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Pauli semigroups and unistochastic quantum channels

Zbigniew Puchała [a,b], Łukasz Rudnicki [c,d,*], Karol Życzkowski [b,d]

[a] Institute of Theoretical and Applied Informatics, Polish Academy of Sciences, ulica Bałtycka 5, 44-100 Gliwice, Poland
[b] Faculty of Physics, Astronomy and Applied Computer Science, Jagiellonian University, ul. Łojasiewicza 11, 30-348 Kraków, Poland
[c] Max-Planck Institute for the Science of Light, Staudtstraße 2, 91058 Erlangen, Germany
[d] Center for Theoretical Physics, Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warsaw, Poland

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ABSTRACT

We adopt the perspective of similarity equivalence, in gate set tomography called the gauge, to analyze various properties of quantum operations belonging to a semigroup, $\Phi = e^{\mathcal{L}t}$, and therefore given through the Lindblad operator. We first observe that the non unital part of the channel decouples from the time evolution. Focusing on unital operations we restrict our attention to the single-qubit case, showing that the semigroup embedded inside the tetrahedron of Pauli channels is bounded by the surface composed of product probability vectors and includes the identity map together with the maximally depolarizing channel. Consequently, every member of the Pauli semigroup is unitarily equivalent to a unistochastic map, describing a coupling with one-qubit environment initially in the maximally mixed state, determined by a unitary matrix of order four.

1. Introduction

Quantum systems interacting with an environment or being subject to a quantum noise can be described within the theory of open quantum systems [1,2]. One applies the notion of mixed quantum state represented by a positive, normalized hermitian matrix [3], which can be considered as a generalization of the classical probability vector.

In the stroboscopic approach, the dynamics is represented in discrete time steps and the formalism of quantum operations, often called *quantum channels*, becomes useful. These completely positive and trace preserving linear maps send the set of mixed quantum states of a given size N into itself. The channel can be considered as a generalization of the unitary evolution of a density matrix, which takes into account interactions of the system with an environment or with a measurement apparatus.

Although in the simplest case of a single qubit system, $N = 2$, the set of quantum operations has 12 dimensions, its structure and geometry is already well understood [4–6]. This contrasts the case of a larger size N, for which the set of quantum operations has $N^4 - N^2$ dimensions and its structure and geometry become difficult to grasp [7].

In an alternative approach, one describes dynamics in continuous time. The most general form of a quantum Markov process, which preserves positivity of quantum states, is given by the equation derived by Gorini, Kossakowski and Sudarshan [8], and independently by Lindblad [9]. Its solution describes a (non)unitary quantum dynamics, $\rho(t) = e^{\mathcal{L}t}[\rho(0)]$, and is determined by the Lindblad generator $\mathcal{L}$ – see e.g. [1]. During the last four decades an approach of quantum dynamical semigroups [10] was successfully used in a broad variety of physical problems. For an interesting account on the history and importance of the GKLS equation consult a recent review [11].

It is natural to ask to which extent both alternative descriptions of quantum dynamics are compatible. In general, this is not a trivial question as it is well known that some quantum channels are not *divisible* [12,13], hence they cannot be represented as concatenation of other channels. Consequently, they do not belong to a semigroup. In spite of several recent related contributions on the structure of quantum Markovian dynamics [14,15] the problem how to describe the set of quantum channels, which belong to a semigroup, remains open even in the simplest case of operations acting on a single qubit [16]. Nevertheless, as quite a lot is known about formal properties of channels ranging from the divisible up to the Markovian ones [12,17], we are not concerned here with the characterization problem. Instead, we assume that a given channel Φ can be a *seed* for a semigroup (see next section for a proper explanation) and we examine construction and properties of associated Lindblad operator.

* Corresponding author.
E-mail addresses: z.puchala@iitis.pl (Z. Puchała), rudnicki@cft.edu.pl (Ł. Rudnicki).

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Our approach pursued in this paper is inspired by gate set tomography [18–20] being an efficient successor of process tomography. In this reconstruction scheme, quantum channels are obtained up to a similarity equivalence, customarily called the gauge, i.e. instead of Φ one recovers $X\Phi X^{-1}$, where X is unknown. It was shown [21] that X itself is a reversible and trace preserving operation, though, it is not necessarily a channel since it does not need to be completely positive.

On the one hand side, some information concerning the character of the discrete evolution corresponding to a quantum operation can be obtained by investigating spectral properties of the corresponding superoperator [21,22]. On the other hand, the gauge symmetry inherent to gate set tomography promotes the spectrum of the superopertor Φ to be the only source of accessible knowledge. Therefore, the aim of this work is to make first steps in learning about the structure of the Lindblad generators related to quantum channels, while being guided by the similarity relation. In Sec. 2 we introduce necessary notation, while in Sec. 3 we initiate the general analysis of the problem. In Sec. 4 we concentrate on the case $N = 2$ and establish some results on the geometric structure of the set $\mathcal{S}$ of one-qubit unital operations which belong to a semigroup. In particular, we demonstrate that any Pauli channel is unitarily equivalent to a unistochastic channel.

