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# SINGULAR VALUE DECOMPOSITION AND MATRIX REORDERINGS IN QUANTUM INFORMATION THEORY

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We review Schmidt and Kraus decompositions in the form of singular value decomposition using operations of reshaping, vectorization and reshuffling. We use the introduced notation to analyze the correspondence between quantum states and operations with the help of Jamiołkowski isomorphism. The presented matrix reorderings allow us to obtain simple formulae for the composition of quantum channels and partial operations used in quantum information theory. To provide examples of the discussed operations, we utilize a package for the *Mathematica* computing system implementing basic functions used in the calculations related to quantum information theory.

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## 1. Introduction

Quantum information theory[1−3] aims to provide methods of harnessing the quantum nature of information carriers to develop more efficient quantum algorithms and more secure communication protocols. Mathematically quantum systems are described using the formalism of density matrices and the most general form of quantum evolution is described by completely positive (CP) operators.[2,4]

In many situations in quantum information theory one deals with vector spaces of the tensor-product form. For example, the description of composite quantum systems is based on a tensor product of spaces describing sub-systems. This is essential for the phenomenon of quantum entanglement, which is one of the most important features of quantum information theory.[5,6] Also the theory of quantum channels, which are used, for example, to describe errors in quantum computation and communication protocols, deals with the composite channels that are described as tensor products of channels. The composition of quantum channels gives rise to another phenomenon unique to quantum information theory, namely the non-additivity of channel capacity.[7,8]

The main aim of this report is to present a uniform view on Schmidt and Kraus decompositions. Both decompositions provide very important tools used in quantum information theory. Schmidt decomposition is used to describe quantum entanglement in the special case of pure quantum states. Kraus decomposition, on the other hand, is used in the analysis of quantum channels. We achieve our goal by presenting both decompositions in the form of singular value decomposition (SVD) and by using some matrix reorderings. As the reorderings are used in many branches of mathematics, physics and computer science, our goal is also to clarify the used notation. The presented concepts form the basis for the package of functions for *Mathematica* computer algebra systems presented in the last part of this report.

This report is organized as follows. In Sec. 2 we review some basic algebraic facts applied in this report. In particular we fix the notions of matrix reshaping, vectorization and reshuffling. In Sec. 3 we use the SVD theorem in the finite-dimensional Hilbert space to obtain Schmidt decomposition for pure quantum states. We also rephrase Schmidt decomposition in any unitary space and apply it to density matrices to obtain the so-called *operator Schmidt decomposition*. In Sec. 4 we use the conditions for quantum channels and SVD to derive the Kraus form of a quantum channel and we analyze the composition of quantum channels and partial operations. Finally, Appendix A contains some examples of the discussed concepts using the package of functions for *Mathematica* computing system.

**Notation.** In what follows we denote by $\mathbf{v}$, elements of finite vector space, and $|\phi\rangle$, pure states. By $\mathbb{M}_{m,n}$ we denote the set of all $m \times n$ matrices over $\mathbf{C}$. The set of square $n \times n$ matrices is denoted by $\mathbb{M}_n$. The set of $n$-dimensional density matrices (normalized, positive semi-definite operators on $\mathbf{C}^n$) is denoted by $\Omega_n$.

The set $\mathbb{M}_n$ has the structure of the Hilbert space with the scalar product given by the formula

$$(A, B) = \operatorname{tr} A^\dagger B. \tag{1}$$

This particular Hilbert space is known as the Hilbert−Schmidt space of operators acting on $\mathbf{C}^n$ and we will denote it by $\mathcal{H}_{\mathrm{HS}}$.

## 2. SVD and Matrix Reorderings

In this section we review some basic algebraic facts used in the following parts of this report. One should note that the operations of reshaping and vectorization, introduced in this section, are used in many areas of science and engineering — see for example Refs. 9 and 10. For this reason in many cases, the naming conventions differ depending on the authors' preferences and backgrounds.

### 2.1. *Singular value decomposition*

For the sake of consistency we start by recalling SVD which is valid for any $n \times m$ matrix over $\mathbf{C}$.[11]

**Theorem 1.** *Let $A \in \mathbb{M}_{m,n}$ has the rank $k \leq m$. Then there exist unitary matrices $U \in \mathbb{M}_m$ and $V \in \mathbb{M}_n$ such that*

$$A = U \Sigma V^\dagger. \tag{2}$$

*The matrix $\Sigma = \{\sigma_{ij}\} \in \mathbb{M}_{m,n}$ is such that*

$$\sigma_{ij} = 0, \quad \text{for } i \neq j, \tag{3}$$

*and*

$$\sigma_{11} \geq \sigma_{22} \geq \cdots \geq \sigma_{kk} > \sigma_{k+1,k+1} = \cdots = \sigma_{qq} = 0, \tag{4}$$

*with $q = \min(m, n)$.*

The numbers $\sigma_{ii} \equiv \sigma_i$ are *singular vales*, i.e. non-negative square roots of the eigenvalues of $AA^\dagger$. The columns of $U$ are eigenvectors of $AA^\dagger$ and the columns of $V$ are eigenvectors of $A^\dagger A$.

In the special case when $A$ is positive semi-definite, the above decomposition is equivalent to the eigendecomposition of $A$.

## 2.2. *Reshaping and vectorization*

SVD provides us with the particular form of a given matrix. This can be directly applied in the case when we deal with linear maps on a finite-dimensional vector space.

In order to use the SVD we need one or more algebraic tools, namely the mapping between $\mathbb{M}_{m,n}$ and $\mathbb{M}_{mn,1}$ (or $\mathbf{C}^{mn}$). We define two functions, which can be used as such mappings.

**Definition 1.** *Let $A = [a_{ij}]_{i,j} \in \mathbb{M}_{m,n}(\mathbf{C})$. We define the reshaping of $A$ as*

$$\mathbf{res}(A) = (a_{11}, a_{12}, \ldots, a_{1n}, a_{21}, a_{22}, \ldots, a_{2n}, \ldots, a_{m1}, a_{m2}, \ldots, a_{mn})^T, \tag{5}$$

*and the vectorization of $A$ as*

$$\mathbf{vec}(A) = (a_{11}, a_{21}, \ldots, a_{m1}, a_{12}, a_{22}, \ldots, a_{m2}, \ldots, a_{1n}, a_{2n}, \ldots, a_{mn})^T \tag{6}$$

*where "$T$" denotes matrix transposition.*

In other words, the vectorization of matrix $A$ means its reordering in column order and reshaping in row order. Note that $\mathbf{res}(A)$ is equivalent to $\mathbf{vec}(A^T)$. Both operations can be achieved using, for example, `Flatten` function in *Mathematica* or `reshape` function in *Matlab* and *GNU Octave*.

