On orthogonal bases in the Hilbert-Schmidt space of matrices

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Abstract
Decomposition of (finite-dimensional) operators in terms of orthogonal bases of matrices has been a standard method in quantum physics for decades. In recent years, it has become increasingly popular because of various methodologies applied in quantum information, such as the graph state formalism and the theory of quantum error correcting codes, but also due to the intensified research on the Bloch representation of quantum states. In this contribution we collect various interesting facts and identities that hold for finite-dimensional orthogonal matrix bases.

1. Introduction
Expansions of finite-dimensional matrices in terms of an orthogonal basis of matrices as a method is ubiquitous in quantum physics, although it is often not explicitly mentioned (e.g., [1–11]). In the past few decades, with the upcoming field of quantum information, there has been increasing attention to techniques based on matrix expansions, for example, in measurement-based quantum computation [12], the formalism of quantum error correcting codes [13–15], the graph state formalism [16], and entanglement theory [17–19]. There is also a renewed interest in the Bloch representation, i.e., a decomposition of the density operators of (usually) multipartite quantum states in terms of matrix bases [20–33].

We start by introducing the most frequently used matrix bases and then discuss the transformation between arbitrary bases. Subsequently we analyze the matrix expansions of the two most important operators in this context, the SWAP operator and the projector onto the Bell state, which give rise to identities containing sums of products of two basis elements. But there exist also relations for products with a larger number of factors. Finally we consider the explicit matrix representations of various interesting maps. We elucidate the simple relations between all these identities and hope to render transparent their sometimes surprising structure.

2. Orthogonal bases of matrices
2.1. Definitions and frequently applied matrix bases
In the following we discuss bases of the space $\mathcal{B}(\mathcal{H}_d)$ of bounded linear operators acting on a $d$-dimensional Hilbert space $\mathcal{H}_d$. The Hermitian adjoint of an operator $A \in \mathcal{B}(\mathcal{H}_d)$ is denoted by $A^\dagger$. The space $\mathcal{B}(\mathcal{H}_d)$ is endowed with the Hilbert-Schmidt inner product

$$\langle A, B \rangle_{\text{HS}} = \text{Tr}(A^\dagger B),$$

where $\text{Tr}$ denotes the trace. Correspondingly, the norm induced by this inner product is called the Hilbert-Schmidt norm (also known as the Frobenius norm). An operator basis in $\mathcal{B}(\mathcal{H}_d)$ has $d^2$ elements, therefore it can be represented by a $d \times d$ matrix. We will use the terms ‘operator’ and ‘matrix’ interchangeably, as it is common in the context of finite-dimensional quantum mechanics. For the elements of the vector space $\mathcal{H}_d$ and the expansion of matrices in a given basis we will use the Dirac bra-ket notation. That is, vectors $\psi \in \mathcal{H}_d$ are written...
as kets $|\psi\rangle$, whereas the elements $\varphi^*$ of the dual space $(\mathcal{H}_d)^*$ are denoted as bras, $\langle \varphi |$. A rank-1 matrix $\psi\varphi^*$ is written as the outer product $|\psi\rangle\langle\varphi|$. The standard basis in $\mathcal{H}_d$ is called the computational basis and denoted by $\{|j\rangle\}$, $j = 0, \ldots (d - 1)$.

To start with an example, an operator (or matrix) basis every physicist is familiar with is given by the Pauli matrices together with the $2 \times 2$ identity matrix, an orthogonal basis for $\mathcal{B}(\mathcal{H}_d)$ in the case $d = 2$,

$$
\begin{align*}
\sigma_0 &= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \\
\sigma_1 &= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \\
\sigma_2 &= \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \\
\sigma_3 &= \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix},
\end{align*}
$$

with the normalization

$$
\text{Tr}(\sigma_j\sigma_k) = 2\delta_{jk}.
$$

A well-known application of this basis is the expansion of a density matrix $\rho^{(2)}$ of a two-level system, the so-called Bloch representation for a qubit,

$$
\rho^{(2)} = \frac{1}{2} \sum_j r_j \sigma_j,
$$

with real coefficients $r_j$ and $r_0 = 1$. There is an obvious second possibility to expand $\rho^{(2)}$ that makes reference to the basis of the Hilbert (vector) space it acts on, the computational basis $\{|0\rangle, |1\rangle\}$,

$$
\rho^{(2)} = \begin{bmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{bmatrix} = \sum_{j,k=0}^1 \rho_{jk} |j\rangle\langle k|.
$$

