_{x=0},$ defined on $\text{dom } K_0.$ Indeed, $\omega \geq 0$ implies $\omega(x,x) \geq 0,$ and if $\omega \in \text{dom } K_0,$ then $\omega(x,0) = \omega(0,y) = 0,$ hence $\omega(0,0) = 0$ and necessarily $d\omega(x,x)|_{x=0} \geq 0.$ But the functional $\omega \to d\omega(x,x)|_{x=0}$ has meaning for a broader domain of trace-class operators $\omega,$ for which the kernel $\omega(x,y)$ need not satisfy the zero boundary condition, and then $\omega \geq 0$ need not imply $d\omega(x,x)|_{x=0} \geq 0.$ An example is $\omega(x,y) = \psi(x)\psi(y),$ where $\psi$ is a square-integrable with $\text{Re } \psi'(0)\psi(0) < 0$ (e.g. $\psi(x) = \exp(-x).$) Formally

$$\frac{d}{dx}\omega(x,x)|_{x=0} = -\langle \delta'|\omega|\delta \rangle - \langle \delta|\omega|\delta' \rangle;$$

for this reason the perturbation term $\Lambda[\omega]$ does not have any generalization of the Kraus form for CP maps.

3.3 The semigroup $S^0_t$

Here we give an explicit expression for $S^0_t$ which however is not needed for the proof of nonstandardness. From (16) it follows that the family $\omega_t = S^0_t[\omega]$ satisfies

$$\frac{d}{dt}(f|\omega_t|g) = 2\langle f'|\omega_t|g' \rangle + \langle f''|\omega_t|g \rangle + \langle f|\omega_t|g'' \rangle, \quad f, g \in \mathcal{D}. \quad (27)$$

Consider the expression (17) for the generator $K_0$ of the semigroup $S^0_t.$ Making change of variables $u = x + y, \; v = x - y,$ one can see that $K_0$ is a restriction to $\mathcal{D}_0$ of the operator

$$K_0[\omega] = 4\frac{\partial^2}{\partial u^2}\omega \left( \frac{u + v}{2}, \frac{u - v}{2} \right) = \frac{d^2}{d\xi^2}\omega(x + \xi, y + \xi)|_{\xi=0} \quad (28)$$

of the second directional derivative at the point $(x, y)$ in the direction $(1, 1),$ defined on a broader domain $\text{dom } K_0.$

The quadrant $Q = \mathbb{R}_+ \times \mathbb{R}_+$ in the variables $u, v$ is given by the inequality $u \geq |v|.$ Consider the Cauchy problem for the degenerate heat equation

$$\frac{\partial \omega_t}{\partial t} = 4\frac{\partial^2 \omega_t}{\partial u^2}, \quad u > |v|, \quad \omega_t|_{\partial Q} = 0, \quad (29)$$
in which the variable \( v \) enters as a parameter. The solution is obtained by the method of reflection. For given \( x, y \), define \( \omega_0(\xi + [x - y]_+, \xi + [y - x]_+) = -\omega_0(-\xi+[x - y]_+, -\xi+[y - x]_+) \) for \( \xi \leq 0 \) – the odd continuation (with respect to the point \( \xi = 0 \)) of \( \omega_0 \) along the line \( u_0 = |x - y| + 2\xi, v_0 = x - y; \xi \in \mathbb{R} \). Then the solution of (29) is given by the Poisson integral

\[
\omega_t(x, y) = \omega_t \left( \frac{u + v}{2}, \frac{u - v}{2} \right) \\
= \frac{1}{4\sqrt{\pi t}} \int_{-\infty}^{\infty} \exp \left\{ -\frac{|u - u_0|^2}{16t} \right\} \omega_0 \left( \frac{u_0 + v}{2}, \frac{u_0 - v}{2} \right) du_0 \\
= \frac{1}{2\sqrt{\pi t}} \int_0^{\infty} \sum_{n=0,1} (-1)^n \exp \left\{ -\frac{\min(x, y) - (-1)^n \xi^2}{4t} \right\} \\
\times \omega_0(\xi + [x - y]_+, \xi + [y - x]_+)d\xi.
\]

The expression (30) should replace the incorrect unnumbered formula at the bottom of p.1 in [13].