Both $\mathbf{vec}(A)$ and $\mathbf{res}(A)$, map $\mathbb{M}_{m,n}$ onto $\mathbb{M}_{mn,1}$. Both operations can also be interchanged as they are connected by the formula

$$\mathbf{res}\, A = \mathbf{vec}\, A^T. \tag{7}$$

Thus, it is rather a matter of taste which one to use.

One should keep in mind that there are several notational conventions in literature for denoting vectorization and reshaping operations. We use the definition of vectorization as provided in Refs. 10, 12 and 13. The reshaping operation defined above agrees with the convention used in Ref. 4 and it corresponds to the row-major order method of turning a matrix into a vector. In Ref. 14 this operation is denoted as **col**. In the recent preprint of Gilchrist *et al.*[15] the authors refer to **res** operation defined above as to vectorization.

Vectorization and reshaping have many useful properties, some of which we are going to use in the following sections. In particular, if $A, B, C \in \mathbb{M}_m$ then we have the following.

(P1) $\mathbf{vec}(A) = \mathbf{res}(A^T)$ for $A \in \mathbb{M}_m$,
(P2) $\mathbf{vec}(ABC) = (C^T \otimes A)\,\mathbf{vec}(B)$ and $\mathbf{res}(ABC) = (A \otimes C^T)\mathbf{res}(B)$,
(P3) $\mathbf{vec}(AB) = (\mathbb{1} \otimes A)\,\mathbf{vec}(B) = (B^T \otimes \mathbb{1})\mathbf{vec}(A)$,
(P4) $\mathbf{vec}(A \circ B) = \mathbf{vec}(A) \circ \mathbf{vec}(B)$, where "∘" denotes the Hadamard product,[11]
(P5) $\operatorname{tr} A^\dagger B = \mathbf{vec}(A)^* \cdot \mathbf{vec}(B) = \mathbf{res}(A)^* \cdot \mathbf{res}(B)$, where "·" denotes the scalar product of two vectors in $\mathbf{C}^n$.

In particular, properties (P2), (P3) and (P4) from the above list also hold for rectangular matrices of appropriate dimensions. According to Ref. 13 the property (P2) appeared for the first time in Ref. 16 and it will be crucial in the next sections.

## 2.3. *Reshuffling*

Our main goal is to use SVD to analyze composite quantum states and the dynamics of quantum systems. In both cases we need to deal with the tensor-product structure. For pure quantum states this structure is fixed by the physical structure of the system we aim to describe. For quantum channels this structure is introduced by Jamiołkowski isomorphism, which uses the operation of *reshuffling*.

Reshuffling can be used to fix particular tensor-product structure in the set of matrices. Roughly speaking a reshuffled matrix is a matrix represented in a particular tensor-product base.

Let us denote by $\{\epsilon_i : i = 1, \ldots, m^2\}$ and $\{\varepsilon_j : j = 1, \ldots, n^2\}$ canonical bases in $\mathbb{M}_m$ and $\mathbb{M}_n$ respectively. This is to say that $\mathbf{res}(\epsilon_i)$ $(\mathbf{res}(\varepsilon_j))$ has 1 at $i$th ($j$th) position and zeros elsewhere and $\mathbf{res}(\epsilon_i \otimes \varepsilon_j)$ has 1 at the $i \times j$th position.

**Definition 2.** Let $A \in \mathbb{M}_k$ with $k = mn$, i.e. $\mathbb{M}_k = \mathbb{M}_m \otimes \mathbb{M}_n$. Matrix with elements

$$\{A^{R(m,n)}\}_{ij} \overset{\text{def}}{=} \operatorname{tr}\big[(\epsilon_i \otimes \varepsilon_j)^\dagger A\big] \tag{8}$$

is called a *reshuffling of matrix A with respect to subspaces* $\mathbb{M}_m$ *and* $\mathbb{M}_n$.

Using **res** operation a reshuffled matrix can be expressed as

$$\{A^{R(m,n)}\}_{ij} = \mathbf{res}(\epsilon_i \otimes \varepsilon_j) \cdot \mathbf{res}(A), \tag{9}$$

where we have used the fact that matrices $\epsilon_i$ and $\varepsilon_j$ are real.

Note that this type of matrix reordering was introduced without any connection to quantum physics in Ref. [17].

One can also introduce the reshuffling operation using transposed canonical bases, which are ordered accordingly in column order. This is to say that $\mathbf{vec}(\epsilon_i^T)$ $(\mathbf{vec}(\varepsilon_j^T))$ has 1 at $i$th ($j$th) position and zeros elsewhere and $\mathbf{vec}(\epsilon_i^T \otimes \varepsilon_j^T)$ has 1 at the $(i \times j)$th position. We define alternative reshuffling by counting matrix elements in column order.

**Definition 3.** Let $A \in \mathbb{M}_k$ with $k = mn$, i.e. $\mathbb{M}_k = \mathbb{M}_m \otimes \mathbb{M}_n$. Matrix with elements

$$\{A^{R'(m,n)}\}_{ij} \stackrel{\text{def}}{=} \text{tr}[(\epsilon_j^T \otimes \varepsilon_i^T)^\dagger A] \tag{10}$$

is called an *alternative reshuffling of matrix $A$ with respect to subspaces* $\mathbb{M}_m$ *and* $\mathbb{M}_n$.

Taking into account that base matrices are real we get

$$\{A^{R'(m,n)}\}_{ij} = \text{tr}[(\epsilon_j \otimes \varepsilon_i)A]. \tag{11}$$

Note that it is also possible to define reshuffling in more general case when matrix $A$ is of the form $A = X \otimes Y$ with $X \in \mathbb{M}_{k,l}$ and $Y \in \mathbb{M}_{m,n}$.

We usually work with a density matrix $\rho$, which is said to be an element of $S(\mathcal{H}_A \otimes \mathcal{H}_B)$. In such case the reshuffling operation is understood with respect to canonical bases in $S(\mathcal{H}_A)$ and $S(\mathcal{H}_B)$.

Moreover, while working with $\rho \in \mathbb{M}_n \otimes \mathbb{M}_n$ we write simply $\rho^R$ as long as the dimensions of matrices in question can be deduced from the context.