2. Preliminaries

We consider a quantum channel $\mathcal{E}$ acting on density matrices of order N. The action of the channel, defined in terms of the Kraus decomposition K_j

$$\mathcal{E}(\rho) = \sum_j K_j \rho K_j^\dagger, \tag{1}$$

leads to the superoperator representation, $\Phi = \sum_j K_j \otimes \bar{K}_j$. Given any hermitian operator basis $\{B_0, \ldots, B_{N^2-1}\}$, such that $B_0 = \mathbb{1}/\sqrt{N}$ and $\operatorname{tr} B_i B_j = \delta_{ij}$, the superoperator further acquires the block form

$$\Phi = \begin{bmatrix} 1 & 0 \\ \kappa & T \end{bmatrix}, \tag{2}$$

provided that we assume the channel $\mathcal{E}$ is trace preserving. Up to unitary rotations in $N^2 - 1$ dimensions, such a basis is formed by the generalized Pauli matrices. The real distortion matrix T of order $N^2 - 1$ acts on the generalized Bloch vector representing a quantum mixed state in the Bloch representation, while the real vector κ accounts for the displacement of the entire set of quantum states. In the case of unital maps, which preserve the maximally mixed state, $\Phi(\mathbb{1}/N) = \mathbb{1}/N$, the translation vector vanishes, $\kappa = 0$. In the case of a unitary map, the matrix T is orthogonal.

A matrix Φ, acting on a composite Hilbert space $\mathcal{H}_N \otimes \mathcal{H}_N$, can alternatively be represented in a product basis, $|m\rangle \otimes |\mu\rangle$ with matrix element written $\Phi_{\substack{m\mu \\ n\nu}} = \langle m\mu|\Phi|n\nu\rangle$. In general, the superoperator matrix Φ is non Hermitian. However, by reshuffling of its four indices one obtains a Hermitian matrix $D_\Phi = \Phi^R$, where $X^R_{\substack{m\mu \\ n\nu}} = X_{\substack{mn \\ \mu\nu}}$ – see [23]. The matrix D_Φ is called dynamical matrix or the Choi matrix, as the theorem of Choi [24] implies that the map Φ is completely positive if and only if the corresponding Choi matrix D_Φ is positive.

For every quantum operation $\mathcal{E}$ its corresponding superoperator Φ of order N^2 enjoys the following spectral properties [3]: a) $\lambda_0(\Phi) = 1$, due to trace preservation; b) other $\lambda_i(\Phi)$, $i = 1, \ldots, N^2 - 1$ are in general complex, though they are either real or come in conjugate pairs, so that $\det \Phi$ and $\operatorname{tr} \Phi$ are real; c) All eigenvalues belong to the unit disk, $|\lambda_k| \leq 1$.

Although the spectrum of the superoperator can be complex, the case $N = 2$ is somewhat special: For any one-qubit channel Φ there exists a unitarily equivalent operation $\tilde{\Phi}$ with real spectrum and diagonal distortion matrix,

$$\tilde{\Phi} = \Psi_U \circ \Phi \circ \Psi_V = (U \otimes \bar{U})\Phi(V \otimes \bar{V}). \tag{3}$$

To show this one uses a known group–theoretical homomorphism, $SU(2) \simeq SO(3)$, which allows to represent a unitary transformation of a complex one–qubit state by an orthogonal proper rotation of the corresponding Bloch vector of length three [6]. This implies the transformation $T \to \tilde{T} = O_U T O_V$, where O_U and O_V denote orthogonal matrices of order three, which are determined by unitary rotation matrices of size two, U and V respectively. An analogous formula with usage of arbitrary orthogonal matrices corresponds to singular value decomposition of T with positive singular values. Since in the case considered, orthogonal matrices do belong to $SO(3)$ and have unit determinant, the transformed matrix is diagonal and real, but may contain also negative entries, $\tilde{T} = \operatorname{diag}(\lambda_1, \lambda_2, \lambda_3)$. The vector $\vec{\lambda}$ describes the distortion of the Bloch ball induced by the operation [3] and forms the spectrum of the operation $\tilde{\Phi}$.

Let us now proceed to the description of quantum dynamics in continuous time. Every quantum Markov evolution can be determined by a linear Lindblad superoperator $\mathcal{L}$,

$$\rho(t) = e^{\mathcal{L}t}[\rho(0)] = \Lambda_t[\rho(0)], \tag{4}$$

which generates a semigroup, $\Lambda_s \Lambda_t = \Lambda_{t+s}$. According to the celebrated GKLS theory [8,9], the action of any Lindblad generator $\mathcal{L}$ can be written in terms of no more than $(N^2 - 1)$ jump operators L_j,

$$\mathcal{L}(\rho) = \sum_{j=1}^{N^2-1} \Big(L_j \rho L_j^\dagger - \frac{1}{2} L_j^\dagger L_j \rho - \frac{1}{2} \rho L_j^\dagger L_j \Big). \tag{5}$$

