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On the Use of Total State Decompositions for the Study of Reduced Dynamics

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Abstract. The description of the dynamics of an open quantum system in the presence of initial correlations with the environment needs different mathematical tools than the standard approach to reduced dynamics, which is based on the use of a time-dependent completely positive trace preserving (CPTP) map. Here, we take into account an approach that is based on a decomposition of any possibly correlated bipartite state as a conical combination involving statistical operators on the environment and general linear operators on the system, which allows one to fix the reduced-system evolution via a finite set of time-dependent CPTP maps. In particular, we show that such a decomposition always exists, also for infinite dimensional Hilbert spaces, and that the number of resulting CPTP maps is bounded by the Schmidt rank of the initial global state. We further investigate the case where the CPTP maps are semigroups with generators in the Gorini-Kossakowski-Lindblad-Sudarshan form; for two simple qubit models, we identify the positivity domain defined by the initial states that are mapped into proper states at any time of the evolution fixed by the CPTP semigroups.

Keywords: Initial correlations, completely positive trace preserving maps, frame theory, positive frame, Schmidt rank.

1. Introduction

The dynamics of open quantum systems in the presence of initial correlations with the environment has been attracting a renewed interest, driven by both fundamental questions and the need for a realistic description of concrete physical systems [17, 33, 2, 25, 20, 30, 34, 29, 42, 38, 26, 28]. Relaxing the assumption that the open system and the environment are uncorrelated at the initial time, the very existence of a reduced dynamics defined in terms

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of a time-dependent map acting on the whole set of open-system states is no longer guaranteed. Most of the recent theoretical literature on the subject has thus been focused on how to extend the notion of dynamical maps to the scenario with initial system–environment correlations, resorting to the identification of a restricted domain of allowed initial states, and possibly preserving the notion of complete positivity in such a scenario [21, 22, 37, 39, 6, 7, 15].

Very recently [32], a different approach has been introduced, which, relying on the frame decomposition of the bipartite initial state, leads to the definition of a set of completely positive trace preserving (CPTP) time-dependent maps that describe the evolution of a precisely identified set of initial states. More specifically, the exploited decomposition relies on the introduction of a positive frame on the set of the open-system Hilbert-Schmidt operators and, provided that such a positive frame exists, it allows one to deal with fully general initial conditions. The number of involved CPTP maps depends on the chosen initial state and it is anyway bounded by the square of the dimensionality of the open system. This approach has been used to devise an efficient control of general open-system evolutions [10] and to characterize multipartite photonic systems [18]; furthermore, it has been combined with perturbative projection-operator techniques [5] to derive an uncoupled system of homogeneous master equations that can be applied under general initial conditions [40].

In this paper, we introduce two different positive decompositions, one starting from the generalized Pauli matrices for a generic finite dimension, and one directly built on any orthonormal basis of a possibly infinite dimensional Hilbert space. The latter, in particular, explicitly shows that the description of the open-system evolution in the presence of initial correlations via a set of time-dependent CPTP maps can be defined in full generality, for any initial global state and for any dimension of the open-system Hilbert space. Moreover, in the finite dimensional case, we prove that the number of needed CPTP maps always coincides with the Schmidt rank of the initial global state, both for pure and mixed states. This clarifies in a quantitative way the enhanced complexity needed to describe open-system dynamics when moving from an initial product state, where one CPTP map is enough, to initially correlated states. In the latter case, CPTP maps can still be used, but at the price of increasing their number according to the Schmidt rank of the initial global state, which will be indeed strictly larger than one in the presence of correlations. Finally, in the last part of the paper, we have considered the case in which the CPTP maps are semigroups with generators in the Gorini-Kossakowski-Lindblad-Sudarshan (GKLS) form. For the case of qubit Pauli channels, we have derived and investigated an explicit condition that defines the set of initial open-system states that are mapped into positive states at any subsequent time of the evolution, when each of the semigroups is applied to a different term of the conical decomposition yielding the initial reduced state.

The rest of the paper is organized as follows. In Sect. 2, we briefly recall the framework of open-system dynamics in the presence of initial system–environment correlations and how it can be described through a family of time-dependent CPTP maps via the approach introduced in [32], and we further recall the elements of the theory of frames that we will exploit in the following. In Sect. 3, we show that this approach can be extended to infinite-dimensional Hilbert spaces of the open-system, and we prove that in the finite dimensional case the number of required CPTP maps can be linked in full generality to the Schmidt rank of the initial global state. In Sect. 4, we specialize our analysis to the case were the CPTP maps are semigroups and we give a detailed characterization of initial reduced states compatible with such a choice, in the case of qubit Pauli channels. Finally, in Sect. 5, the conclusions of our work are presented.

2. One-Sided Positive Decomposition

2.1. Open quantum system dynamics via completely positive maps

We consider the standard framework to describe the dynamics of an open quantum system [5]. We have a bipartite global system, consisting of the open system S, which is associated with the Hilbert space $\mathcal{H}_S$, and the environment E, associated with $\mathcal{H}_E$, so that the global system is associated with the tensor product Hilbert space $\mathcal{H}_S \otimes \mathcal{H}_E$. Moreover, the global system is assumed to evolve unitarily, i.e., the joint system–environment evolution is fixed by the unitary operators $U(t)$ (here and in the following, $t_0 = 0$ is the initial time). Let $\mathcal{S}(\mathcal{H})$ denote the set of statistical operators, i.e. positive linear operators with unit trace, on $\mathcal{H}$. The reduced open-system state $\rho_S(t)$ can be written at any time t as a map from $\mathcal{S}(\mathcal{H}_S \otimes \mathcal{H}_E)$ to $\mathcal{S}(\mathcal{H}_S)$,

$$\rho_S(t) \;=\; \mathrm{Tr}_E \left[U(t)\rho_{SE}U^\dagger(t) \right], \tag{1}$$

where Tr_E is the partial trace on the environmental degrees of freedom. The map defined in (1) is CPTP, but its domain involves the whole $\mathcal{S}(\mathcal{H}_S \otimes \mathcal{H}_E)$, while when dealing with the evolution of an open quantum system, one would like to describe the dynamics via maps defined on $\mathcal{S}(\mathcal{H}_S)$ only.

This goal is achieved in [32], relying on the the decomposition of the bipartite statistical operator $\rho_{SE} \in \mathcal{S}(\mathcal{H}_S \otimes \mathcal{H}_E)$ as

$$\rho_{SE} \;=\; \sum_{\alpha=1}^{\mathfrak{N}} \omega_\alpha D_\alpha \otimes \rho_\alpha \,, \tag{2}$$

where $\rho_\alpha \in \mathcal{S}(\mathcal{H}_E)$ and $\omega_\alpha \geq 0$, while the D_α are operators within the set $\mathcal{L}_2(\mathcal{H}_S)$ of Hilbert-Schmidt operators on $\mathcal{H}_S$, i.e., the trace of the square of their absolute value is finite; note that these operators are indeed not necessarily positive. We will call the representation of ρ_{SE} in (2) *one-sided positive decomposition* (OPD), to stress that positive operators on the environmental side are needed; we will further call *cost* of the OPD the minimum number $\mathfrak{N}$ of terms with which the sum in (2) can be expressed. If the D_α are positive operators, ρ_{SE} in (2) is a separable state [3]; if, in addition, the D_α or the ρ_α or both are given by a family of orthogonal projections, ρ_{SE} is a zero discord state [31, 19, 29]. On the other hand, let us stress once more that general bipartite states, including any kind of classical or quantum correlations, can be decomposed via (infinitely many) OPDs.