**Example 1.** To give a simple example of reshuffling operation one can use a square matrix $A \in \mathbb{M}_{n^2}$. For example, if $A \in \mathbb{M}_4$ it is given as

$$A = \begin{pmatrix} \alpha_{1,1} & \alpha_{1,2} & \alpha_{1,3} & \alpha_{1,4} \\ \alpha_{2,1} & \alpha_{2,2} & \alpha_{2,3} & \alpha_{2,4} \\ \alpha_{3,1} & \alpha_{3,2} & \alpha_{3,3} & \alpha_{3,4} \\ \alpha_{4,1} & \alpha_{4,2} & \alpha_{4,3} & \alpha_{4,4} \end{pmatrix}, \tag{12}$$

then we have

$$A^{R(2,2)} = \begin{pmatrix} \alpha_{1,1} & \alpha_{1,2} & \alpha_{2,1} & \alpha_{2,2} \\ \alpha_{1,3} & \alpha_{1,4} & \alpha_{2,3} & \alpha_{2,4} \\ \alpha_{3,1} & \alpha_{3,2} & \alpha_{4,1} & \alpha_{4,2} \\ \alpha_{3,3} & \alpha_{3,4} & \alpha_{4,3} & \alpha_{4,4} \end{pmatrix}. \tag{13}$$

On the other hand taking the alternative definition of reshuffling we get

$$A^{R'(2,2)} = \begin{pmatrix} \alpha_{1,1} & \alpha_{3,1} & \alpha_{1,3} & \alpha_{3,3} \\ \alpha_{2,1} & \alpha_{4,1} & \alpha_{2,3} & \alpha_{4,3} \\ \alpha_{1,2} & \alpha_{3,2} & \alpha_{1,4} & \alpha_{3,4} \\ \alpha_{2,2} & \alpha_{4,2} & \alpha_{2,4} & \alpha_{4,4} \end{pmatrix}. \tag{14}$$

**Example 2.** Reshuffling operation is a linear map on $\mathbb{M}_n$ and as such it can be represented as a matrix. For example the operation $\rho \mapsto \rho^{R(2,2)}$ on $\mathbb{M}_4$ has the

following matrix representation

$$M_{R(2,2)} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \tag{15}$$

One can note that reshuffling and alternative reshuffling are connected by the relation[4]

$$A^{R'} = (SA^R S)^T, \tag{16}$$

where $S$ is the swap operation.

In the next section we use the following simple fact connecting reshuffling and the tensor product.

**Proposition 1.** *Let $A \in \mathbb{M}_n$ and $B \in \mathbb{M}_m$. Then we have*

$$\mathbf{res}((A \otimes B)^R) = \mathbf{res}(A) \otimes \mathbf{res}(B) \tag{17}$$

*and*

$$\mathbf{vec}((A \otimes B)^{R'}) = \mathbf{vec}(A) \otimes \mathbf{vec}(B). \tag{18}$$

Proposition 1 follows directly from the definition of reshuffling and it allows us to interchange between product base in Hilbert−Schmidt space and the one in $\mathbf{C}^n$.

## 3. Schmidt Decomposition

Now we are ready to use the introduced tools for deriving some important results from quantum information theory.

Our first goal is to prove a particular representation of vectors in finite-dimensional vector space with inner product. This representation is known in quantum information theory as *Schmidt decomposition*.[4,18]

Schmidt decomposition was first stated for an infinite-dimensional Hilbert space,[19],[20] but it is more often used in a version which deals with finite-dimensional spaces only. It is frequently used in quantum information theory to distinguish between separable and entangled states.[6]

### 3.1. *Schmidt decomposition for pure states*

We start with Schmidt decomposition for pure states, i.e. unit vectors in a finite-dimensional Hilbert space $\mathbf{C}^{mn} = \mathbf{C}^m \otimes \mathbf{C}^n$. This form is used in quantum information theory to study quantum entanglement.

**Theorem 2.** *Any pure state* $|\psi\rangle \in \mathbf{C}^m \otimes \mathbf{C}^n$ *can be represented as*

$$|\psi\rangle = \sum_{i=1}^{k} \sqrt{\lambda_i} |\alpha_i\rangle \otimes |\beta_i\rangle, \tag{19}$$

*where* $\{|\alpha_i\rangle\} \in \mathbf{C}^m$ *and* $\{|\beta_i\rangle\} \in \mathbf{C}^n$ *are orthogonal in respective Hilbert spaces and* $k \leq \min(m, n)$.

**Proof.** We can always represent $|\psi\rangle \in \mathbf{C}^m \otimes \mathbf{C}^n$ using canonical basis as

$$|\psi\rangle = \sum_{i=1}^{m} \sum_{j=1}^{n} C_{ij} |e_i\rangle \otimes |f_j\rangle, \tag{20}$$

where $\{|e_i\rangle\} \in \mathbf{C}^m$ and $\{|f_j\rangle\} \in \mathbf{C}^m$ are canonical bases in respective subspaces, $C \in \mathbb{M}_{m,n}$ and vectors $|e_i\rangle \otimes |f_j\rangle$, $i = 1, \ldots, m$, $j = 1, \ldots, n$ have the following form

$$|e_i\rangle \otimes |f_j\rangle = (0, \ldots, 0, 1, 0, \ldots, 0)^T, \tag{21}$$

with 1 at position $ij$ and zeros elsewhere. In this particular basis $|\psi\rangle = \mathbf{res}(C)$. Using the SVD and the property (P2) for the reshaping operation we get

$$|\psi\rangle = \mathbf{res}(U \Sigma V^\dagger) = (U \otimes V^*) \mathbf{res}(\sigma_{ij} \delta_{ij}) \tag{22}$$

and by using the canonical basis we get

$$|\psi\rangle = (U \otimes V^*) \sum_{i=1}^{m} \sum_{j=1}^{n} \sigma_{ij} \delta_{ij} |b_{ij}\rangle \tag{23}$$

$$= \sum_{i=1}^{k} \sigma_{ii} U |e_i\rangle \otimes V^* |f_i\rangle, \tag{24}$$

where $k$ is the order of $C$. Since $\sigma_{ii}$ are square roots of eigenvalues of positive matrix $CC^\dagger$ we can write

$$|\psi\rangle = \sum_{i=1}^{k} \sqrt{\lambda_i} |\alpha_i\rangle \otimes |\beta_i\rangle, \tag{25}$$

with $\sigma_{ii} = \sqrt{\lambda_i}$, $|\alpha_i\rangle = U |e_i\rangle$ and $|\beta_i\rangle = V^* |f_i\rangle$. $\qquad\square$

**Definition 4.** Number $k$ of elements in Schmidt decomposition is often referred to as the *Schmidt number*.

States of bipartite systems are among the most interesting objects in quantum information theory. This is because the tensor-product structure of state space results in the presence of states which cannot be mimicked using classical theory. These special states are called *entangled states* and are used in quantum protocols and algorithms.