A product of any three matrices, $Y = ABC$, can also be written as $Y = \Psi B$, where the superoperator reads $\Psi = A \otimes C^T$ and B is transformed to a vectorized form. Thus, the Lindblad generator can be explicitly represented by a matrix of order N^2,

$$\mathcal{L} = \sum_j L_j \otimes \overline{L}_j - \frac{1}{2} \sum_j L_j^\dagger L_j \otimes \mathbb{1} - \frac{1}{2} \sum_j \mathbb{1} \otimes L_j^T \overline{L}_j. \tag{6}$$

Let us now merge both pictures by setting $\Phi = \Lambda_1$, so that $\mathcal{L} = \log \Phi$. We assume that Φ fulfills all the requirements to be a seed for the semigroup, what means that $\Lambda_t = e^{t \log \Phi}$ gives the proper quantum channel for all $t \geq 0$. Under a similarity transformation $\Phi \mapsto X\Phi X^{-1}$, we get

$$\mathcal{L} \mapsto X \log \Phi X^{-1}, \qquad \Lambda_t \mapsto X e^{t \log \Phi} X^{-1}. \tag{7}$$

Clearly, the similarity transformation might spoil complete positivity of both the seed channel and the semigroup, however, it does not mingle with the time evolution.

3. General channels

First of all, we consider the general channel given by Eq. (2) acting on a system of size N. We observe that, as long as the matrix $(T - \mathbb{1})$ is invertible, the following decomposition holds:

$$\begin{aligned} \Phi &= \begin{bmatrix} 1 & 0 \\ \kappa & T \end{bmatrix} \\ &= \begin{bmatrix} 1 & 0 \\ (\mathbb{1} - T)^{-1}\kappa & \mathbb{1} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & T \end{bmatrix} \begin{bmatrix} 1 & 0 \\ (T - \mathbb{1})^{-1}\kappa & \mathbb{1} \end{bmatrix}, \end{aligned} \tag{8}$$

and the last matrix on the right hand side is the inverse of the first one therein. Since Eq. (8) constitutes the similarity relation, we immediately conclude that the non unital contribution from κ does not complicate the time evolution (however, one needs to remember that κ does play a role in assuring complete positivity of the channel Λ_t). Moreover, since the logarithm of the unital part in the middle term above is equal to diag $(0, \log T)$, the multiplication from the left will trivialize leading to the results:

$$\mathcal{L} = \log\Phi = \begin{bmatrix} 1 & 0 \\ (\mathbb{1}-T)^{-1}\kappa & \mathbb{1} \end{bmatrix}\begin{bmatrix} 0 & 0 \\ 0 & \log T \end{bmatrix}\begin{bmatrix} 1 & 0 \\ (T-\mathbb{1})^{-1}\kappa & \mathbb{1} \end{bmatrix} \equiv \begin{bmatrix} 0 & 0 \\ 0 & \log T \end{bmatrix}\begin{bmatrix} 1 & 0 \\ (T-\mathbb{1})^{-1}\kappa & \mathbb{1} \end{bmatrix}, \tag{9}$$

and

$$\Lambda_t = \begin{bmatrix} 1 & 0 \\ (\mathbb{1}-T)^{-1}\kappa & \mathbb{1} \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & T^t \end{bmatrix}\begin{bmatrix} 1 & 0 \\ (T-\mathbb{1})^{-1}\kappa & \mathbb{1} \end{bmatrix} \equiv \begin{bmatrix} 1 & 0 \\ (T^t-\mathbb{1})(T-\mathbb{1})^{-1}\kappa & T^t \end{bmatrix}. \tag{10}$$

The above simple and at the same time general formula, if T is diagonal, could be intuitively rewritten in terms of the N^2-1 non-trivial eigenvalues $\lambda_i(\Phi)$, which for diagonal distortion matrices are real. If an *a priori* given channel $\Phi = \Phi(\lambda_i, \kappa_i)$, with $i = 1, \ldots, N^2-1$ is an admissible seed to a semigroup, then the following relation holds for an arbitrary dimension N

$$\Lambda_t = \Phi\left(\lambda_i^t, \frac{1-\lambda_i^t}{1-\lambda_i}\kappa_i\right). \tag{11}$$

Obviously, for $t = 1$ this formula yields the seed quantum operation Φ.