From the point of view of the description of open-system dynamics, the key advantage of the OPD is that, starting from it, the reduced state at time t can always be obtained by means of a family of time-dependent CPTP maps defined on operators acting on $\mathcal{H}_S$ only. Replacing (2) into (1), we have in fact

$$\rho_S(t) = \sum_{\alpha=1}^{\mathfrak{N}} \omega_\alpha \Phi_\alpha(t)[D_\alpha], \tag{3}$$

where

$$\begin{aligned} \Phi_\alpha(t) : \mathcal{L}_2(\mathcal{H}_S) &\longrightarrow \mathcal{L}_2(\mathcal{H}_S) \\ A &\longmapsto \Phi_\alpha(t)[A] = \mathrm{Tr}_E[U(t) A \otimes \rho_\alpha U(t)^\dagger]. \end{aligned} \tag{4}$$

The initial reduced state

$$\rho_S = \sum_{\alpha=1}^{\mathfrak{N}} \omega_\alpha D_\alpha \tag{5}$$

is mapped into the reduced state at time t by the $\mathfrak{N}$ CPTP maps $\{\Phi_\alpha(t)\}_{1,\ldots,\mathfrak{N}}$ on $\mathcal{L}_2(\mathcal{H}_S)$. An initial product state corresponds to the case $\mathfrak{N} = 1$, which directly reduces to the usual description in terms of a single CPTP map [5, 36]. The presence of initial correlations implies that generally $\mathfrak{N} > 1$ CPTP maps are needed; on the other hand, the same set $\{\Phi_\alpha(t)\}_{1,\ldots,\mathfrak{N}}$ of maps can be used for all the states connected by any local operation on S [32].

2.2. Theory of frames: reconstruction formula and positive frames

Here, we briefly present the main features of the theory of frames that will be relevant for our purposes, directly referring to the set $\mathcal{L}_2(\mathcal{H}_S)$; we will further restrict to frames consisting of a countable set of operators, but, indeed, extensions to uncountable sets are possible. For a more general treatment of frame theory, the interested reader is referred to [1, 35].

Consider the Hilbert space of Hilbert-Schmidt operators $\mathcal{L}_2(\mathcal{H}_S)$ equipped with the scalar product

$$(A, B) \;=\; \mathrm{Tr}_S[A^\dagger B]\,, \quad A, B \in \mathcal{L}_2(\mathcal{H}_S)\,, \tag{6}$$

where Tr_S denotes the trace over $\mathcal{H}_S$, and a family of operators $\{F_\alpha\}_{\alpha\in I}$, where each $F_\alpha \in \mathcal{L}_2(\mathcal{H}_S)$ and the index α takes values in the countable set I, such that

$$\sum_{\alpha\in I} |(F_\alpha, A)|^2 \;<\; \infty \tag{7}$$

for every $A \in \mathcal{L}_2(\mathcal{H}_S)$. The associated map on $\mathcal{L}_2(\mathcal{H}_S)$

$$\begin{aligned} \Xi : \mathcal{L}_2(\mathcal{H}_S) \;&\longrightarrow\; \mathcal{L}_2(\mathcal{H}_S) \\ A \;&\longmapsto\; \Xi[A] \;=\; \sum_{\alpha\in I} (F_\alpha, A)\, F_\alpha \end{aligned} \tag{8}$$

is called *frame map*; the operators F_α are indeed not necessarily orthogonal, nor linearly independent. Now, one says that the family of operators $\{F_\alpha\}_{\alpha\in I}$ is a *frame* of $\mathcal{L}_2(\mathcal{H}_S)$ whenever (7) holds and the corresponding frame map Ξ satisfies the following lower and upper bound:

$$m\|A\|_2 \;\le\; (A, \Xi[A]) \;\le\; M\|A\|_2\,, \quad \forall\, A \in \mathcal{L}_2(\mathcal{H}_S)\,, \tag{9}$$

for some $0 < m \le M < \infty$, where $\|A\|_2 = \mathrm{Tr}_S\left[A^\dagger A\right]$ is the Hilbert-Schmidt norm induced by the scalar product in (6); in particular, the lower bound with m strictly larger than zero implies that $\{F_\alpha\}_{\alpha\in I}$ spans $\mathcal{L}_2(\mathcal{H}_S)$. On the whole, the definition of frame is equivalent to the requirement that Ξ is bounded and invertible, with bounded inverse Ξ^{-1}. Using such properties, so that we can write

$$A \;=\; \Xi^{-1}\left[\Xi[A]\right] \;=\; \sum_{\alpha\in I} (F_\alpha, A)\, \Xi^{-1}\left[F_\alpha\right],$$

we decompose any Hilbert-Schmidt operator according to

$$A \;=\; \sum_{\alpha\in I} (F_\alpha, A)\widetilde{F}_\alpha\,, \quad A \in \mathcal{L}_2(\mathcal{H}_S)\,, \tag{10}$$

where we defined

$$\widetilde{F}_\alpha \;=\; \Xi^{-1}[F_\alpha]\,. \tag{11}$$

Importantly, (10) allows us to reconstruct any operator in $\mathcal{L}_2(\mathcal{H}_S)$ in terms of the elements of the chosen frame. Indeed, this is a generalization of the reconstruction formula of any vector of a Hilbert space by means of an orthonormal basis. In fact, orthonormal bases are a special case of frames, for which Ξ corresponds to the identity map and thus (9) holds with $m = M = 1$.[a]

It is easy to see that the family $\{\widetilde{F}_\alpha\}_{\alpha\in I}$ is itself a frame, whose frame map coincides with Ξ^{-1}, so that the corresponding reconstruction formula reads

$$A = \sum_{\alpha\in I}(\widetilde{F}_\alpha, A)F_\alpha\,, \quad A \in \mathcal{L}_2(\mathcal{H}_S)\,;$$

$\{\widetilde{F}_\alpha\}_{\alpha\in I}$ is called the *canonical dual frame* of $\{F_\alpha\}_{\alpha\in I}$. More in general, a dual frame of $\{F_\alpha\}_{\alpha\in I}$ is a frame $\{D_\alpha\}_{\alpha\in I}$, such that for any operator A the following reconstruction formula holds:

$$A = \sum_{\alpha\in I}(F_\alpha, A)D_\alpha = \sum_{\alpha\in I}(D_\alpha, A)F_\alpha\,, \quad A \in \mathcal{L}_2(\mathcal{H}_S)\,; \tag{12}$$

as seen, every frame has at least one dual frame, which is the canonical dual frame.

We can now move back to the bipartite setting that is of interest for us, so that, besides the open system S, we also consider the environment E and we deal with Hilbert-Schmidt operators on the tensor product $\mathcal{H}_S \otimes \mathcal{H}_E$, i.e., $O_{SE} \in \mathcal{L}_2(\mathcal{H}_S \otimes \mathcal{H}_E)$. Given a frame of operators referred to the open system, $\{F_\alpha\}_{\alpha\in I}$, and a dual frame $\{D_\alpha\}_{\alpha\in I}$, with $F_\alpha, D_\alpha \in \mathcal{L}_2(\mathcal{H}_S)$, together with a frame of environmental operators, $\{X_\beta\}_{\beta\in J}$, along with a dual frame $\{Y_\beta\}_{\beta\in J}$, with $X_\beta, Y_\beta \in \mathcal{L}_2(\mathcal{H}_E)$, one can readily see that $\{F_\alpha \otimes X_\beta\}_{\alpha\in I,\beta\in J}$ and $\{D_\alpha \otimes Y_\beta\}_{\alpha\in I,\beta\in J}$ provide us with a frame of $\mathcal{L}_2(\mathcal{H}_S \otimes \mathcal{H}_E)$ and its dual. We can thus apply the reconstruction formula to any system–environment Hilbert-Schmidt operator,

$$\begin{aligned} O_{SE} &= \sum_{\alpha\in I,\beta\in J}(F_\alpha \otimes X_\beta, O_{SE})D_\alpha \otimes Y_\beta \\ &= \sum_{\alpha\in I,\beta\in J}\mathrm{Tr}_{SE}\left[(F_\alpha^\dagger \otimes X_\beta^\dagger)O_{SE}\right]D_\alpha \otimes Y_\beta \\ &= \sum_{\alpha\in I} D_\alpha \otimes \left\{\sum_{\beta\in J}\mathrm{Tr}_E\left[\mathrm{Tr}_S[(F_\alpha^\dagger \otimes \mathbb{1}_E)O_{SE}]X_\beta^\dagger\right]Y_\beta\right\}, \end{aligned}$$

where in the second identity we used the definition of the Hilbert-Schmidt scalar product of $\mathcal{L}_2(\mathcal{H}_S \otimes \mathcal{H}_E)$, as in (6) but where the trace is now taken over all the global $S-E$ degrees of freedom, while in the third identity we used that $\mathrm{Tr}_{SE}[(F_\alpha^\dagger \otimes X_\beta^\dagger)O_{SE}] = \mathrm{Tr}_E[\mathrm{Tr}_S[(F_\alpha^\dagger \otimes \mathbb{1}_E)O_{SE}]X_\beta^\dagger]$, with $\mathbb{1}_E$ the identity operator on $\mathcal{H}_E$. Hence, noting that the expression in the curly brackets