Theorem 2 allows us to distinguish entangled pure states from non-entangled (or separable) pure states. We have the following theorem, which provides us with the simplest *separability criterion*.[5,6]

**Theorem 3.** *Pure state is separable iff its Schmidt number is equal to* 1.

### 3.2. *Schmidt decomposition for unitary spaces*

As one can easily see the line of reasoning used in the proof of Theorem 2, it can be repeated for any finite-dimensional vector space $\mathcal{H}$ with scalar product. All we need is a particular representation of elements in this space in the base of the tensor-product form. This is to say that $\mathcal{H}$ has to be of the form $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. Moreover, we do not need Hilbert spaces to spell-out this theorem. We require only for $\mathcal{H}_A$ and $\mathcal{H}_B$ to be finite-dimensional vector spaces over **C** with inner product, i.e. $\mathcal{H}_A$ and $\mathcal{H}_B$ have to be unitary spaces. Thus we can easily reformulate Schmidt decomposition in somehow more universal language.

**Theorem 4.** *Let $\mathcal{H}_A$ and $\mathcal{H}_B$ be unitary spaces. Any element $\mathbf{v} \in \mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ can be represented as*

$$\mathbf{v} = \sum_{i=1}^{k} \sqrt{\lambda_i} \mathbf{u}_i \otimes \mathbf{w}_i, \tag{26}$$

*where vectors $\mathbf{u}_i \in \mathcal{H}_A$ and $\mathbf{w}_i \in \mathcal{H}_B$, $i = 1, 2, \ldots, k$ are mutually orthogonal in respective spaces and $k \leq \min(\dim \mathcal{H}_A, \dim \mathcal{H}_B)$.*

**Proof.** The line of reasoning is analogous to the one used to prove Theorem 2. In this case $\lambda_i$ are singular values of the matrix

$$C_{ij} = (\mathbf{e}_i \otimes \mathbf{e}_j, \mathbf{v}), \tag{27}$$

with $(\cdot, \cdot)$ being scalar product on $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. □

This form of Schmidt decomposition allows us to use it not only for pure states, but also for any space with an introduced scalar product. In many situations it is convenient, however, to use the isomorphism defined by reshaping (or vectorization).

Recently Schmidt decomposition applied to two-qubit unitary gates has been used to study the properties of this particular set.[21] Using this tool it was found, for example, that locally equivalent non-local gates possess the same set of Schmidt coefficients.

### 3.3. *Example: Bipartite density matrices*

In quantum mechanics only a small fraction of states can be represented by normalized vectors in some Hilbert space $\mathbf{C}^n$. Especially when we are interested in interactions of the system in question with the environment, we have to represent the states of the system as density matrices, i.e. positive operators with unit trace.

As an example of Theorem 4 we will use it to analyze the space of bipartite density matrices. Let us start by recalling the definition of bipartite separable state.[22,6]

**Definition 5.** Let $\rho$ be a state of a bipartite quantum system, $\rho \in \mathcal{S}(\mathcal{H}_A \otimes \mathcal{H}_B)$. We say that $\rho$ is *separable* if it can be represented as a convex combination

$$\rho = \sum_{i=1}^{k} p_i \rho_i^{(A)} \otimes \rho_i^{(B)}, \tag{28}$$

with $\sum p_i = 1$, and for all $i = 1, \ldots, k$ we have $\rho_i^{(A)} \in \mathcal{S}(\mathcal{H}_A)$ and $\rho_i^{(B)} \in \mathcal{S}(\mathcal{H}_B)$. If $\rho$ cannot be represented in this form we say that it is *entangled*.

Although the space $\Omega_m \otimes \Omega_n$ of density matrices is not a vector space, we can exploit the linear structure it inherits as a subset of $\mathcal{H}_{\mathrm{HS}} = \mathbb{M}_{mn}$.

Any element $\rho \in \Omega_m \otimes \Omega_n \subset \mathbb{M}_{mn}$ can be written using the standard basis as

$$\rho = \sum_{i=1}^{m^2} \sum_{k=1}^{n^2} C_{ij} \epsilon_i \otimes \varepsilon_j, \tag{29}$$

where $\epsilon_i \in \mathbb{M}_m$, $i = 1, \ldots, m^2$ and $\varepsilon_j \in \mathbb{M}_n$, $j = 1, \ldots, n^2$ are standard bases in respective spaces.

Using Schmidt decomposition 4 we can rewrite $\rho$ as

$$\rho = \sum_{l=1}^{k} \sigma_l \epsilon'_l \otimes \varepsilon'_l, \tag{30}$$

where $\sigma_i$ are singular values of the matrix

$$C_{ij} = \mathrm{tr}\left[\rho^\dagger (\epsilon_i \otimes \varepsilon_j)\right] = \mathbf{res}(\rho)^* \cdot \mathbf{res}(\epsilon_i \otimes \varepsilon_j). \tag{31}$$

This representation can be also obtained using the isomorphism $\mathbb{M}_{mn} \simeq \mathbf{C}^{m^2 n^2}$ and by representing elements of $\mathbb{M}_n$ as vectors in $\mathbf{C}^{m^2 n^2}$ with the help of reshaping operation

$$|X\rangle \stackrel{\mathrm{def}}{=} \mathbf{res}\, X, \tag{32}$$

so that $|X\rangle \in \mathbf{C}^{m^2 n^2}$ for $X \in \mathbb{M}_{mn}$. Using this reasoning one can see directly how to construct base vectors in Eq. (30).[4]

The representation given by Eq. (30) is sometimes referred to as an *operator Schmidt decomposition*,[23] but, as one can see, it provides only an example of the application of Schmidt decomposition as presented in Theorem 4.

## 4. Quantum Channels

Since we aim to apply SVD to quantum channels, we need to introduce some basic facts about them. We restrict ourselves to the finite-dimensional case and the special subclass of trace-preserving (TP) quantum channels.

A state in quantum mechanics is described using density matrices and thus any quantum evolution $\Phi$ has to transform initial density matrix $\rho_{\text{in}} \in \Omega_m$ into density matrix $\Phi(\rho_{\text{in}}) = \rho_{\text{out}} \in \Omega_n$.