The general question, whether a given channel (1) defines a proper semigroup, is beyond the scope of this work. Nevertheless, we shall briefly scrutinize few immediate restrictions. First of all, referring now to the Bloch form (2) of the superoperator, we see that if all real eigenvalues of Φ are positive the desired expression $\log T$ can be defined. Moreover, existence of $(T-\mathbb{1})^{-1}$ forces that all eigenvalues (except λ_0), if real, are strictly smaller than 1. For a qubit case, $N = 2$, it is known that [21]

$$\|\kappa\|^2 \le 1 - |\lambda_1|^2 - |\lambda_2|^2 - |\lambda_3|^2 + 2\lambda_2\lambda_2\lambda_3, \tag{12}$$

is a necessary condition for complete positivity of Φ. Note that it stems from a related condition expressed through singular values of T [6]. From this result we easily infer, that if $\kappa \neq 0$, then

$$\max\{|\lambda_1|, |\lambda_2|, |\lambda_3|\} < 1, \tag{13}$$

so that the second requirement is always satisfied. To prove the assertion, without loss of generality, we assume that $\max\{|\lambda_1|, |\lambda_2|, |\lambda_3|\} = |\lambda_1|$. Then if $|\lambda_1| = 1$ we obtain

$$\|\kappa\|^2 \le -|\lambda_2|^2 - |\lambda_3|^2 + 2|\lambda_2\lambda_3| \le 0, \tag{14}$$

which enforces the contradiction $\kappa = 0$. The last inequality used is arithmetic-geometric. A similar property could potentially hold for $N > 2$, however, further studies are needed to substantiate that hope.

4. Qubit channels

In the second part we consider the simplest but fairly non-trivial one-qubit problem, $N = 2$. In this case the three eigenvalues of T are either all real or of the form: $\lambda_1(\Phi) = x \in \mathbb{R}$ and $\lambda_2(\Phi) = z$, $\lambda_3(\Phi) = \bar{z}$ with $z \in \mathbb{C}$. In what follows we concentrate on the first case, leaving the second one as an open problem for the future.

Above, we have already shown that every channel (also beyond the qubit case) is similar to its own unital variant, obtained by letting $\kappa \to 0$. Moreover, every unital qubit channel with four real eigenvalues $(\lambda_0 \equiv 1, \lambda_1, \lambda_2, \lambda_3)$ is similar (see Eq. (40) in ref. [21]) to the channel

$$\Xi = \sum_{i=0}^{3} p_i\sigma_i \otimes \bar{\sigma}_i = \begin{pmatrix} p_0+p_3 & 0 & 0 & p_1+p_2 \\ 0 & p_0-p_3 & p_1-p_2 & 0 \\ 0 & p_1-p_2 & p_0-p_3 & 0 \\ p_1+p_2 & 0 & 0 & p_0+p_3 \end{pmatrix}. \tag{15}$$

Note that, for further convenience, Ξ is given in the product basis (not in the Pauli basis) so it is not of the form (2). However, for the sake of the spectrum, the choice of the basis is of no relevance. The eigenvalues are related to the probabilities $p_0, \ldots, p_3$ in the following way:

$$\begin{aligned} \lambda_0 &= p_0 + p_1 + p_2 + p_3 \equiv 1, \\ \lambda_1 &= p_0 + p_1 - p_2 - p_3 = 1 - 2(p_2 + p_3), \\ \lambda_2 &= p_0 - p_1 + p_2 - p_3 = 1 - 2(p_1 + p_3), \\ \lambda_3 &= p_0 - p_1 - p_2 + p_3 = 1 - 2(p_1 + p_2). \end{aligned} \tag{16}$$

In other words, every single-qubit unital map is similar to a Pauli channel — mixed unitary operation, defined as convex combination of rotations with respect to the Pauli matrices, $\Xi : \rho \mapsto \sum_{i=0}^{3} p_i\sigma_i\rho\sigma_i^\dagger$, with $\sigma_0 = \mathrm{id}, \sigma_1 = \sigma_x, \sigma_2 = \sigma_y, \sigma_3 = \sigma_z$. For such a channel the Kraus operators can be chosen as $K_i = \sqrt{p_i}\sigma_i$. In fact, taking into account the results presented in the previous section, every qubit channel is similar to Ξ, with the similarity transformation X being given by concatenation of the transformation from Eq. (8) and the rotation which brings the intermediate unital channel to the form (15).

Quite naturally, every channel (non unital and of any dimension) is also similar to diag$(1, \lambda_1, \ldots, \lambda_{N^2-1})$, so that from this fundamental perspective, the time evolution does only depend on the eigenvalues. However, the observations made so far point towards the less obvious approach, in which for qubits, the burden and actual complexity are both to be lifted to the level of the Pauli channels. Therefore, in the next four subsections we discuss various semigroup-related properties of this special class of channels.

4.1. The Pauli semigroup

It is easy to check that the probabilities defining the Pauli channel are non-negative whenever $\lambda_3^\downarrow \ge \lambda_1^\downarrow + \lambda_2^\downarrow - 1$, where $\lambda^\downarrow$ denotes the vector $(\lambda_1, \lambda_2, \lambda_3)$ ordered decreasingly. In fact, this is a necessary and sufficient condition for complete positivity of this channel, derived in terms of the eigenvalues [21]. Moreover, if we employ the condition $\lambda_{\min} \ge 0$, which holds whenever $p_i + p_j \le \frac{1}{2}$ for $i, j \in \{1, 2, 3\}; i \neq j$, the logarithm of Ξ is well-defined. These conditions imply that p_0 is the largest component of vector p.