[a]Whenever (9) holds with $m = M = 1$, the frame $\{F_\alpha\}_{\alpha\in I}$ is called a Parseval frame, as (10) reduces to $A = \sum_{\alpha\in I}(F_\alpha, A)F_\alpha$; interestingly, there are Parseval frames that are *not* orthonormal bases.

in the last line is simply the reconstruction formula for the environmental operator $\mathrm{Tr}_S[(F_\alpha^\dagger \otimes \mathbb{1}_E)O_{SE}]$ on the frame $\{X_\beta\}_{\beta\in J}$ and its dual $\{Y_\beta\}_{\beta\in J}$, we conclude that any global S–E Hilbert-Schmidt operator $O_{SE} \in \mathcal{L}_2(\mathcal{H}_S \otimes \mathcal{H}_E)$ can be decomposed as

$$O_{SE} \;=\; \sum_{\alpha\in I} D_\alpha \otimes \mathrm{Tr}_S\left[(F_\alpha^\dagger \otimes \mathbb{1}_E)O_{SE}\right]; \tag{13}$$

in other terms, a frame of open-system operators naturally induces a decomposition formula for the global operators.

Comparing (13) with (2), we see that in order to define an OPD we have to guarantee that when we focus on system–environment states, $\rho_{SE} \in \mathcal{S}(\mathcal{H}_S \otimes \mathcal{H}_E) \subset \mathcal{L}_2(\mathcal{H}_S \otimes \mathcal{H}_E)$, the decomposition can be expressed in terms of environmental statistical operators and positive coefficients. Indeed, this is the case if we have a *positive frame*, i.e., a frame $\{F_\alpha\}_{\alpha\in I}$ made up of positive operators, $F_\alpha \geq 0$ for any α, which implies that $\mathrm{Tr}_S[(F_\alpha^\dagger \otimes \mathbb{1}_E)\rho_{SE}] = \mathrm{Tr}_S[(F_\alpha \otimes \mathbb{1}_E)\rho_{SE}] \geq 0$. In fact, introducing the trace of these operators

$$\omega_\alpha \;=\; \mathrm{Tr}_E\left[\mathrm{Tr}_S[(F_\alpha^\dagger \otimes \mathbb{1}_E)\rho_{SE}]\right] \;\geq\; 0 \tag{14}$$

and defining the environmental statistical operators $\rho_\alpha \in \mathcal{S}(\mathcal{H}_E)$ via the assignment

$$\omega_\alpha \rho_\alpha \;=\; \mathrm{Tr}_S\left[(F_\alpha^\dagger \otimes \mathbb{1}_E)\rho_{SE}\right] \tag{15}$$

(so that ρ_α is arbitrary when $\mathrm{Tr}_S[(F_\alpha^\dagger \otimes \mathbb{1}_E)\rho_{SE}] = 0$), we end up with an OPD. Furthermore, we note that the coefficients ω_α only depend on the reduced system state $\rho_S = \mathrm{Tr}_E[\rho_{SE}]$, since they are equivalently expressed by

$$\omega_\alpha \;=\; \mathrm{Tr}_S[F_\alpha^\dagger \rho_S]\,. \tag{16}$$

In the next section, we present two different explicit choices of positive operators allowing us to express every initial global state with an OPD, but before that let us note the following. Once we have assigned a certain initial global state ρ_{SE}, there is a (slightly) weaker sufficient condition than using a positive frame to define an OPD. We could allow some elements of the frame not to be positive, as long as the corresponding environmental operator $\mathrm{Tr}_S[(F_\alpha^\dagger \otimes \mathbb{1}_E)\rho_{SE}]$ is equal to the null operator, and then also the corresponding ω_α as in (14) is equal to zero. More in general, it might be useful to consider an OPD where the frame is chosen according to the specific initial state (or set of initial states) at hand, and possibly even according to the global unitary evolution, so as to simplify the dynamical representation in (3) as much as possible. We leave the study of how to optimize the choice of the frame in the sense now indicated for future investigation.

3. Existence and Cost of the Decomposition

3.1. Positive decomposition in finite and infinite-dimensional systems

We introduce now two different constructions of an OPD valid for any global state ρ_{SE}; the first one is referred to a finite dimensional Hilbert space $\mathcal{H}_S$ and relies on the definition of a positive frame, which generalizes straightforwardly the frame for qubit systems introduced in [32]. The second OPD, instead, includes fully general Hilbert spaces $\mathcal{H}_S$ and is defined in terms of a family of positive operators that, in the infinite dimensional case, do not constitute a frame but still allow us to exploit a reconstruction formula as in (13).

Let us then first consider a d-dimensional $\mathcal{H}_S$, with $d < \infty$, and the d^2 generalized Pauli matrices (also known as generalized Gell-Mann matrices) [23]

$$\begin{aligned}
\mathfrak{f}_{kj}^{(d)} &= \frac{1}{\sqrt{2}}\begin{cases} |k\rangle\langle j| + |j\rangle\langle k|; & \text{for} \quad k>j \\ -i(|j\rangle\langle k| - |k\rangle\langle j|); & \text{for} \quad k<j \end{cases} \\
\mathfrak{h}_{k}^{(d)} &= \begin{cases} \frac{1}{\sqrt{d}}\mathbb{1}_d; & \text{for} \quad k=1 \\ \mathfrak{h}_k^{(d-1)} \oplus 0; & \text{for} \quad k=2,\dots,d-1 \\ \frac{1}{\sqrt{d(d-1)}}[\mathbb{1}_{(d-1)} \oplus (1-d)]; & \text{for} \quad k=d\,, \end{cases}
\end{aligned} \tag{17}$$

where $\{|k\rangle\}_{k=1,\dots,d}$ is an orthonormal basis of $\mathcal{H}_S$ and $\oplus$ denotes the matrix direct sum; these matrices are Hermitian and traceless, apart from $\mathfrak{h}_1^{(d)}$ with trace $\sqrt{d}$, and they correspond to the Pauli and Gell-Mann matrices for $d=2$ and $d=3$, respectively. A positive frame is thus defined by setting (with a mapping of the index α to the couple (k,j))

$$\begin{aligned}
F_{11}^{(d)} &= \mathfrak{h}_1^{(d)}; \\
F_{kk}^{(d)} &= \sqrt{d}\sqrt{\frac{k-1}{k}}\mathfrak{h}_1^{(d)} + \mathfrak{h}_k^{(d)}; \quad \text{for} \quad k=2,\dots,d \\
F_{kj}^{(d)} &= \frac{1}{\sqrt{2}}\mathbb{1}_d + \mathfrak{f}_{kj}^{(d)}; \quad \text{for} \quad k \neq j = 1,\dots,d.
\end{aligned} \tag{18}$$