### 4.1. *Definitions*

The set of quantum operations has some particular structure.[4,18] First of all we assume that any such map $\Phi : \rho_{\text{in}} \mapsto \rho_{\text{out}}$ has to be linear. This is motivated by the fact that any mixed state can be represented as a convex combination of other states in infinitely many possible ways. The linearity of quantum channel $\Phi$ means that its action does not depend on the particular representation of input density matrix.

The main condition, however, for a linear map to be a proper quantum operation follows from the positivity of input and output states. In order to get more information about the form of $\Phi$ we need to use some physical arguments.

It is clear that any physical map $\Phi$ (i.e. any operation that can be implemented in a laboratory) has to preserve positivity. However, by performing an operation $\Phi$ on our system, we perform $\Phi \otimes \mathbb{1}$ on our system and on environment. As such, any physical map has to be *completely positive* (CP), i.e. any extension of $\Phi$ of the form $\Phi \otimes \mathbb{1}_m$ with $\mathbb{1}_m \in \mathbb{M}_m$ and $m = 1, 2, \ldots$ has to be positive.

**Definition 6.** A map $\Phi$ is called CP if it preserves positivity and for any $n = 1, 2, \ldots$ the map

$$\Phi \otimes \mathbb{1}_n, \tag{33}$$

where $\mathbb{1}_n$ is an identity operation on $n$-dimensional space of states, also preserves positivity.

This definition introduces the Kronecker product of channels, which is described in more details in Sec. 4.3.

Using the above definition we can define a *quantum channel*, which describes the most general form of the evolution of quantum systems.

**Definition 7.** Any CP-map preserving trace is called a *quantum channel* or a *quantum operation*.

We use the isomorphism $\mathbb{M}_{mn} \simeq \mathbf{C}^{m^2 n^2}$ to calculate the elements of its matrix representation. As a linear map any $\Phi : \Omega_n \mapsto \Omega_n$, $\Phi(\rho_{\text{in}}) = \rho_{\text{out}}$, can be written as a matrix $M_\Phi \in \mathbb{M}_{n^2}$

$$\mathbf{res}(\rho_{\text{out}}) = M_\Phi \, \mathbf{res}(\rho_{\text{in}}), \tag{34}$$

where

$$M_\Phi = \{(\epsilon_k, \Phi(\epsilon_l))\}_{k,l=1,\ldots,n^2} = \{\mathrm{tr}[\epsilon_k^\dagger \Phi(\epsilon_l)]\}_{k,l=1,\ldots,n^2}, \tag{35}$$

has $n^4$ elements. Here again we have used the canonical basis $\{\epsilon_k\}_{k=1,\ldots,n^2}$ in $\mathbb{M}_{n^2}$.

Surprisingly more information about the positivity of a given map can be obtained if we represent map $\Phi$ in a specific basis, namely the one obtained as a tensor product of base matrices in subspaces of dimension $n^2$. To exploit this structure we define so-called *dynamical matrix* of the map $\Phi$.

**Definition 8.** Let $\Phi$ be a linear map on $\mathbb{M}_n$. The dynamical matrix for $\Phi$ is defined as a matrix $D_\Phi \in \mathbb{M}_{n^2}$

$$D_\Phi = \{\mathrm{tr}[(\epsilon_i \otimes \epsilon_j) M_\Phi]\}_{i,j=1,\ldots,n}, \tag{36}$$

where $\{\epsilon_i\}_{i=1,\ldots,n}$ is a canonical basis in $\mathbb{M}_n$, or, equivalently

$$D_\Phi = M_\Phi^{R(n,n)}. \tag{37}$$

One should note that the elements of the matrix $D_\Phi$ can be calculated according to the formula

$$\langle (i-1)n+j|D_\Phi|(k-1)n+l\rangle = \mathrm{tr}\big[(\epsilon_i \otimes \epsilon_j)^\dagger \Phi(\epsilon_k \otimes \epsilon_l)\big]. \tag{38}$$

Note that this allows to use a four-index notation as introduced in Ref. 4. This notation allows to express the idea behind reshuffling as (see Ref. 4)

$$\langle k|\Phi(|i\rangle\langle j|)|l\rangle = \langle k \otimes i|D_\Phi|l \otimes j\rangle. \tag{39}$$

For quantum information theory the most important fact expressed using the dynamical matrix is known as *Choi theorem*.[24]

**Theorem 5.** *Linear map $\Phi$ is CP if and only if $D_\Phi$ is positive.*

This theorem allows us to check easily if a given map is CP. The detailed discussion of the CP conditions is presented in Refs. 4 and 18 for one-qubit quantum channels and in Ref. 25 for one-qutrit channels.

**Example 3.** The operation of matrix transposition $T(\rho) = \rho^T$ on $\mathbf{C}^2$ can be expressed as

$$M_T = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{40}$$

which is equivalent to SWAP for a two-qubit system. In this case we have $D_T = M_T^R = M_T$ and, since the spectrum of this matrix is $\{-1, 1, 1, 1\}$, we can see that the transposition is not CP.

In general, the transposition operation can be introduced on $\mathbb{M}_{m,n}$. The general form of this operation is given by the following theorem.[13]

**Theorem 6.** *For a matrix $A \in \mathbb{M}_{mn}$ there exists a unique matrix $P(m, n)$ such that*

$$\mathbf{res}\, A^T = P(m, n)\, \mathbf{res}\, A \tag{41}$$

*given by formula*

$$P(m, n) = \sum_{i=1}^{m} \sum_{j=1}^{n} \epsilon_{ij} \otimes \epsilon_{ij}^{T} \tag{42}$$

*where $\{\epsilon_{ij}\}$, with $i = 1, \ldots, m$ and $j = 1, \ldots, n$ is a standard basis in $\mathbb{M}_{mn}$ and $P(m, n)$ is a permutation matrix.*

Note that, as it preserves the spectrum, the transposition is a positive map. Operations which are positive, but not CP, play an important role in quantum information theory since they are used to detect quantum entanglement.[6]

Another interesting feature of quantum theory is the correspondence between quantum states and quantum channels.[26]

The dynamical matrix for the operations $\Phi$ is defined as $D_\Phi = M_\Phi^R$, where "$R$" denotes a *reshuffling* operation.[4] The dynamical matrix for the TP operation acting on $N$-dimensional system is an $N^2 \times N^2$ positive defined matrix with trace $N$. We can introduce the natural correspondence between such matrices and density matrices on $N^2$ by normalizing $D_\Phi$. Such a correspondence is known as *Jamiołkowski isomorphism.*[26,27]

Let $\Phi$ be a completely positive map acting on density matrices. We define Jamiołkowski matrix of $\Phi$ as

$$\rho_\Phi = \frac{1}{N} D_\Phi. \tag{43}$$

Jamiołkowski matrix has the same mathematical properties as a quantum state i.e. it is a semi-definite positive matrix with a trace equal to one. It is sometimes referred to as *Jamiołkowski operation matrix.*[27]

### 4.2. *Kraus decomposition*

Now we are ready to use the SVD to obtain a special representation of quantum channels known as the *Kraus form* as we will see the Kraus decomposition of an operation obtained as Schmidt decomposition of its linear representation.