Let us introduce an orthogonal matrix O_4, an explicit form of which is of no relevance here, that allows to diagonalize the superoperator in question, $E = O_4 \Xi O_4^\top = \mathrm{diag}(1, \lambda_1, \lambda_2, \lambda_3)$. Under all the conditions listed above, the Lindblad generator is

$$\mathcal{L} = O_4^\top \log E \; O_4. \tag{17}$$

The associated semigroup is then given by

$$\Lambda_t = e^{\mathcal{L}t} = O_4^\top e^{t\log E} O_4 = \frac{1}{2}\begin{pmatrix} 1+\lambda_3^t & 0 & 0 & 1-\lambda_3^t \\ 0 & \lambda_1^t+\lambda_2^t & \lambda_1^t-\lambda_2^t & 0 \\ 0 & \lambda_1^t-\lambda_2^t & \lambda_1^t+\lambda_2^t & 0 \\ 1-\lambda_3^t & 0 & 0 & 1+\lambda_3^t \end{pmatrix}. \tag{18}$$

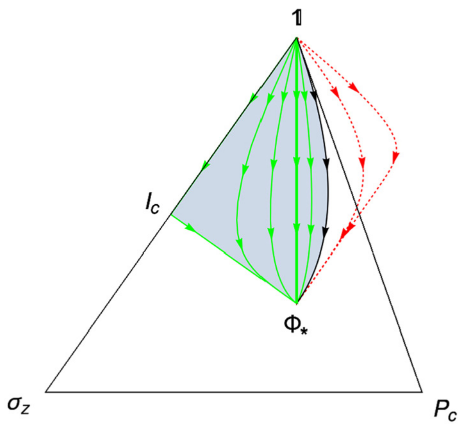

Fig. 1. Cross-section of the simplex of one–qubit Pauli channels determined by the identity map $\mathbb{1}$, the completely depolarizing channel Φ_*, and the z-rotation corresponding to the map $\Phi_z = \sigma_z \otimes \sigma_z$ which includes also classical channels: $I_c = (\mathbb{1} + \Phi_z)/2 = \mathrm{diag}(1,0,0,1)$ and $P_c = (\Phi_x + \Phi_y)/2 = \mathrm{diag}(0,1,1,0)$. The set $\mathcal{S}$ of channels belonging to a semigroup is shown in gray, and its right boundary corresponds to the product relation, $p_0 p_3 = p_1 p_2$. Some exemplary semigroups leading from $\mathbb{1}$ to Φ_*, are represented by solid arrowed lines. Dashed (red) lines going through a channel $\Psi \notin \mathcal{S}$ do not correspond to a semigroup, as it leaves the simplex of CP maps for some initial time $t > 0$. (For interpretation of the colours in the figure(s), the reader is referred to the web version of this article.)

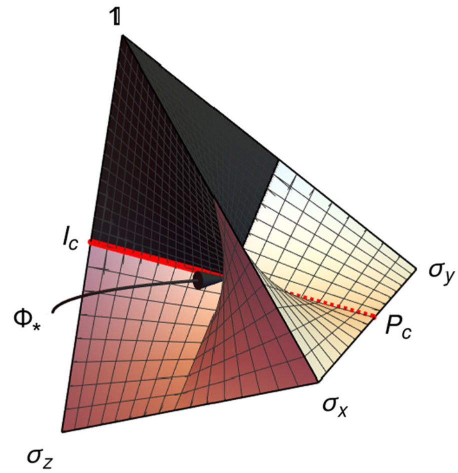

Fig. 2. The tetrahedron of Pauli channels spanned by three Pauli matrices and identity contains a proper set of maps bounded by the classical 4-point probability vectors with a product structure. Dark region, including identity map $\mathbb{1}$ and the completely depolarizing channel Φ_*, represents probability vectors for which the corresponding Pauli channel $\Phi_{\vec{p}}$ belongs to a semigroup. Dashed (red) line represents maps corresponding to classical action of bistochastic matrices of size $N = 2$, while solid line denotes maps from the classical semigroup $[I_c, \Phi_*]$. The map P_c represents negation of the classical state.

In order to check if this is a completely positive operation for all $t \geq 0$, we construct the corresponding Choi matrix

$$D_{\Lambda_t} = \Lambda_t^R = \frac{1}{2}\begin{pmatrix} 1+\lambda_3^t & 0 & 0 & \lambda_1^t+\lambda_2^t \\ 0 & 1-\lambda_3^t & \lambda_1^t-\lambda_2^t & 0 \\ 0 & \lambda_1^t-\lambda_2^t & 1-\lambda_3^t & 0 \\ \lambda_1^t+\lambda_2^t & 0 & 0 & 1+\lambda_3^t \end{pmatrix}, \qquad (19)$$

and study its positivity. As recalled in Section 2, for any four-index matrix Y the symbol Y^R denotes the matrix with reshuffled indices [23]; such an involution transforms a non-hermitian super-operator matrix Φ into the hermitian dynamical matrix D_Φ. The above matrix is positive iff the following three relations are satisfied for all times $t \geq 0$:

$$\begin{aligned} 1+\lambda_3^t &\geq \lambda_1^t + \lambda_2^t, \\ 1+\lambda_2^t &\geq \lambda_1^t + \lambda_3^t, \\ 1+\lambda_1^t &\geq \lambda_2^t + \lambda_3^t. \end{aligned} \qquad (20)$$