The positivity of the frame elements in (18) directly follows from the fact that the minimum eigenvalue of $\mathfrak{h}_k^{(d)}$ is $-\sqrt{(k-1)/k}$, while $\sqrt{d}\,\mathfrak{h}_1^{(d)}$ is equal to the identity matrix, and the minimum eigenvalue of $\mathfrak{f}_{kj}^{(d)}$ is $-1/\sqrt{2}$. The inverse of the frame map provides us with the canonical dual frame, see (11),

$$D_{11}^{(d)} = \mathfrak{h}_1^{(d)} - \sqrt{d}\sum_{k=2}^{d}\sqrt{\frac{k-1}{k}}\mathfrak{h}_k^{(d)} - \sqrt{\frac{d}{2}}\sum_{j\neq k}\mathfrak{f}_{kj}^{(d)};$$

$$\begin{aligned} D_{kk}^{(d)} &= \mathfrak{h}_k^{(d)}; \quad \text{for} \quad k = 2, \dots, d \\ D_{kj}^{(d)} &= \mathfrak{f}_{kj}^{(d)}; \quad \text{for} \quad k \neq j = 1, \dots, d\,. \end{aligned} \tag{19}$$

We will then call *Pauli-OPD* the decomposition in (2) fixed by the positive frame in (18) and its dual in (19), see also (14) and (15). Importantly, we note that since $D_{11}^{(d)}$ is the only element of the dual frame with non-vanishing trace, (2) implies that $\rho_E = \mathrm{Tr}_S[\rho_{SE}]$ coincides with the first environmental statistical operator appearing in the Pauli-OPD, $\rho_E = \rho_1$.

Let us now consider a possibly infinite dimensional Hilbert space $\mathcal{H}_S$ and an orthonormal basis $\{|k\rangle\}_{k=1,\dots,d;k\in\mathbb{N}}$ (where the first set of values of k refers to a finite d-dimensional Hilbert space and the second to an infinite dimensional one; to simplify the notation, from now on the range of values of k will be implied). We start by defining

$$\begin{aligned} \mathfrak{b}_{kj} &= \frac{1}{\sqrt{2}} \begin{cases} |k\rangle\langle j| + |j\rangle\langle k|\,; & \text{for} \quad k > j \\ -i(|j\rangle\langle k| - |k\rangle\langle j|)\,; & \text{for} \quad k < j \end{cases} \\ \mathfrak{b}_{kk} &= |k\rangle\langle k|\,, \end{aligned} \tag{20}$$

that is an orthonormal basis of Hermitian operators in $\mathcal{L}_2(\mathcal{H}_S)$; note that in d dimensions this basis differs from the basis of generalized Pauli operators only in its diagonal elements. Using a basis of $\mathcal{L}_2(\mathcal{H}_S \otimes \mathcal{H}_E)$ made of tensor product operators between the elements of, respectively, the basis in (20) and a basis of $\mathcal{L}_2(\mathcal{H}_E)$ (analogously to what has been done to derive (13)), we can decompose any $O_{SE} \in \mathcal{L}_2(\mathcal{H}_S \otimes \mathcal{H}_E)$ as

$$O_{SE} = \sum_{kj} \mathfrak{b}_{kj} \otimes \mathrm{Tr}_S\left[(\mathfrak{b}_{kj} \otimes \mathbb{1}_E) O_{SE}\right]. \tag{21}$$

If we now consider two families of operators $P_{kj} = \sum_{k'j'} M_{kj}^{k'j'} \mathfrak{b}_{k'j'}$ and $Q_{kj} = \sum_{k'j'} N_{kj}^{k'j'} \mathfrak{b}_{k'j'}$ such that the corresponding real coefficients satisfy

$$\sum_{k''j''} M_{k''j''}^{kj} N_{k''j''}^{k'j'} = \delta_{kk'}\delta_{jj'}\,, \tag{22}$$

equation (21) is equivalent to

$$O_{SE} = \sum_{kj} Q_{kj} \otimes \mathrm{Tr}_S\left[(P_{kj} \otimes \mathbb{1}_E) O_{SE}\right]; \tag{23}$$

indeed, if the operators P_{kj} are positive, with the same reasoning as the one at the end of Sect. 2.2, we can conclude that the previous relation provides any $\rho_{SE} \in \mathcal{L}_2(\mathcal{H}_S \otimes \mathcal{H}_E)$ with a valid OPD. Our choice for the positive operators, aimed at reproducing the non-diagonal elements of (18) and using simple diagonal operators, is the following:

$$
\begin{aligned}
P_{kk} &= |k\rangle\langle k| ; \\
P_{kj} &= \frac{1}{\sqrt{2}}\mathbb{1} + \mathfrak{b}_{kj} \quad \text{for} \quad k \neq j \,.
\end{aligned} \tag{24}
$$

Using (22), we can thus complete the decomposition in (23) with the family of operators

$$
\begin{aligned}
Q_{kk} &= |k\rangle\langle k| - \frac{1}{\sqrt{2}}\sum_{k\neq j}\mathfrak{b}_{kj} ; \\
Q_{kj} &= \mathfrak{b}_{kj} \quad \text{for} \quad k \neq j \,.
\end{aligned} \tag{25}
$$

We will call the OPD fixed by (23)–(25) *basis-induced OPD*, to stress its connection with the initial choice of the basis $\{|k\rangle\}$ of $\mathcal{H}_S$. Such an OPD can be used both for finite and infinite dimensional systems, but we stress that only in the former case the family of operators defined in (24) is actually a frame. In the infinite dimensional case, in fact, the upper bound in (9) does not hold, as, e.g., if we consider the operator $A = \mathfrak{b}_{kk} = |k\rangle\langle k|$ we find the divergent series

$$
\sum_{k'j'} |\mathrm{Tr}_S[\mathfrak{b}_{kk} P_{k'j'}]|^2 \;=\; 1 + \sum_{k'\neq j'} \frac{1}{2} \,.
$$

Thus, the basis-induced OPD shows that, strictly speaking, frames are not necessary to define a proper OPD, the key point rather being the definition of a reconstruction formula as in (13), or, equivalently, (23) via a family of positive open-system operators (F_α or P_{kj}).

3.2. Cost of the decomposition and Schmidt rank of the initial global state

Moving back to a finite-dimensional Hilbert space $\mathcal{H}_S$ with dimension d, both the Pauli and the basis-induced OPD allow us to express any global state by means of an OPD with d^2 terms. On the other hand, assigned a certain state ρ_{SE}, it might well be that it is possible to write it equivalently via an OPD with a lower number of terms. Recall that we denote with $\mathfrak{N}$ the minimal number of terms appearing in the OPD of a given state ρ_{SE}, that is the cost of the OPD of ρ_{SE}; moreover, since we deal now with finite-dimensional Hilbert spaces, we will consider OPDs induced by positive frames. Here, we show that the cost $\mathfrak{N}$ of the OPD of a given state ρ_{SE} is equal to the Schmidt rank of ρ_{SE}.