That is, also the elements

$$
\tilde{e}_{00} = |0\rangle\langle 0|, \quad \tilde{e}_{01} = |0\rangle\langle 1|, \\
\tilde{e}_{10} = |1\rangle\langle 0|, \quad \tilde{e}_{11} = |1\rangle\langle 1|,
$$

form an orthogonal basis of $\mathcal{B}(\mathcal{H}_d)$, however, with normalization $\text{Tr}(\tilde{e}_{jk}\tilde{e}_{km}) = \delta_{jk}\delta_{km}$. This is the so-called standard basis.

By comparing equations (2) and (6) we note that often for the enumeration of a matrix basis a single index $j = 0 \ldots (d^2 - 1)$ is used (for example, also for $\lambda_1 \ldots \lambda_8$, the Gell-Mann matrices in $d = 3$). On the other hand, the standard basis indicates that two indices would be a more natural choice (or equivalently a two-digit base-$d$ number). Throughout this paper we will adhere to the two-index enumeration.

For the sake of completeness we include here the general definitions for three frequently used matrix bases in $d$ dimensions: the standard matrix basis, the Gell-Mann basis, and the Weyl operator basis. Importantly, we will normalize all the matrix bases to the dimension $d$. As the basis of the underlying Hilbert (vector) space $\mathcal{H}_d$ we use the computational basis $\{|0\rangle, |1\rangle \ldots |d-1\rangle\}$. In contrast to the Hilbert space $\mathcal{H}_d$ we refer to $\mathcal{B}(\mathcal{H}_d)$ as the Hilbert–Schmidt space.

The standard matrix basis. It is straightforward to generalize equation (6) to obtain the standard basis in $d$ dimensions (yet with different normalization),

$$
e_k = \sqrt{d} |j\rangle\langle k|, \quad j = k = 0, 1 \ldots (d - 1).
$$

The (generalized) Gell-Mann basis. The only matrix of this basis with non-vanishing trace is $\Lambda_{00}^{(d)} \equiv I_d$. The other $(d^2 - 1)$ traceless elements are Hermitian and correspond to the generators of SU($d$). They are defined by

$$
\begin{align*}
\Lambda_{kl}^{(d)} &\equiv x_{kl} = \sqrt{\frac{d}{2}} \left(|k\rangle \langle l| + |l\rangle \langle k|\right), \\
\Lambda_{lk}^{(d)} &\equiv y_{kl} = \sqrt{\frac{d}{2}} \left(-i|k\rangle \langle l| + i|l\rangle \langle k|\right), \\
\Lambda_{jl}^{(d)} &\equiv z_{jl} = \sqrt{\frac{d}{l(l+1)}} \left(-i|l\rangle \langle j| + \sum_{j=0}^{l-1} |j\rangle \langle j|\right),
\end{align*}
$$

with $k < l = 1 \ldots (d - 1)$. The Pauli basis is a special case of the Gell-Mann basis for $d = 2$. Note that the ordering as well as the normalization in $d = 3$ is different from the standard one used in high-energy physics.

The Weyl operator basis. Another highly interesting basis was introduced in the quantum mechanics context by Weyl [34] and discussed also by Schwinger [3]. It consists of unitary matrices which are generated by the clock operator $Z$ and the shift operator $X$,
\[
Z\hat{j} = \omega^j \hat{j}, \quad X\hat{j} = |j + 1\rangle,
\]
where \(\omega = e^{2\pi i/d}\) and the addition is taken mod \(d\). The basis elements are defined as
\[
D_{jk} = Z^j X^k \omega^{-\frac{j+k}{2}}, \quad j, k = 0 \ldots (d - 1).
\]
These operators are traceless. Moreover, they have a group structure. Also here, the Pauli matrices arise as the special case \(d = 2\), that is, they are both Hermitian and unitary.