Let us now consider quantum channel $\Phi$ acting on $\Omega_n$. Its matrix representation $M_\Phi$ is an element of $\mathbb{M}_{n^2}$ and so is its dynamical matrix $D_\Phi$.

One can represent $D_\Phi$ in the basis

$$\{\epsilon_i \otimes \epsilon_j : i, j = 1, \ldots, n^2\}, \tag{44}$$

composed of tensor products of elements of canonical bases in $\mathbb{M}_n$. We get

$$M_\Phi = \sum_{i=1}^{n^2} \sum_{j=1}^{n^2} D_{\Phi_{ij}} \epsilon_i \otimes \epsilon_j. \tag{45}$$

By taking into account the fact that the matrix $D_\Phi$ is positive and by using Schmidt decomposition (Theorem 4) we get

$$M_\Phi = \sum_{i=1}^{k} \sigma_i \kappa_i \otimes \kappa_i^*, \tag{46}$$

where $\kappa_i$, $i = 1, \ldots, k$ are mutually orthogonal elements of Hilbert$-$Schmidt space of operators. Recall that $M_\Phi$ acts on $\rho \in \Omega_n$ according to Eq. 34. Combining this with Property 2 we get

$$\mathbf{res}(\rho_{\text{out}}) = \mathbf{res}\Phi(\rho_{\text{in}}) = M_\Phi \, \mathbf{res}(\rho_{\text{in}}) = \sum_{i=1}^{k} \sigma_i \kappa_i \otimes \kappa_i^* \mathbf{res}(\rho_{\text{in}})$$

$$= \sum_{i=1}^{k} \sigma_i \, \mathbf{res}(\kappa_i \rho_{\text{in}} \kappa_i^\dagger) = \mathbf{res}\left( \sum_{i=1}^{k} \sigma_i \kappa_i \rho_{\text{in}} \kappa_i^\dagger \right). \tag{47}$$

Thus we have obtained the following representation of quantum channels.

**Theorem 7.** *Any CP map $\Phi : \Omega_N \to \Omega_N$ can be represented as*

$$\Phi(\rho) = \sum_{i=1}^{k} \sigma_i \kappa_i \rho \kappa_i^\dagger, \tag{48}$$

*where $\kappa_i$ are un-reshaped singular vectors of $D_\Phi$ and $\sigma_i$ are singular values of $D_\Phi$.*

For an alternative proof based on Stinespring dilatation theorem see e.g. Ref. 18.

Operators $\{K_i = \sqrt{\sigma_i} \kappa_i : i = 1, 2, \ldots, k\}$ in the above decomposition are known as *Kraus operators*.

The Kraus form of a quantum channel is non-unique. We can choose another set of operators $\{\nu_i : i = 1, \ldots, l\}$ such that it represents an action of channel $\Phi$, i.e.

$$\Phi(\rho_{\text{in}}) = \sum_{i=1}^{l} \nu_i \rho_{\text{in}} \nu_i^\dagger. \tag{49}$$

Operators $K_i = \sqrt{\sigma_i} \kappa_i$ are usually referred to as canonical Kraus operators.

**Example 4.** Let us consider the completely depolarizing channel $\Delta_{n,p} : \Omega_n \mapsto \Omega_n$[28] defined as

$$\Delta_{n,p}(\rho) = p\rho + (1 - p) \frac{\mathbb{1}}{n} \operatorname{tr} \rho, \tag{50}$$

with $n = 1, 2, \ldots$ and $0 \le p \le 1$. A depolarizing channel acting on initial state

$$\rho_{\text{in}} = \begin{pmatrix} a & b + ic \\ b - ic & 1 - a \end{pmatrix} \tag{51}$$

results in an output state

$$
\rho_{\text{out}} = \begin{pmatrix} \frac{1}{2} + \left(a - \frac{1}{2}\right)p & (b+ic)p \\ (b-ic)p & \frac{1}{2} - \left(a - \frac{1}{2}\right)p \end{pmatrix}. \tag{52}
$$

In one-qubit case the dynamical matrix of $\Delta_{2,p}$ reads

$$
D_{\Delta_{2,p}} = \begin{pmatrix} \frac{p+1}{2} & 0 & 0 & p \\ 0 & \frac{1-p}{2} & 0 & 0 \\ 0 & 0 & \frac{1-p}{2} & 0 \\ p & 0 & 0 & \frac{p+1}{2} \end{pmatrix}, \tag{53}
$$

and it has singular values

$$
\left\{ \frac{p}{2}, \frac{p}{2}, \frac{p}{2}, \frac{1}{2}(4-3p) \right\}. \tag{54}
$$

Un-reshaped singular vectors of $D_{\Delta_{2,p}}$ are

$$
\left\{ \begin{pmatrix} -\frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} \end{pmatrix} \right\}, \tag{55}
$$

and we obtain the following collection of Kraus operators

$$
\left\{ \begin{pmatrix} -\frac{\sqrt{p}}{2} & 0 \\ 0 & \frac{\sqrt{p}}{2} \end{pmatrix}, \begin{pmatrix} 0 & \sqrt{\frac{p}{2}} \\ 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 \\ \sqrt{\frac{p}{2}} & 0 \end{pmatrix}, \begin{pmatrix} \frac{1}{2}\sqrt{4-3p} & 0 \\ 0 & \frac{1}{2}\sqrt{4-3p} \end{pmatrix} \right\}. \tag{56}
$$

It can be also easily checked that $\Delta_{2,p}$ can be also represented by Kraus operators[2]

$$
\left\{ \frac{\sqrt{1+3p}}{2} \mathbb{1}, \frac{\sqrt{1-p}}{2}\sigma_x, \frac{\sqrt{1-p}}{2}\sigma_y, \frac{\sqrt{1-p}}{2}\sigma_z \right\}, \tag{57}
$$

where $\sigma_x, \sigma_y$ and $\sigma_z$ are Pauli matrices. This representation is more appealing from the physical point of view.