As first step, we show that given a bipartite statistical operator ρ_{SE}, the cost $\mathfrak{N}$ of its OPD equals the number $\mathfrak{I}$ of linearly independent operators in the set of environmental states ρ_α associated with non-zero coefficients ω_α. Importantly, this number does not depend on the specific frame chosen to perform the decomposition and therefore the cost is a property of the operator itself. Hence, consider any positive frame $\{F_\alpha\}_{\alpha=1,\ldots,\mathfrak{D}}$ of $\mathcal{L}_2(\mathcal{H}_S)$, with $\mathfrak{D}$ elements ($\mathfrak{D} \geq d^2$ as the frame spans $\mathcal{L}_2(\mathcal{H}_S)$), along with a dual frame $\{D_\alpha\}_{\alpha=1,\ldots,\mathfrak{D}}$. As shown Sect. 2.2, given any bipartite statistical operator ρ_{SE}, we can write its OPD with respect to this frame as

$$\rho_{SE} = \sum_{\alpha=1}^{N} \omega_\alpha D_\alpha \otimes \rho_\alpha\,,$$

where ρ_α are environmental statistical operators defined via (15) and we have ordered the frame elements such that the first $N \leq \mathfrak{D}$ coefficients ω_α defined as in (14) are strictly positive, while the last $\mathfrak{D} - N$ are equal to zero. Now, let us denote as $\mathfrak{I}$ the number of linearly independent ρ_α in the set $\{\rho_\alpha\}_{\alpha=1,\ldots,N}$, which indeed coincides with the number of linearly independent operators in the set $\{\omega_\alpha\rho_\alpha\}_{\alpha=1,\ldots,\mathfrak{D}}$; if $N > \mathfrak{I}$, we can write $\rho_N = \sum_{\alpha=1}^{N-1} c_\alpha \rho_\alpha$ for some coefficients $c_\alpha \in \mathbb{R}$, from which it follows that ρ_{SE} is equivalently represented by

$$\rho_{SE} = \sum_{\alpha=1}^{N-1} \omega_\alpha \overline{D}_\alpha \otimes \rho_\alpha\,,$$

where we introduced the new frame

$$\begin{aligned} \overline{D}_\alpha &= D_\alpha + \frac{\omega_N}{\omega_\alpha} c_\alpha D_N \quad \text{for} \quad 1 \leq \alpha \leq N-1 \\ \overline{D}_\alpha &= D_\alpha \quad \text{for} \quad N \leq \alpha \leq \mathfrak{D}\,. \end{aligned} \tag{26}$$

Correspondingly, the duality relation is preserved if we also define

$$\begin{aligned} \overline{F}_\alpha &= F_\alpha \quad \text{for} \quad 1 \leq \alpha \leq N-1 \\ \overline{F}_N &= F_N - \sum_{\alpha=1}^{N-1} \frac{\omega_N}{\omega_\alpha} c_\alpha F_\alpha \\ \overline{F}_\alpha &= F_\alpha \quad \text{for} \quad N+1 \leq \alpha \leq \mathfrak{D}\,. \end{aligned} \tag{27}$$

This frame is not necessarily positive since $\overline{F}_N$ may have negative eigenvalues, but this does not affect the resulting OPD, as

$$\mathrm{Tr}_S[(\overline{F}_N \otimes \mathbb{1}_E)\rho_{SE}] = 0\,; \tag{28}$$

compare with the discussion at the end of Sect. 2.2. Indeed, this procedure can be repeated if also $\{\rho_\alpha\}_{\alpha=1,\ldots,N-1}$ are linearly dependent, i.e., $N-1 > \mathfrak{I}$, and so on: if there are $\mathfrak{I}$ linear independent operators in $\{\rho_\alpha\}_{\alpha=1,\ldots,N}$, it is always possible to write an OPD with only $\mathfrak{I}$ terms. Crucially, no further reduction is possible as can be shown by reductio ad absurdum. Suppose, in fact, that one can construct a different OPD with $\mathfrak{I}' < \mathfrak{I}$ terms $\rho_{SE} = \sum_{\beta=1}^{\mathfrak{I}'} \lambda_\beta Q_\beta \otimes \eta_\beta$, starting from a possibly different frame of operators $\{Q_\beta\}_{\beta=1,\ldots,\mathfrak{D}'}$, dual to a positive frame $\{P_\beta\}_{\beta=1,\ldots,\mathfrak{D}'}$. For what seen above, the set of statistical operators $\{\eta_\beta\}_{\beta=1,\ldots,\mathfrak{I}'}$ can be taken linearly independent and $\lambda_\beta = \mathrm{Tr}_{SE}\left[(P_\beta \otimes \mathbb{1}_E)\rho_{SE}\right] = 0$ for $\beta > \mathfrak{I}'$, see (28), without loss of generality. But then using the decomposition of F_α on the frame $\{P_\beta\}_{\beta=1,\ldots,\mathfrak{D}'}$, $F_\alpha = \sum_{\beta=1}^{\mathfrak{D}'} q_{\beta\alpha} P_\beta$, we obtain

$$\omega_\alpha \rho_\alpha \;=\; \mathrm{Tr}_S[(F_\alpha \otimes \mathbb{1}_E)\rho_{SE}] \;=\; \sum_{\beta=1}^{\mathfrak{D}'} q_{\beta\alpha}\lambda_\beta \eta_\beta \;=\; \sum_{\beta=1}^{\mathfrak{I}'} q_{\beta\alpha}\lambda_\beta \eta_\beta \,. \quad (29)$$

Eq. (29) states that the set of linearly independent vectors $\{\omega_\alpha\rho_\alpha\}_{\alpha=1,\ldots,\mathfrak{I}}$ is generated by a family $\{\lambda_\beta\eta_\beta\}_{\beta=1,\ldots,\mathfrak{I}'}$ with $\mathfrak{I}' < \mathfrak{I}$, which is a contradiction. We can thus conclude that, starting from any OPD, it is always possible to reduce the number of terms appearing in it to the number $\mathfrak{I}$ of independent operators in the set $\{\omega_\alpha\rho_\alpha\}_{\alpha=1,\ldots,\mathfrak{D}}$, but not more, i.e., $\mathfrak{N} = \mathfrak{I}$; note that the reasoning used in the reductio ad absurdum also implies that $\mathfrak{I}$ does not depend on the specific frame used to define the OPD of ρ_{SE}.

The connection between the cost $\mathfrak{N}$ of an OPD and the number $\mathfrak{I}$ of linearly independent environmental states appearing in the OPD directly leads us to link $\mathfrak{N}$ with the Schmidt rank. Any bipartite state $\rho_{SE} \in \mathcal{S}(\mathcal{H}_S \otimes \mathcal{H}_E)$ can be associated with a Schmidt decomposition, which reads:

$$\rho_{SE} \;=\; \sum_{k=1}^{\mathfrak{R}} \lambda_k G_k^S \otimes G_k^E \,, \quad (30)$$

with $\lambda_k > 0$ and $\{G_k^{S,E}\}_{k=1,\ldots,\mathfrak{R}}$ orthonormal Hermitian operators on $\mathcal{H}_S, \mathcal{H}_E$; $\mathfrak{R}$ is the *Schmidt rank* of ρ_{SE} and $\mathfrak{R} \leq d^2$; importantly, the Schmidt rank is directly related with the amount of correlations in ρ_{SE} [8, 9]. Now, from (30) it follows

$$\lambda_k G_k^E \;=\; \mathrm{Tr}_S[(G_k^S \otimes \mathbb{1}_E)\rho_{SE}] \quad (31)$$

and that the operators $\{\lambda_k G_k^E\}_{k=1,\ldots,\mathfrak{R}}$ are linearly independent. For an OPD, see (2), we have the similar relation (15) and we can always take into account a minimal OPD of ρ_{SE} such that the $\mathfrak{N}$ operators $\{\omega_\alpha\rho_\alpha\}_{\alpha=1,\ldots,\mathfrak{N}}$ are linearly independent, as discussed above. In addition, we consider, respectively, an orthonormal basis $\{G_k^S\}_{k=1,\ldots,d^2}$ of $\mathcal{L}_2(\mathcal{H}_S)$ whose first $\mathfrak{R}$ elements coincide with the open-system Schmidt operators in (30), also implying $\mathrm{Tr}_S\left[(G_k^S \otimes \mathbb{1}_E)\rho_{SE}\right] = 0$ for $k = \mathfrak{R}+1, \ldots, d^2$, and a complete frame $\{F_\alpha\}_{\alpha=1,\ldots,\mathfrak{D}}$ whose first $\mathfrak{N}$ elements coincide with those defining the minimal

OPD, while the others satisfy $\mathrm{Tr}_S\left[(F_\alpha \otimes \mathbb{1}_E)\rho_{SE}\right] = 0$ for $\alpha = \mathfrak{N}+1,\ldots,\mathfrak{D}$, see (28). Exploiting the decompositions, $G_k^S = \sum_{\alpha=1}^{\mathfrak{D}} g_{k\alpha} F_\alpha$ and $F_\alpha = \sum_{k=1}^{d^2} f_{\alpha k} G_k^S$, we thus obtain from (15) and (31)

$$\begin{aligned} \lambda_k G_k^E &= \sum_{\alpha=1}^{\mathfrak{N}} g_{k\alpha}\omega_\alpha\rho_\alpha\,; \\ \omega_\alpha\rho_\alpha &= \sum_{k=1}^{\mathfrak{R}} f_{\alpha k}\lambda_k G_k^E\,. \end{aligned} \tag{32}$$

Hence, since the linearly independent sets $\{\lambda_k G_k^E\}_{k=1,\ldots,\mathfrak{R}}$ and $\{\omega_\alpha\rho_\alpha\}_{\alpha=1,\ldots,\mathfrak{N}}$ generate each other, they have the same number of elements, i.e., $\mathfrak{N} = \mathfrak{R}$. We thus conclude that the cost $\mathfrak{N}$ of the OPD coincides with the Schmidt rank of the global statistical operator ρ_{SE}, in this way generalizing to mixed states the link between Schmidt rank and OPD discussed in [32] for pure global states.