There is an interesting observation regarding these three bases. Each of them can be divided in two subsets, one of \(d\) diagonal and the other of \(d(d - 1)\) matrices with vanishing main diagonal. Another noteworthy aspect is the difference between the standard matrix basis on the one hand, and Gell-Mann basis as well as Weyl operators on the other: While the latter contain —except the identity matrix —only traceless elements the former has several elements with nonvanishing trace. This property singles out matrix bases of \((d^2 - 1)\) traceless elements (such as the Gell-Mann and the Weyl operator bases) for the use in the Bloch decomposition of density matrices, in particular of multipartite states. The reason is that the expansion into traceless operators generates a structure into so-called sectors and subsectors \([32, 33]\) that clearly specify which parts of the expansion describe the reduced state across any possible cut in the set of parties.

2.2. Transformation between matrix bases
A natural question is: What is the rule according to which two matrix bases transform into one another? The answer is straightforward. Suppose we are given two orthogonal matrix bases \(\{g_{jk}\}\) and \(\{h_{lm}\}\), \(j, k, l, m = 0\ldots (d - 1)\), with
\[
\text{Tr}(g_{jk}^\dagger h_{lm}) = d \delta_{jj'} \delta_{kk'},
\]
\[
\text{Tr}(h_{lm}^\dagger h_{mn}) = d \delta_{ll'} \delta_{mm'},
\]
and a \(d^2 \times d^2\) matrix \(S\),
\[
h_{jk} = \sum_{lm} S_{jk,lm} g_{lm}.
\]
Note that this relation does not describe an action of \(S\) on the \(g_{lm}\). It simply is the coefficient matrix that determines the linear combinations of the \(g_{lm}\) to produce the new basis elements \(h_{jk}\). Application of the orthogonality relations yields
\[
\delta_{jj'} \delta_{kk'} = \sum_{lm} S_{jk,lm}^\dagger S_{j'k',lm},
\]
which is nothing but the definition of a unitary matrix acting on a two–party space \(\mathbb{C}^d \otimes \mathbb{C}^d\). What is of particular interest for the following is the transformation between an arbitrary basis \(\{g_{jk}\}\) and the standard basis,
\[
g_{jk} = \sqrt{d} \sum_{lm} U_{jk,lm} |l\rangle\langle m|, \tag{13a}
\]
\[
\sqrt{d} |j\rangle\langle k| = \sum_{lm} U_{j'k,lm}^\dagger g_{lm}, \tag{13b}
\]
with a two–party unitary matrix \(U\) \([35, 36]\) as described above. If \(\{g_{jk}\}\) has the property that there are \(d\) diagonal elements and the others with vanishing diagonal, the matrix \(U\) has block structure: There is a \(d \times d\) block \(\mathcal{D}\) transforming between the diagonal elements of \(\{g_{jk}\}\) and the \(|l\rangle\langle l|, l = 0\ldots (d - 1)\), and another \(d(d - 1) \times d\) \((d - 1)\) block \(\mathcal{O}\) for the offdiagonal elements.

3. SWAP operator and maximally entangled state
In this section we analyze various matrix decompositions that are related to the SWAP operator. As the SWAP decomposition is one of the most frequently occurring ‘tricks’ it is the appropriate example to highlight the fact that the origin of the structure of many matrix basis expansions is the unitary transformation law, equation \(13\).