Expanding these equations in power series around $t = 0$ we see that it is sufficient to check the inequalities for small $t > 0$ – see also Eq. (51) in the work of Wolf and Cirac [12]. This gives three independent conditions on the eigenvalues of the Bloch transition matrix T entering Eq. (2), which need to be fulfilled to assure positivity of the Choi matrix:

$$\lambda_3 \geq \lambda_1\lambda_2, \quad \lambda_2 \geq \lambda_1\lambda_3, \quad \lambda_1 \geq \lambda_2\lambda_3. \qquad (21)$$

4.2. The geometric picture

As we shall see below, each of the conditions (21) determines a surface inside the tetrahedron of the Pauli channels and forms a part of the boundary of the set $\mathcal{S}$ of operations belonging to a semigroup. For any point outside the set $\mathcal{S}$ one can try to find a continuous trajectory starting at identity, but for some finite time t it will leave the tetrahedron of completely positive maps — see Fig. 1.

The relations (16) allow us to translate the inequalities (21) concerning eigenvalues λ_i into constraints for components of the probability vector:

$$p_0 p_3 \geq p_1 p_2, \quad p_0 p_2 \geq p_1 p_3, \quad p_0 p_1 \geq p_2 p_3. \qquad (22)$$

Boundary of the set $\mathcal{S}$ is met, whenever one of these inequalities becomes saturated. This happens if the classical probability vector of length four has a product structure. For example, the choice

$$\vec{p} = (a, a') \times (b, b') = (ab, ab', a'b, a'b'), \qquad (23)$$

where $a' = 1 - a$ and $b' = 1 - b$, renders $p_0 p_3 = aba'b' = p_1 p_2$. Other two equalities would correspond to permutations of the components of $\vec{p}$.

Interestingly, these product vectors form three fragments of a hyperboloid – a ruled surface inside the tetrahedron which is spanned by its two opposite sides. This manifold is useful to visualize the set of two-qubit separable states in a 3D cross-section through the 6D space of two-qubit pure states [3,25] and to identify the maximally entangled states, which are located as far from this manifold as possible.

The region $\mathcal{S}$ for which constraints (22) are satisfied contains two special points: $(1,0,0,0)$, corresponding to identity channel, and $(1,1,1,1)/4$, representing the maximally depolarizing channel Φ_*. The region in question is also bounded by three surfaces consisting of product probability vectors — see Fig. 2. Below we prove a proposition concerned with the shape of S, which stems from the product structure mentioned in the previous sentence.

Proposition 1. *The set $\mathcal{S}$ is star-shaped with respect to any point on the interval*

$$\beta(1,0,0,0) + (1-\beta)\frac{1}{4}(1,1,1,1), \ \ \textit{for} \ \ \beta \in [0,1]. \qquad (24)$$

Proof. We will show, that the intervals connecting any boundary point of $\mathcal{S}$ with an arbitrary point from the interval (24), represented by a bold interval in Fig. 1, belongs to $\mathcal{S}$. The boundary of the set $\mathcal{S}$ is solely formed by permutations of product vectors, so to fix the attention we consider a part of the boundary given by $(pq, p(1-q), (1-q)p, (1-p)(1-q))$, with $\frac{1}{2} \leq p, q \leq 1$. For every point from the interval (24) we consider a line to the above generic boundary point, which is parameterized as

$$\vec{r} = \gamma[\beta(1,0,0,0) + (1-\beta)\frac{1}{4}(1,1,1,1)] + (1-\gamma)(pq, p(1-q), (1-q)p, (1-p)(1-q)) \quad \text{for } \beta,\gamma \in [0,1]. \tag{25}$$

With the help of elementary inequalities one can check that under our assumptions the condition $r_0 r_3 \geq r_1 r_2$ holds. Consequently, $\vec{r} \in \mathcal{S}$ for all $\beta,\gamma \in [0,1]$. □

4.3. Lindblad dynamics associated with Pauli semigroups

Consider now a special example of the Pauli semigroup $\Lambda_s^z = \exp(\mathcal{L}_z s)$ associated with a single jump operator $L_1 = \sigma_z$. It describes the effects of decoherence as it gradually diminishes the off-diagonal entries of the density matrix. Define also two accompanying semigroups: $\Lambda_t^x = \exp(\mathcal{L}_x t)$ describing decoherence with respect to the basis along the x axis and corresponding to the jump operator $L_1 = \sigma_x$. The third Pauli semigroup, $\Lambda_u^y = \exp(\mathcal{L}_y u)$ is defined analogously. Since the tensor squares of the Pauli matrices commute, $[\sigma_i \otimes \sigma_i, \sigma_j \otimes \sigma_j] = 0$, the corresponding Lindblad generators commute as well, $[\mathcal{L}_i, \mathcal{L}_j] = 0$ for $i, j = x, y, z$, and so do the semigroups. Therefore, the order of operations is not important and will not influence the following key observation concerning a composition of two or three semigroups:

Proposition 2. *For any choice of the times (t, s) the map $\Lambda_s^z \Lambda_t^x$ gives a Pauli channel for which the vector $\vec{p}$ has a product structure (23). This map forms a part of the boundary of the set $\mathcal{S}$. Two other parts of this boundary are obtained by the remaining two-factor concatenations $\Lambda_s^z \Lambda_u^y$ and $\Lambda_u^y \Lambda_t^x$.*

Proof. Using the fact that tensor squares of Pauli matrices do commute, we arrive at a simple result

$$\Lambda_s^z \Lambda_t^x = O_4^\top \operatorname{diag}(1, e^{-2s}, e^{-2(s+t)}, e^{-2t}) O_4. \tag{26}$$

Therefore $\Lambda_s^z \Lambda_t^x$ is a Pauli channel for which the corresponding probability vector:

$$\begin{aligned} p_0 &= 2e^{-(s+t)} \cosh(s)\cosh(t), \\ p_1 &= 2e^{-(s+t)} \cosh(s)\sinh(t), \\ p_2 &= 2e^{-(s+t)} \sinh(s)\sinh(t), \\ p_3 &= 2e^{-(s+t)} \sinh(s)\cosh(t), \end{aligned} \tag{27}$$

enjoys the product structure $p_0 p_2 = p_1 p_3$. Other two conditions for a product vector p correspond to remaining choices of two generators and two other parts of the boundary of $\mathcal{S}$. □

Proposition 3. *For any point $\vec{p}$ in the interior of the set $\mathcal{S}$ of quantum operations belonging to the semigroup, there exist a triple $(s, t, u > 0)$ such that the corresponding Pauli channel is given by a composition $\Phi_{\vec{p}} = \Lambda_s^z \Lambda_t^x \Lambda_u^y$.*

Proof. For a given probability vector $\vec{p} \in \mathcal{S}$ we resort to (16) in order to find its accompanying distortion vector $\vec{\lambda}$. In the next step we set:

$$\begin{aligned} s &= \frac{1}{2}\log\sqrt{\frac{\lambda_3}{\lambda_1\lambda_2}}, \\ t &= \frac{1}{2}\log\sqrt{\frac{\lambda_1}{\lambda_2\lambda_3}}, \\ u &= \frac{1}{2}\log\sqrt{\frac{\lambda_2}{\lambda_1\lambda_3}}. \end{aligned} \tag{28}$$

For points in the interior, relations (21) are satisfied as strict inequalities, the arguments of the logarithms are greater than unity so that the times s, t, u are positive.

Now utilizing the trivial commutation relation, we get

$$\Lambda_s^z \Lambda_t^x \Lambda_u^y = O_4^\top \operatorname{diag}(1, e^{-2(s+u)}, e^{-2(s+t)}, e^{-2(t+u)}) O_4, \tag{29}$$

which gives $\Phi_{\vec{p}}$. Note that the entries of the diagonal matrix reveal time dependence of the vector λ. □

4.4. Dynamical semigroups and unistochastic maps

Let us recall here that a unital quantum operation acting on an N dimensional system and determined by a unitary matrix U of order N^2, which describes the coupling of the system with environment initially in the maximally mixed state followed by the partial trace over the environment B,

$$\rho' = \Phi_U(\rho) = \operatorname{tr}_B\Big(U(\rho \otimes \frac{\mathbb{I}_N}{N})U^\dagger\Big), \tag{30}$$

is called *unistochastic* [23]. It is known that the set of one-qubit unistochastic maps forms a non-convex proper subset of the tetrahedron of Pauli channels [26] which is bounded by the manifold of probability vectors with a tensor product structure as shown in Fig. 1. Therefore, the set of Pauli channels belonging to a semigroup forms a quarter of the set of unistochastic maps which contains the identity operation. More formally, we arrive at the following statement.

Proposition 4. *Any bistochastic one qubit Pauli channel $\Phi : \rho \mapsto \sum_{i=0}^3 p_i \sigma_i \rho \sigma_i^\dagger$ belongs to a dynamical semigroup, and can be written in the Lindblad form, $\Lambda_t = e^{\mathcal{L}t}$, if and only if Λ_t is unistochastic and the identity component p_0 is the largest component of the probability vector $\vec{p} = (p_0, p_1, p_2, p_3)$.*

To shed some light on the above result we will make use of the notion of locally equivalent gates and apply the canonical form of a two-qubit quantum gate. Two unitary matrices U and V of order four, are called *locally equivalent*, if there exist four unitary matrices W_i of order two such that

$$V \sim U = (W_1 \otimes W_2) V (W_3 \otimes W_4). \tag{31}$$

Observe that unistochastic maps Φ_U and Φ_V, generated by two locally equivalent unitary matrices, $U \sim V$, lead to unitarily equivalent channels (3).