4. Case Study: Combination of Semigroup Maps

We now provide an explicit example of an open-system evolution fixed by a family of CPTP maps $\Phi_\alpha(t)$ according to (3). In [40] we exploited the possible relevance of OPD in order to obtain a perturbative expansion of a microscopically motivated open system dynamics in the presence of initial correlations. We will here take a complementary phenomenological approach, exploring whether convenient choices of the CPTP maps $\Phi_\alpha(t)$ can lead to a well defined description of the system evolution. In particular, we take the maps $\Phi_\alpha(t)$ to be CPTP semigroups, i.e.,

$$\Phi_\alpha(t) \;=\; e^{\mathcal{L}_\alpha t}, \tag{33}$$

where $\mathcal{L}_\alpha$ are generators in the GKLS form [24, 16]

$$\mathcal{L}_\alpha[\rho] \;=\; \sum_{j=1}^{d^2-1} \gamma_{\alpha,j}\left(L_{\alpha,j}\rho L_{\alpha,j}^\dagger - \frac{1}{2}\left\{L_{\alpha,j}^\dagger L_{\alpha,j}, \rho\right\}\right), \tag{34}$$

with $\gamma_{\alpha,j} \geq 0$ and $L_{\alpha,j}$ linear independent linear operators on $\mathcal{H}_S$, and we recall that d is the finite dimension of the open-system Hilbert space $\mathcal{H}_S$.

The idea of combining a family of semigroup maps to go beyond the description of Markovian dynamics has been used by Chruściński and Kossakowski in several pioneering works [11, 12, 13], aiming at the identification of well-defined integro-differential master equations accounting for non-Markovian dynamics. In [4] a system of GKSL evolutions was used to take into account statistical correlations between system and environment leading to a non-Markovian dynamics within a projection operator approach. Here, by using Eq.(3) to connect the initial reduced state with its value at a generic time, we explore whether a family of semigroups can be exploited in the context of open-system dynamics in the presence of initial correlations with the environment. Indeed, while every $e^{\mathcal{L}_\alpha t}$ is CPTP, so that also a convex combination of these maps would be CPTP, we are now applying each $e^{\mathcal{L}_\alpha t}$ to a distinct element of the dual frame D_α, which needs not to be positive. As a consequence, it is a-priori not guaranteed that even though we start from an initial positive state ρ_S in (5), the state at time t fixed by (3) will be positive, too. In the following, we show that it is actually possible to identify a proper set of initial states that are mapped into states at any time t, for a relevant class of two-level system dynamics. Let us stress that, as common in phenomenological approaches, the fact that we can introduce a well-defined evolution on open-system states does not mean by itself that the evolution can be derived from a full microscopic model. Within the formalism exploited here, the existence of a microscopic model would consist in the presence of initial global states and a global unitary evolution such that the action of the maps $\Phi_\alpha(t)$ could be expressed as in (4); whether this is the case is a challenging question, which we leave for future investigation.

4.1. Pauli channels

We consider a two-level open quantum system and we further exploit the positive frame induced by the Pauli basis of operators, introduced in Sec.3.1. In particular, the dual-frame operators D_α are as in (19), which for the case $d = 2$ we are dealing with simply read

$$\begin{aligned} D_0 &= \frac{1}{\sqrt{2}}\Big(\sigma_0 - \sum_{\alpha=1}^{3}\sigma_\alpha\Big)\,, \\ D_\alpha &= \frac{1}{\sqrt{2}}\sigma_\alpha \quad \text{for} \quad \alpha = 1,2,3\,, \end{aligned} \tag{35}$$

where σ_0 is the identity, the σ_α, $\alpha = 1, 2, 3$ are the usual Pauli matrices, and we reordered the frame indices as $\alpha = 0, \ldots, 3$. Given a reduced operator of the form (compare with (5))

$$\rho_S = \frac{1}{\sqrt{2}}\sum_{\alpha=0}^{3} \upsilon_\alpha D_\alpha\,, \tag{36}$$

where for the sake of convenience we have set $\upsilon_\alpha = \sqrt{2}\omega_\alpha$ with ω_α as in (5), it has trace one if and only if $\upsilon_0 = 1$, while its positivity is ensured by the validity of

$$(1 - v_1)^2 + (1 - v_2)^2 + (1 - v_3)^2 \; \leq \; 1 \, . \tag{37}$$

Hence, the initial positivity domain, that is the set of points $\{v_1, v_2, v_3\}$ for which ρ_S as in (36) can be taken as a proper initial state, is a ball with radius 1 and origin in the point $\{1, 1, 1\}$.

Our goal is then to determine whether there is a subset of the initial positivity domain such that the state $\rho_S(t)$ obtained via (3) is positive at any time t. In particular, we take into account the maps corresponding to the so-called Pauli channels [41, 14], whose generators are given by

$$\mathcal{L}_\alpha[\rho] \; = \; \sum_{j=1}^{3} \gamma_{\alpha,j}(t) \left(\sigma_j \rho \sigma_j - \rho \right) . \tag{38}$$

When the rates $\gamma_{\alpha,j}(t)$ are non-negative and time independent each of this generator corresponds to a GKSL master equation, otherwise the dynamics can be highly non-Markovian also for a single $\mathcal{L}_\alpha$ [27]. Here, as said, we restrict to semigroups; note that while the coefficients $\gamma_{\alpha,j}$ can be different for the different $\mathcal{L}_\alpha$s, the Lindblad operators are always the same, i.e., the Pauli matrices. The corresponding CPTP maps take the form

$$\phi_\alpha(t)[\rho] \; = \; \sum_{j=0}^{3} p_{\alpha,j}(t) \sigma_j \rho \sigma_j \, , \tag{39}$$

where the coefficients $p_{\alpha,j}(t)$ are readily expressed by introducing the vectors $\vec{p}_\alpha(t)$, whose components are $(\vec{p}_\alpha(t))_j = p_{\alpha,j}(t)$, so that one has

$$\vec{p}_\alpha(t) \; = \; \frac{1}{4} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix} \vec{\lambda}_\alpha(t) \, , \tag{40}$$

where $(\vec{\lambda}_\alpha(t))_j = \lambda_{\alpha,j}(t)$ with

$$\lambda_{\alpha,0} = 1, \quad \lambda_{\alpha,j} = e^{-2(\gamma_{\alpha,k} + \gamma_{\alpha,m})t}, \quad j \neq k \neq m = 1, 2, 3, \tag{41}$$

i.e., the exponential decays characterizing semigroup dynamics. Note that the $\{\lambda_{\alpha,j}(t)\}_{j=0,\ldots,3}$ are eigenvalues of the map $\phi_\alpha(t)$

$$\phi_\alpha(t)[\sigma_j] \; = \; \lambda_{\alpha,j}(t) \sigma_j \, , \tag{42}$$

while the coefficients $\{p_{\alpha,j}(t)\}_{j=0,\ldots,3}$ form a probability distribution, i.e. $p_{\alpha,j}(t) \geq 0$ and $\sum_{j=0}^{3} p_{\alpha,j}(t) = 1$.