**Proposition 8** The Cauchy problem (29) is equivalent to the Cauchy problem for the equation (27).

**Proof (Sketch).** Denoting \( F(x, y) = g(y) \overline{f(x)} \) we have

\[
\langle f|\omega_t|g \rangle = \int_0^\infty \int_0^\infty \omega_t(x, y)F(x, y)dxdy \\
= \int \int_Q \omega_t \left( \frac{u + v}{2}, \frac{u - v}{2} \right) F \left( \frac{u + v}{2}, \frac{u - v}{2} \right) dudv.
\]

From (29) we obtain

\[
\frac{d}{dt} \langle f|\omega_t|g \rangle = 4 \int \int_Q \left[ \frac{\partial^2}{\partial u^2} \omega_t \left( \frac{u + v}{2}, \frac{u - v}{2} \right) \right] F \left( \frac{u + v}{2}, \frac{u - v}{2} \right) dudv. \quad (31)
\]

Integrating by parts, the righthand side is equal to

\[
4 \int \int_Q \omega_t \left( \frac{u + v}{2}, \frac{u - v}{2} \right) \frac{\partial^2}{\partial u^2} F \left( \frac{u + v}{2}, \frac{u - v}{2} \right) dudv + 4 \int \frac{\partial}{\partial u} F ds.
\]

Taking into account zero boundary values of \( \omega_t \) on \( \partial Q \), we obtain

\[
\frac{d}{dt} \langle f|\omega_t|g \rangle = 4 \int \int_Q \omega_t \left( \frac{u + v}{2}, \frac{u - v}{2} \right) \frac{\partial^2}{\partial u^2} F \left( \frac{u + v}{2}, \frac{u - v}{2} \right) dudv \quad (32)
\]

\[
= 2 \int_0^\infty \int_0^\infty f'(x) \omega_t(x, y)g'(y)dxdy \\
+ \int_0^\infty \int_0^\infty f''(x) \omega_t(x, y)g(y)dxdy + \int_0^\infty \int_0^\infty f(x) \omega_t(x, y)g''(y)dxdy.
\]

12
whence (27) follows.

Conversely, starting from (27) we obtain (32). Since the linear span of the products $F(x, y) = g(y)f(x)$ is dense in the space of test functions, this means that

$$\frac{d}{dt} \int_Q \omega_t F \, dudv = 4 \int_Q \omega_t \frac{\partial^2}{\partial u^2} F \, dudv$$

for all test functions $F$ in $Q$. Taking $F$ as a product $a(u)b(v)$, we obtain that for almost all $v$ the function $\omega_t$ is the weak solution of the heat equation (29). But the weak solution of the heat equation coincides with the classical solution [18], hence we can perform partial integration to obtain

$$\int_{\partial Q} \omega_t \frac{\partial}{\partial u} F \, ds = 0 \quad (33)$$

for all $F \in D_0$. Taking $F(x, y) = g(y)f(x)$, where $f, g \in AC_0^2(\mathbb{R}_+)$, we obtain

$$\frac{\partial}{\partial u} \bigg|_{\partial Q} F = \frac{1}{2} \begin{cases} g'(0)f(x), & x > 0, y = 0, \\ g(y)f'(0) & x = 0, y > 0 \end{cases}$$

Therefore we can choose $f, g$ such that $\frac{\partial}{\partial u} \big|_{\partial Q} F$ is an arbitrary function from $AC_0^2(\mathbb{R}_+)$. From (33) it follows that $\omega_t \big|_{\partial Q} = 0$. Then we can modify $\omega_t$ by changing it on a set of zero Lebesgue measure in $Q$ so that it will be a solution of the Cauchy problem (29). □

In this way we can also prove one part of the following statement:

**Proposition 9** $\text{dom} \, K_0$ consists of trace-class operators $\omega$ with kernels $\omega(x, y)$ such that for almost all $(x, y)$ the function $\omega(x + \xi, y + \xi)$ as a function of $\xi$ is absolutely continuous, vanishes for $\xi = 0$ and has second generalized derivative $\sigma(x, y) = \frac{d^2}{d\xi^2} \omega(x + \xi, y + \xi)|_{\xi=0}$, which is a kernel of a trace-class operator in $H$.