Any unitary matrix $U \in U(4)$ is locally equivalent to a two–qubit gate written in the canonical Cartan form [27,28],

$$U \sim V = e^{i\sum_{j=1}^3 \alpha_j \sigma_j \otimes \sigma_j}, \tag{32}$$

and the vector of $(\alpha_1, \alpha_2, \alpha_3)$ called *information content* can be chosen from the Weyl chamber, $\frac{\pi}{4} \geq \alpha_1 \geq \alpha_2 \geq |\alpha_3| \geq 0$. Thus, we are going to restrict our attention to the unistochastic maps Φ_U corresponding to unitary matrices in the above Cartan form.

Consider a unistochastic channel Φ_U determined by a unitary $U \in U(4)$. The corresponding Choi matrix can be written with use of the reshuffled matrix, $D_U = \frac{1}{2}U^R(U^R)^\dagger$, so that the superoperator reads [26], $\Phi_U = \frac{1}{2}[U^R(U^R)^\dagger]^R$. Taking U in the form Eq. (32) we arrive at the following expression for the superoperator

$$\Phi_U = O_4^\top \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(2\alpha_2)\cos(2\alpha_3) & 0 & 0 \\ 0 & 0 & \cos(2\alpha_1)\cos(2\alpha_3) & 0 \\ 0 & 0 & 0 & \cos(2\alpha_1)\cos(2\alpha_2) \end{pmatrix} O_4. \tag{33}$$

Since the eigenvalues of Φ_U do satisfy (21) this channel belongs to a semigroup. On the other hand for a qubit unital channel with positive eigenvalues, satisfying constraints (21), we can find unitary matrix U, such that the channel can be written as Φ_U. It is enough to take the angles $\alpha_1, \alpha_2, \alpha_3$

$$\alpha_1 = \frac{1}{2}\arccos(\sqrt{\frac{\lambda_2\lambda_3}{\lambda_1}}),$$
$$\alpha_2 = \frac{1}{2}\arccos(\sqrt{\frac{\lambda_1\lambda_3}{\lambda_2}}), \tag{34}$$
$$\alpha_3 = \frac{1}{2}\arccos(\sqrt{\frac{\lambda_1\lambda_2}{\lambda_3}}),$$

as due to relations (21) the arguments of the square roots do not exceed the unity. In this way we have shown that every unistochastic channel (up to a unitary rotation) belongs to a semigroup. This concludes a constructive proof of Proposition 4.

5. Concluding remarks

The results of the present work, motivated by the similarity equivalence (gauge) inherent to gate set tomography, touched upon the general case of non unital quantum maps of arbitrary dimension and studied in more detail the set $\mathcal{S}$ of single-qubit quantum Pauli channels which belong to a semigroup. A conceptual novelty of the results is that the Pauli channels are shown to be a handy way of encoding relevant features of qubit channels.

To synthetically summarize the findings of geometrical nature: the set $\mathcal{S}$ forms a subset of a quarter of the tetrahedron of Pauli channels bounded by the surfaces consisting of 4-point probability vectors with the tensor product structure. Although this set is not convex, it is star-shaped. Since this set contains unistochastic channels [26], which correspond to the coupling with a one-qubit environment initially in the maximally mixed state [23], we conclude that every map accessible through the continuous semigroup is unitarily equivalent to a unistochastic channel.

Note that for any quantum operation acting on quantum states of size N one can find the corresponding classical map represented by a stochastic transition matrix of order N. This matrix is obtained by reshaping the diagonal of the Choi matrix, which may be interpreted as a result of the decoherence acting in the space of quantum maps [29,30]. Hence the problem studied in this work can be considered as a quantum analogue of the question, which bistochastic matrix allows for a continuous dynamics, $B = \exp(\mathcal{L}t)$, such that the trajectory does not leave the Birkhoff polytope $\mathcal{B}_N$ of bistochastic matrices [31]. Although for $N = 2$ this question is fairly easy, [the answer is $B_a = (1-a, a;\ a, 1-a)$ with $a \leq 1/2$ represented by interval $[I_c, \Phi_*]$ in Fig. 2], already for $N = 3$ the problem becomes interesting [32,33]. In fact one can study also a simpler question, asking for the set of bistochastic matrices, such that its square root (or roots of a higher order) are bistochastic and formulate the corresponding quantum problem, looking for bistochastic operations such that its square root (or higher order roots) forms bistochastic operations [32,34]. Any divisible map, which belongs to a semigroup, is included inside this set.

It will be a challenge to find out, which of the above results can be extended to a more general class of systems. In particular, in the case of unital quantum channels it is clear that the set of the bistochastic maps acting on $\mathcal{H}_N$, which belong to a semigroup, includes the maps corresponding to the action of bistochastic matrices of size N, which belong to classical semigroups [31,33].

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