For the sake of simplicity, we now restrict to two different semigroup maps, one for the dual frame element D_0, which we denote as $\phi(t) := \phi_0(t)$, and another for the other elements, which we denote as $\tilde{\phi}(t) := \phi_1(t) = \phi_2(t) = \phi_3(t)$; accordingly all the parameters referred to the first (second) map will be indicated without (with) a tilde. The state at time t obtained via (3) then reads

$$\begin{aligned} \rho_S(t) &= \frac{1}{2}\Big(\mathbb{1} + (\tilde{\lambda}_1(t)v_1 - \lambda_1(t))\sigma_1 + (\tilde{\lambda}_2(t)v_2 - \lambda_2(t))\sigma_2 \\ &\quad + (\tilde{\lambda}_3(t)v_3 - \lambda_3(t))\sigma_3\Big)\,, \end{aligned} \tag{43}$$

so that the positivity domain at a generic time is specified by the condition

$$(\lambda_1(t) - \tilde{\lambda}_1(t)v_1)^2 + (\lambda_2(t) - \tilde{\lambda}_2(t)v_2)^2 + (\lambda_3(t) - \tilde{\lambda}_3(t)v_3)^2 \;\leq\; 1\,, \tag{44}$$

which defines the interior of an axis-aligned ellipsoid with semiaxes lengths $1/\tilde{\lambda}_1(t)$, $1/\tilde{\lambda}_2(t)$ and $1/\tilde{\lambda}_3(t)$, centered at the point $(\lambda_1(t)/\tilde{\lambda}_1(t), \lambda_2(t)/\tilde{\lambda}_2(t), \lambda_3(t)/\tilde{\lambda}_3(t))$.

4.2. Results

Summarizing the previous discussion, our primary goal is thus to find the values $\{v_1, v_2, v_3\}$ that satisfy both (37) and (44), where the former inequality defines the initial positivity domain, while the latter depends on the dynamical parameters $\lambda_\alpha(t)$ and $\tilde{\lambda}_\alpha(t)$.

To this aim, it is advantageous to decouple the quantities referred to, respectively, $\phi(t)$ and $\tilde{\phi}(t)$. Note that we can interpret (44) as an equation of a ball with the axis rescaled by $\tilde{\lambda}$s:

$$(\lambda_1(t) - \tilde{x}(t))^2 + (\lambda_2(t) - \tilde{y}(t))^2 + (\lambda_3(t) - \tilde{z}(t))^2 \;\leq\; 1\,. \tag{45}$$

We call the set of points $\{\tilde{x}(t), \tilde{y}(t), \tilde{z}(t)\}$ satisfying this inequality an evolved positivity ball, as for $t = 0$ it gives the initial positivity domain as in (37). On the other hand, (37) after such rescaling takes the form

$$\frac{1}{\tilde{\lambda}_1^2(t)}\left(\tilde{\lambda}_1(t) - \tilde{x}(t)\right)^2 + \frac{1}{\tilde{\lambda}_2^2(t)}\left(\tilde{\lambda}_2(t) - \tilde{y}(t)\right)^2 + \frac{1}{\tilde{\lambda}_3^2(t)}\left(\tilde{\lambda}_3(t) - \tilde{z}(t)\right)^2 \;\leq\; 1\,, \tag{46}$$

and the set of all evolved initial points is an axis-aligned ellipsoid centered at $(\tilde{\lambda}_1(t), \tilde{\lambda}_2(t), \tilde{\lambda}_3(t))$ with semiaxes lengths $\tilde{\lambda}_1(t)$, $\tilde{\lambda}_2(t)$ and $\tilde{\lambda}_3(t)$. Accordingly, the intersection of this ellipsoid with the evolved positivity ball with radius 1 and origin in $(\lambda_1(t), \lambda_2(t), \lambda_3(t))$ gives the wanted set of vs. If the whole ellipsoid is contained within the evolved positivity ball at a given time t, all initial density operators ρ_S stay positive at this point of time. By virtue of

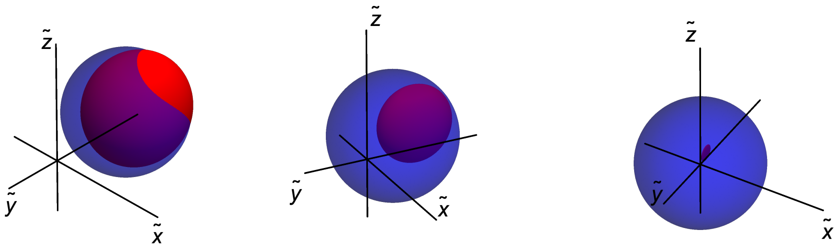

Fig. 1: Example 1: evolved initial points (red) and the evolved positivity ball (blue). Left: $\gamma t = 1/10$, Middle: $\gamma t = 1/2$, Right: $\gamma t = 2$.

the rescaling introduced above, the form and location of the ellipsoid is only governed by the $\tilde{\lambda}$s, while the positivity ball evolves according to the λs.

In Fig. 1 and 2 we report the ellipsoid of evolved intial points defined by (46) (in red) and the evolved positivity ball defined by (45) (in blue), for two different choices of the parameters defining the semigroup maps.

EXAMPLE 1 In a generic case all the λs and $\tilde{\lambda}$s describe exponential decay, i.e. according to (41) at most one of the γs and $\tilde{\gamma}$s is zero. In this case the centers of both the evolved positivity ball and the evolved ellipsoid converge to $(0, 0, 0)$. Additionally, the ellipsoid asymptotically shrinks to a point, while the size of the evolved positivity ball does not change. Hence, for large enough times the ellipsoid will be completely contained into the positivity ball. For intermediate times, a portion of the ellipsoid can leave the evolved positivity ball, as seen in Fig. 1 for the following choice of the parameters: $\gamma_1 = \tilde{\gamma}_1 = 0$, $\gamma_2 = \gamma_3 = 2\tilde{\gamma}_2 = 2\tilde{\gamma}_3 = \gamma$, which correspond to

$$\begin{aligned} \lambda_1(t) = e^{-4\gamma t}, \quad \lambda_2(t) = e^{-2\gamma t}, \quad \lambda_3(t) = e^{-2\gamma t}, \\ \tilde{\lambda}_1(t) = e^{-2\gamma t}, \quad \tilde{\lambda}_2(t) = e^{-\gamma t}, \quad \tilde{\lambda}_3(t) = e^{-\gamma t}. \end{aligned} \tag{47}$$

The larger values of the γs with respect to the $\tilde{\gamma}$s result in a quicker motion of the positivity ball than of the ellipsoid. Accordingly, some of the states in the initial positivity domain will anyhow lead to temporarily negative evolved matrix $\rho_S(t)$.