3.1. Decomposition of the SWAP operator
The SWAP operator exchanges the parties of a pure two–party product state. Let \(|\psi\rangle, |\varphi\rangle \in \mathcal{H}_d\), then
\[
\text{SWAP} |\psi\rangle \otimes |\varphi\rangle = |\varphi\rangle \otimes |\psi\rangle.
\]
By applying equations (12), (13) we find the decomposition in another matrix basis \( \{ g_{lm} \} \),
\[
\text{SWAP} = \frac{1}{d} \sum_{jklmpq} U^+_{jkl,m} g_{lm} \otimes (U^+_{j:lpq} g_{pq})^\dagger = \frac{1}{d} \sum_{lm} g_{lm} \otimes g_{lm}^*.
\]

The dagger in equation (16) could equally well be assigned to the first tensor factor. The simplicity of the ‘diagonal’ decomposition in any orthogonal matrix basis hinges upon the unitarity of the transformation matrix \( U \). It is the same reason why the maximally entangled state has the same form for any local basis (and therefore is called ‘isotropic’ [37]). While the decomposition in equation (16) might appear surprising, the unitarity of \( U \) implies that it can be read as if it were written in the standard matrix basis—where it is not surprising at all.

We may comment also on the case that the unitary \( U \) has the block structure discussed in section 2.2 and the basis \( \{ g_{jk} \} \) can be subdivided in diagonal and strictly offdiagonal matrices. By appropriately choosing the order of the columns in \( U \) we can achieve that the matrices \( g_{jj} \) are diagonal and
\[
g_{jj} = \sqrt{d} \sum_k D_j |k\rangle \langle k|\text{ with the unitary } d \times d \text{ matrix } D.\]

An analogous expression can be found for the offdiagonal part of SWAP.

The two-party property of SWAP gives rise to another interesting relation if we apply the partial trace, e.g., on the first party on the left-hand side of equation (16),
\[
d \text{ Tr}[ \text{SWAP} ] = \sum_{lm} \text{Tr}(g_{lm}^*) \otimes g_{lm} = d \quad 1_d,
\]

where \( T \) denotes the transposition. Tracing out the remaining party leads to
\[
d^2 = \sum_{lm} | \text{Tr}(g_{lm}^*) |^2 .
\]

Finally, by looking at equation (15) one might wonder whether it is possible to get an analogous matrix expansion also for the identity operator \( \mathbf{1}_d \otimes \mathbf{1}_d = \sum_{jk}|j\rangle \langle j| \). The answer is affirmative and can be found by exploiting the relation
\[
\text{SWAP} \cdot \text{SWAP} = \mathbf{1}_d \otimes \mathbf{1}_d.
\]

Substituting equation (16) gives
\[
\mathbf{1}_d \otimes \mathbf{1}_d = \frac{1}{d^2} \sum_{jklab} g_{ab}^\dagger \cdot g_{kl} \otimes g_{ab} \cdot g_{kl}^\dagger,
\]

where again several combinations of placing the daggers are possible. The structure of this equation is somewhat unexpected, because in general a matrix basis does not have group properties, that is, the products \( \hat{g}_{ab} \cdot \hat{g}_{kl} \) bear no obvious relation with one another and in particular do not reproduce the elements of a basis (consider the case, e.g., that the \( g_{jk} \) are the Gell-Mann matrices). Also here we can take the partial trace as in equation (19) and

\[\text{1 In a high-energy physics context (e.g., [38]) this relation is often called the completeness relation for the generators of SU(d) and spelled out in components (the dagger could be dropped because of the hermiticity of the generators)}\]
obtain

\[ d^1 \mathbf{1}_d = \sum_{jkab} \text{Tr} (\mathbf{g}_{jk}^d \cdot \mathbf{g}_{jk}^d), \]

\[ d^2 \mathbf{1}_d = \sum_{jk} \mathbf{g}_{jk} \cdot \mathbf{g}_{jk}^d. \]

(24)

### 3.2. Further results related to the SWAP operator

There is an intriguing identity including the SWAP operator [39], which is at the heart of the Choi-Jamiolkowski isomorphism, namely

\[ \text{Tr}_{[2]}(A \otimes B \cdot \text{SWAP}) = A \cdot B, \]