Using Kraus representation we can characterize specific types of quantum channels. First of all we can distinguish a class of TP operations.

**Definition 9.** A channel $\Psi$ given as a collection of Kraus operators $\{A_i\}_{i=1}^n$ is TP if

$$\sum_{i=1}^n A_i A_i^\dagger = \mathbb{1}. \tag{58}$$

Another important class of quantum channels are random unitary channels.

**Definition 10.** A channel $\Phi$ is called a *random unitary* if it can be represented as

$$\Phi(\rho) = \sum_{i=1}^k p_i U_i \rho U_i^\dagger, \tag{59}$$

where operators $U_i, i = 1, \ldots, k$ are unitary, $0 \leq p_i, i = 1, \ldots, k$ and $\sum_i p_i = 1$.

An important example of a random unitary channel is given by *generalized Pauli channel*,[28] which is an extension to any dimension of the one-qubit Pauli channel.

**Example 5.** We define two families of unitary operators:

$$X_d = \sum_0^{d-1} |j - 1 \bmod d\rangle\langle j|, \tag{60}$$

and

$$Z_d = \mathrm{diag}(1, e^{2i\pi/d \times 1}, \ldots, e^{2i\pi/d \times (d-1)}). \tag{61}$$

The action of generalized Pauli channel $\Pi_d$ of dimension $d$ is defined as

$$\Pi_d(\rho) = \sum_{i,j=0}^{d-1} p_{i,j} X_d^i Z_d^j \rho (X_d^i Z_d^j)^\dagger, \tag{62}$$

where $0 \leq p_{i,j} \leq 1$ and $\sum p_{i,j} = 1$.

Generalized Pauli channel is an example of unital channel, i.e. it satisfies the condition $\Pi_d(\mathbb{1}) = \mathbb{1}$.

## 4.3. *Composition of channels*

To this point we have been dealing with simple quantum channels (i.e. channels acting on the whole analyzed system) only. However, some features unique to quantum information theory can be observed when one deals with *composite* quantum channels.

Choi Theorem 5 deals with the extensions of a given map to a higher-dimensional space. Such extensions are maps on $\mathbb{M}_m \otimes \mathbb{M}_n$.

**Definition 11.** Let $\Phi$ and $\Psi$ be quantum channels. Quantum channel $\Phi \otimes \Psi$ is defined using its matrix representation as

$$M_{\Phi \otimes \Psi} = M_{R^{-1}}(M_\Phi \otimes M_\Psi)M_R, \tag{63}$$

where $M_{R^{-1}} = M_R^{-1} = M_R$ is the matrix representation of the reshuffling map $\rho \mapsto \rho^R$ given in Eq. (15) or, equivalently, as a channel acting on the initial state $\rho$ as

$$\mathbf{res}((\Phi \otimes \Psi)(\rho)) = (M_\Phi \otimes M_\Psi(\mathbf{res}(\rho^R)))^R. \tag{64}$$

As the reshuffling operation represents the exchange between canonical and tensor-product base, this definition is simply the standard definition known from the standard multi-linear algebra.

### 4.4. *Partial operations*

Representation (63) can be used to calculate composition $\Phi \otimes \Psi$ of any two quantum channels $\Phi$ and $\Psi$. If we take one of them to be identity $\Psi = \mathbb{1}$ we get so-called *partial operations*.

**Definition 12.** Let $\Phi$ be a quantum channel acting on $m$-dimensional state space. We say that the channel

$$\Phi \otimes \mathbb{1}_n \tag{65}$$

is a partial application of $\Phi$ on $m \times n$-dimensional space or that it is an extension of $\Phi$ to $m \times n$-dimensional space.

Partial operations are used extensively in quantum information theory, especially in the context of quantum entanglement.[5]

Let us return to the transposition operation on one-qubit system and let us see how it behaves under the extension to a two-qubit system.

**Example 6.** We define a partial transposition on the first subsystem as $T_1 = T \otimes \mathbb{1}_2$. This map has a matrix representation

$$M_{T_1} = M_{R^{-1}}(M_T \otimes \mathbb{1}_4)M_R, \tag{66}$$

where $M_R = M_R^{-1}$ is a matrix representation of the reshuffling operations given by Eq. (15) and matrix representation of transposition $M_T$ is given by Eq. (40). In this case

$$M_{T_1} = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1
\end{pmatrix}. \tag{67}$$

See Appendix for more examples.

The operation of partial transposition is important in quantum information theory due to the Peres−Horodecki criterion for distinguishing separable and entangled states. In the particular case of $\mathbf{C}^2 \otimes \mathbf{C}^2$ system (i.e. two qubits), this criterion states that the state $\rho \in \mathcal{S}(\mathbf{C}^2 \otimes \mathbf{C}^2)$ is separable if and only if $\rho^{T_1}$ is positive.

## 5. Summary

We have presented a simple derivation of Schmidt decomposition for pure states and density matrices and Kraus decomposition for quantum channels. Using matrix reordering one can easily construct matrices corresponding to the composition of quantum channels. In particular we have discussed partial operations, which play a prominent role in quantum information theory.

The main advantage of the presented formulae is that they can be used directly in computer algebra systems. Full implementation of the procedures discussed in this report can be found in the source code of the *Mathematica* package.[29] For the sake of consistency we provide some examples of the discussed procedures in Appendix A.

## Appendix A. Examples in *Mathematica*

Below we provide some examples of the discussed procedures using *Mathematica* computing system (see e.g. Ref. 30 for an introduction to *Mathematica*). The following examples are based on the `QI` package for *Mathematica*, which can be freely downloaded from the project home page. This package provides the implementation of various procedures helpful during the calculation related to quantum information processing. For the full list of functions implemented in this package see Ref. 29.

After the proper installation the package can be loaded as

```
<<QI`
```

After loading the package one should get some information about the used version and release date. The examples provided in this report were tested with the version 0.3.21 of the package.

### A.1. *Matrix reorderings*

`QI` Package provides four functions for the matrix operations described in Sec. 2.

- `Res` — reshaping operation,
- `Vec` — vectorization operation,
- `Unres` — inverse map for reshaping,
- `Unvec` — inverse map for vectorization.

In the above functions it is assumed that vectors can be rearranged into square matrices. Nevertheless, it is possible to rearrange a vector into a general $m \times n$ matrix by specifying the second argument in `Unres` and `Unvec` functions.