EXAMPLE 2 If, on the other hand, two of the $\tilde{\gamma}$s equal zero, one can see a qualitatively different behaviour, as some of the choices of initial points lead to eternally negative evolved matrix $\rho_S(t)$. For example, for $\gamma_1 = \tilde{\gamma}_1 = \tilde{\gamma}_2 = 0$, $\gamma_2 = \gamma_3 = \tilde{\gamma}_3 = \gamma$, which correspond to

$$\begin{aligned} \lambda_1(t) = e^{-4\gamma t}, \quad \lambda_2(t) = e^{-2\gamma t}, \quad \lambda_3(t) = e^{-2\gamma t}, \\ \tilde{\lambda}_1(t) = e^{-2\gamma t}, \quad \tilde{\lambda}_2(t) = e^{-2\gamma t}, \quad \tilde{\lambda}_3(t) = 1\,, \end{aligned} \tag{48}$$

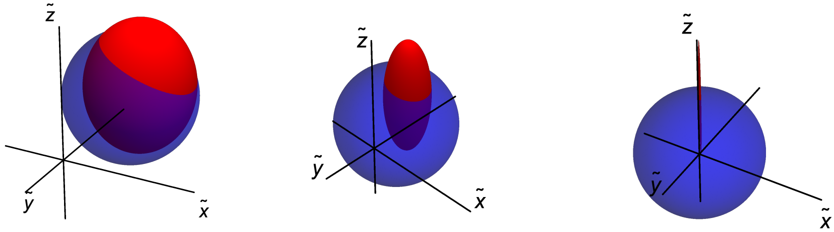

Fig. 2: Example 2: evolved initial points (red) and the evolved positivity ball (blue). Left: $\gamma t = 1/10$, Middle: $\gamma t = 1/2$, Right: $\gamma t = 2$.

the z-coordinate of the initial points is constant: $(e^{-2\gamma t}v_1, e^{-2\gamma t}v_2, v_3)$. Accordingly, the semi-axes length in this direction of the ellipsoid does not change in time and its center remains on the same x-y plane, see Fig. 2. All of the choices of points with $v_3 > 1$ will at some point of the evolution leave the evolved positivity ball forever.

5. Conclusion

In this paper, we have considered an approach to describe the dynamics of open quantum systems that allows one to take into account fully general initially correlated system–environment states. The starting point is the OPD decomposition of the initial global state, which involves positive and normalized operators on the environmental side and fixes the evolution of the open system through a set of time-dependent CPTP maps. Such a decomposition can be defined via a positive frame on the open quantum system and it is in general highly non-unique. In particular, we introduced two OPD decompositions, one that is based on the generalized Pauli matrices and one directly on the basis elements of the open-system Hilbert space; notably, the latter can be defined also for infinite-dimensional Hilbert spaces, thus showing how the OPD-based approach to open-system dynamics is not restricted to the finite-dimensional case. In addition, we have demonstrated that the cost of the decomposition, that is the number of terms involved in it and thus the number of resulting CPTP maps fixing the reduced dynamics, is always bounded by the Schmidt rank of the initial global state. This is a particularly useful feature of the approach, since it implies that the open-system evolution can be fixed by a number of equations, for example as in [40], that is a direct expression of the amount of correlations between the open system and the environment and it is ultimately bounded by the dimensionality of the open system. Finally, we have studied the case where the CPTP maps defining the reduced dynamics along with the OPD decomposition are semigroups fixed by the Gorini-Kossakowski-Lindblad-Sudarshan form. In particular, in the case of qubit Pauli channels, we have derived explicit conditions identifying the positivity domain defined by the initial reduced states that are mapped to proper states at any time and we have distinguished two qualitatively different regimes; one where all the states compatible with a given initial decomposition are eventually mapped into proper states after a transient time interval, and one where some states lead to eternally negative evolved matrices.

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Bibliography

[1] S. T. Ali, J.-P. Antoine, and J.-P. Gazeau, *Coherent States, Wavelets, and Their Generalizations.* Theor. Math. Physics, Springer, 2000.

[2] R. Alicki, Phys. Rev. Lett. **75**, 3020 (1995).

[3] I. Bengtsson and K. Życzkowski, *Geometry of quantum states: an introduction to quantum entanglement*, Cambridge Univ. Press, 2006.

[4] H.-P. Breuer, Phys. Rev. A **75**, 022103 (2007).

[5] H.-P. Breuer and F. Petruccione, *The Theory of Open Quantum Systems.* Oxford Univ. Press, 2002.

[6] A. Brodutch, A. Datta, K. Modi, A. Rivas, and C. A. Rodríguez-Rosario, Phys. Rev. A **87**, 042301 (2013).

[7] F. Buscemi, Phys. Rev. Lett. **113**, 140502 (2014).

[8] D. Cariello, Quantum Inf. Comput. **14**, 1308 (2014).

[9] D. Cariello, Quantum Inf. Comput. **15**, 812 (2015).

[10] T. Chalermpusitarak, B. Tonekaboni, Y. Wang, L. M. Norris, L. Viola, and G. A. Paz-Silva, PRX Quantum **2**, 030315 (2021).

[11] D. Chruściński and A. Kossakowski, Phys. Rev. Lett. **104**, 070406 (2010).

[12] D. Chruściński and A. Kossakowski, Int. J. Quant. Inf. **09**, 129 (2011).

[13] D. Chruściński and A. Kossakowski, EPL **97**, 20005 (2012).

[14] D. Chruściński and F. A. Wudarski, Phys. Lett. A **377**, 1425 (2013).

[15] J. M. Dominy and D. A. Lidar, Quant. Inf. Proc. **15**, 1349 (2016).

[16] V. Gorini, A. Kossakowski, and E. C. G. Sudarshan, J. Math. Phys. **17**, 821 (1976).

[17] H. Grabert, P. Schramm, and G.-L. Ingold, Phys. Rep. **168**, 115 (1988).

[18] S. Hamedani Raja, K. P. Athulya, A. Shaji, and J. Piilo, Phys. Rev. A **101**, 042127 (2020).

[19] L. Henderson and V. Vedral, J. Phys. A: Math. and Gen. **34**, 6899 (2001).

[20] P. Štelmachovič and V. Bužek, Phys. Rev. A **64**, 062106 (2001).

[21] T. F. Jordan, A. Shaji, and E. C. G. Sudarshan, Phys. Rev. A **70**, 052110 (2004).

[22] T. F. Jordan, A. Shaji, and E. C. G. Sudarshan, Phys. Rev. A **73**, 012106 (2006).

[23] G. Kimura, Phys. Lett. A **314**, 339 (2003).

[24] G. Lindblad, Commun. Math. Phys. **48**, 119 (1976).

[25] G. Lindblad, J. Phys. A: Math. Gen. **29**, 4197 (1996).

[26] M. Majeed and A. Z. Chaudhry, Eur. Phys. J. D **73**, 16 (2019).

[27] N. Megier, D. Chruściński, J. Piilo, and W. T. Strunz, Sci. Rep. **7**, 6379 (2017).

[28] M. Merkli, arXiv:2107.02515 (2021).

[29] K. Modi, A. Brodutch, H. Cable, T. Paterek, and V. Vedral, Rev. Mod. Phys. **84**, 1655 (2012).

[30] P. Myöhänen, A. Stan, G. Stefanucci, and R. van Leeuwen, EPL **84**, 67001 (2008).

[31] H. Ollivier and W. H. Zurek, Phys. Rev. Lett. **88**, 017901 (2001).

[32] G. A. Paz-Silva, M. J. W. Hall, and H. M. Wiseman, Phys. Rev. A **100**, 042120 (2019).

[33] P. Pechukas, Phys. Rev. Lett. **73**, 1060 (1994).

[34] A. Pomyalov, C. Meier, and D. Tannor, Chem. Phys. **370**, 98 (2010).

[35] J. M. Renes, R. Blume-Kohout, A. J. Scott, and C. M. Caves, J. Math. Phys. **45**, 2171 (2004).

[36] Á. Rivas, S. F. Huelga, and M. B. Plenio, Rep. Progr. Phys. **77**, 094001 (2014).

[37] C. A. Rodríguez-Rosario, K. Modi, A. Kuah, A. Shaji, and E. C. G. Sudarshan, J. Phys. A: Math. Theor. **41**, 205301 (2008).

[38] D. Schmid, K. Ried, and R. W. Spekkens, Phys. Rev. A **100**, 022112 (2019).

[39] A. Shabani and D. A. Lidar, Phys. Rev. Lett. **102**, 100402 (2009).

[40] A. Trevisan, A. Smirne, N. Megier, and B. Vacchini, Phys. Rev. A **104**, 052215 (2021).

[41] B. Vacchini, J. Phys. B: Atomic, Molecular and Optical Physics **45**, 154007 (2012).

[42] B. Vacchini and G. Amato, Sci. Rep. **6**, 37328 (2016).