**Proof (Sketch).** Indeed, if $\omega \in \text{dom} \, K_0$ then taking $t = 0$ in (16) we obtain

$$\langle f|K_0[\omega]|g \rangle = 2\langle f'\omega|g' \rangle + \langle f''\omega|g \rangle + \langle f|\omega|g'' \rangle, \quad f, g \in AC_0^2(\mathbb{R}_+),$$

which is equal to (32) for $t = 0$. It follows that

$$\int \int_Q \sigma F \, dudv = 4 \int \int_Q \omega \frac{\partial^2}{\partial u^2} F \, dudv,$$

for arbitrary test function $F$, where $\sigma$ denotes kernel of the trace-class operator $K_0[\omega]$. This implies that $\sigma$ is the generalized second derivative of $\omega$ (see [16]),

$$\sigma(x, y) = K_0[\omega](x, y) = \frac{d^2}{d\xi^2}\omega(x + \xi, y + \xi)|_{\xi=0}, \quad \omega \in \text{dom} \, K_0.$$  

Moreover, integrating by parts and taking into account that $\frac{\partial}{\partial u} F$ can be arbitrary, we obtain the boundary condition $\omega_t \big|_{\partial Q} = 0$. Thus $K_0 \subseteq \tilde{K}_0$, the operator [28] with the domain described in the Proposition 9.
To prove converse inclusion, one can verify the resolvent relations (14) (in fact, only the second one) for the operator $\tilde{K}_0$, with the resolvent

$$R_\lambda[\omega] = \int_0^\infty e^{-\lambda t} S^t_0[\omega] dt$$

computed according to (30), see [19]. This can be done similarly to the proof of Proposition 1.

Acknowledgement. The author acknowledges discussions with R.F. Werner which stimulated revival of the author’s interest to unbounded generators of quantum dynamical semigroup and led to substantial clarifications of the mechanism of nonstandardness. This work is supported by the Russian Science Foundation under grant 14-21-00162.

References

[1] W. Arveson, The domain algebra of a CP-semigroup, Pacific. J. Math. 203, 1 67-77 (2002).

[2] S. Alazzawi, B. Baumgartner, Generalized Kraus operators and generators of quantum dynamical semigroups, [arXiv:1306.4531](https://arxiv.org/abs/1306.4531)

[3] B. V. Bhat, K. R. Parthasarathy, Markov dilations of nonconservative dynamical semigroups and quantum boundary theory, Ann. Inst. H. Poincare, ser. B 31, 601-652 (1995).

[4] A. M. Chebotarev, Sufficient conditions for conservativity of the minimal dynamical semigroups, Theor. Math. Phys. 80, 192-211 (1989).

[5] A. M. Chebotarev, Lectures on quantum probability, Sociedad Matematica Mexicana, Textos 14, Mexico 2000.

[6] A. M. Chebotarev, F. Fagnola, Sufficient conditions for conservativity of quantum dynamical semigroups, J. Funct. Anal. 118, 131-153 (1993).

[7] E. B. Davies, Quantum dynamical semigroups and the neutron diffusion equation, Rep. Math. Phys. 11, 169–188 (1977).

[8] W. Feller, An introduction to probability theory and its applications, vol. I, II, John Wiley, NY.

[9] V. Gorini, A. Kossakowski, E. C. G. Sudarshan, Completely positive dynamical semigroups of N-level systems, J. Math. Phys. 17, 821-825 (1976).

[10] A. S. Holevo, Excessive maps, “arrival times” and perturbations of dynamical semigroups, Izvestiya: Mathematics 59:6, 1311-1325 (1995).

[11] A. S. Holevo, On the structure of covariant dynamical semigroups, J. Funct. Anal. 131, 255-278 (1995).
[12] A. S. Holevo, On dissipative stochastic equations in a Hilbert space, Probab. Theory Rel. Fields 104, 483-500 (1996).

[13] A. S. Holevo, There exists a nonstandard dynamical semigroup on $\mathfrak{B}(\mathcal{H})$, Uspekhi Mat. Nauk. 51(6), 225-226 (1996).

[14] G. Lindblad, On generators of quantum dynamical semigroups, Commun. Math. Phys. 48, 119–130 (1976).

[15] A. Mohari, K. B. Sinha, Stochastic dilation of minimal quantum dynamical semigroup, Proc. Indian Acad. Sci., 102, 159-173 (1992).

[16] S.M. Nikol’sky, Approximation of functions of several variables and embedding theorems, Nauka, Moscow 1977, §4.1.

[17] M. Reed, B. Simon, Methods of modern mathematical physics. II. Fourier analysis and self-adjointness, AP, NY 1975.

[18] V. S. Vladimirov, Equations of mathematical physics, 5-th edition, Nauka, Moscow, 1988.

[19] I. Siemon, A. S. Holevo, R. F. Werner, Unbounded generators of dynamical semigroups, Open Syst. Inf. Dyn. 24 (4), 1740015 (2017).