In the simple case of $\mathbb{M}_4$ we can use the above functions as

```
mA = SymbolicMatrix[a, 4];
vA = Res[mA];
mB = SymbolicMatrix[b, 4];
vB = Vec[mB];
```

Here function `SymbolicMatrix[a,4]` returns $4 \times 4$ matrix filled with elements $a_{i,j}$.

The reshuffle operation can be implemented directly using the Definition 2. Unfortunately this implementation is inefficient as it requires the calculation of $m^2 \times k^2$ matrix elements in order to reshuffle the matrix from $\mathbb{M}_{mk}$.

`QI` Package provides three methods for performing the reshuffle operation in matrices:

- `Reshuffle` — functions based on the Definition 2 and can be used to construct the reshuffle matrix,
- `ReshuffleGeneral` — functions based on the index manipulation and can be used to reshuffle matrices which are not necessarily square,
- `ReshufflePermutation` — can be used to construct permutation matrices for reshuffling operation.

For example with

```
mA = SymbolicMatrix[a, 4];
mR = ReshufflePermutation[2, 2];
```

the following should return `True`

```
Unres[mR.Res[mA]] == Reshuffle2[mA, 2, 2];
```

Each function implementing the reshuffle operation has an equivalent function implementing the alternative reshuffling given by Definition 3 (e.g. `Reshuffle` and `Reshuffle2`).

### A.2. *Schmidt decomposition*

Usually Schmidt decomposition is used in the context of vectors (i.e. elements of $\mathbf{C}^N$). If we define maximally entangled pure state as

```
vA = MaxEnt[4]
```

we can obtain its Schmidt decomposition as

```
vAsd = SchmidtDecomposition[vA, 2, 2];
```

The initial vector can be reconstructed as

```
Plus @@ Table[
  vAsd[[i]][[1]](vAsd[[i]][[2]]⊗vAsd[[i]][[3]])
  {i, 1, 2}
]
```

The meaning of the "⊗" symbol is defined in the `QI` package to provide the required shape of the output.

To demonstrate Schmidt decomposition on the space of matrices we use the maximally entangled mixed state on $\mathbb{M}_n(4)$.

```
mA = Proj[MaxEnt[4]];
```

Its decomposition can be obtained as

```
mAsd = SchmidtDecomposition[mA, 2, 2];
```

The initial matrix can be easily reconstructed.

```
Plus @@ Table[
  mAsd[[i]][[1]](mAsd[[i]][[2]]⊗mAsd[[i]][[3]]),
  {i, 1, 4}
]
```

Note that `SchmidtDecomposition` function works for vectors as well as for matrices. However, it is possible to use `VectorSchmidtDecomposition` and `OperatorSchmidtDecomposition` for an appropriate input instead.

### A.3. *Quantum channels*

`QI` Package defines quantum channels using *pure functions* mechanism. For example, the transposition map can be implemented as

```
TransposeChannel =
 IdentityMatrix[#1].Transpose[#2]&;
```

and its matrix representation can be obtained as

```
mT = ChannelToMatrix[TransposeChannel[#]&, 4];
```

for a map acting on $\mathbb{M}_4$.

Similar construction for the swap operation reads

```
SwapChannel = Swap[#1].(#2).Swap[#1] &;
```

and this function requires information about the system dimension. Here we have used the `SWAP` gate predefined in the package. For example the SWAP operation on two qubits is defined as

```
cS4 = SwapChannel[4,#];
```

Again, one can obtain a matrix representation of this channel as

```
mS = ChannelToMatrix[cS4, 4];
```

Alternatively, the same result can be obtained using

```
mS = Superoperator[cS4, 4];
```

### A.3.1. *Spontaneous emission channel for qutrits*

Following Ref. 31, `QI` package provides a definition of a spontaneous emission channel for a three-level system (qutrit).

```
seK = QutritSpontaneousEmissionKraus[A1,A2,t];
```

Here `A1` and `A2` are Einstein coefficients.

This channel was used as e.g. in Ref. 32 to investigate the behavior of quantum games under decoherence.

The superoperator corresponding to the above channel can be obtained as

```
seS = Superoperator[seK];
```

Note that the `Superoperator` function has two forms and can be used to obtain matrix representation of the channel either from the list of Kraus operators or from the pure function.

### A.3.2. *Partial operations*

The notion of partial operation is very common in quantum information theory and the presented package allows to construct and analyze such operations in a very straightforward manner.

Let us consider an operation $\Psi$ on $n$-dimensional system defined as a pure function `fPsi`. In order to obtain the operation $\Psi \otimes \mathbb{1}$ acting on $n \times m$-dimensional system one needs to

- construct the matrix representation of the map $\Psi$:

  ```
  sPsi = Superoperator[fPsi,n]
  ```

- construct the reshuffle matrix in order to transform the obtained matrix to a new base matrix of the appropriate size:

  ```
  mR = ReshufflePermutation[n n, m m]
  ```

- use the matrix `sPsi` according to the Definition 11, using the $\mathbb{1}$-channel on the second subsystem:

  ```
  extPsi = mR.(sPsi ⊗ IdentityMatrix[m^2]).mR
  ```

The extension of the operation constructed in the above procedure acts on the $n \times m$-dimensional states $\rho$ as

```
Unres[extPsi.Res[ρ]]
```

Note that this procedure requires to construct a matrix of dimension which grows like $\mathcal{O}(n^4)$ and can be slow for larger systems.

The simplest case of such construction is the partial transposition on $n^2$-dimensional space. The matrix representation of the transposition operation of dimension $n$, is a SWAP operation on $n^2$-dimensional system. The matrix representation of the partial transposition can be obtained as

```
mR = ReshufflePermutation[n n, n n];
tA = mR.(Swap[n n]⊗IdentityMatrix[n n]).mR
```

Similar procedure is implemented in `QI` as `PartialTraceA` function. However, as this implementation is not very efficient, `QI` provides an alternative version of this operation as a `PartialTraceGeneral` function, which operates on indices. For example, for a given matrix

```
mA = SymbolicHermitianMatrix[a, 4]
```

the results of

```
PartialTraceA[mA, 2, 2]
```

and

```
PartialTraceGeneral[mA, 2, 2, 1]
```

are identical.

The matrix representation of the partial transposition with respect to the first subsystem, given in Eq. (67), can be obtained as

```
Superoperator[PartialTransposeA[#, 2, 2] &, 4]
```
Here `PartialTransposeA[#,2,2]` is a map which is not positive.

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