(25)

with single-party operators \( A, B \in \mathcal{B}(\mathcal{H}_d) \). It is readily verified by expanding SWAP in the standard matrix basis. This is also helpful to elucidate the workings of this relation: \( \text{Tr}_{[2]}(A \otimes B \cdot \text{SWAP}) = \sum_{ijkl} A_{ij} |j\rangle |k\rangle \langle j| \langle k| B_{kl} = \sum_{jk} A_{jk} |j\rangle |k\rangle B_{jk} |j\rangle |k\rangle. \)

Alternatively, we may look at equation (25) from the point of view of the decomposition equation (16). To this end, it is useful to keep in mind the Bloch representation of \( B \) in the matrix basis \( \{ \mathbf{g}_{jk} \} \),

\[ B = \frac{1}{d} \sum_{jk} b_{jk} \mathbf{g}_{jk}, \quad b_{jk} = \text{Tr} (\mathbf{g}_{jk}^d B), \]

(26)

\[ \text{Tr}_{[2]}(\mathbb{I} \otimes B \cdot \text{SWAP}) = \frac{1}{d} \sum_{jk} \mathbf{g}_{jk} \cdot \text{Tr} (B \cdot \mathbf{g}_{jk}^d) = B, \]

(27)

so that equation (27) can be interpreted in the sense of decomposing \( B \) into its Bloch components on the second party and rebuilding it on the first (and equation (25) follows trivially through multiplication by \( A \) from the left).

If we set \( A = B^\dagger \) and take the trace over both parties separately in equation (25) we immediately find with the matrix decomposition of SWAP

\[ \text{Tr} (B^\dagger \otimes B \cdot \text{SWAP}) = \frac{1}{d} \sum_{jk} |b_{jk}|^2 = \text{Tr} (B^\dagger B), \]

(28)

which links the length of the Bloch vector of \( B \) to the purity of the operator.

Proceeding along these lines we can combine equations (16), (22) and (25),

\[ d^2 \mathbf{1}_d = d \text{Tr}_{[2]}(\text{SWAP} \cdot \text{SWAP}) = \sum_{jk} \text{Tr}_{[2]}(\mathbf{g}_{jk} \otimes \mathbf{g}_{jk}^d \cdot \text{SWAP}) = \sum_{jk} \mathbf{g}_{jk} \cdot \mathbf{g}_{jk}^d = \sum_{jk} \mathbf{g}_{jk} \cdot \mathbf{g}_{jk}, \]

(29)

which again leads us to equation (24), with a slightly different interpretation. This equality demonstrates that the elements of a matrix basis constitute (up to prefactors) the Kraus operators of a unital channel, the depolarizing channel.

By reading equation (29) in terms of the standard basis we see that there is a more direct way to obtain this identity: We could have used \( d^1 \mathbf{1}_d = d \sum_{jk} |j\rangle \langle k| \cdot |j\rangle \langle k| \cdot (|j\rangle \langle k|)^d \) and applied the transformation equation (13).

Moreover, it is also possible to derive equalities that contain inner products of four basis elements. For this purpose, we substitute equation (23) into equation (16) and find

\[ \mathbf{1}_d = \text{Tr}_{[2]}(\mathbb{I}_d \otimes \mathbf{1}_d \cdot \text{SWAP}) = \frac{1}{d^2} \sum_{jkab} \text{Tr}_{[2]}(\mathbf{g}_{ab}^d \cdot \mathbf{g}_{jk} \otimes \mathbf{g}_{ab} \cdot \mathbf{g}_{jk}^d \cdot \text{SWAP}) = \frac{1}{d^2} \sum_{jkab} \mathbf{g}_{ab}^d \cdot \mathbf{g}_{jk} \cdot \mathbf{g}_{ab} \cdot \mathbf{g}_{jk}^d. \]

(30)
3.3. The maximally entangled state

The maximally entangled state (or Bell state) in a \(d \times d\)-dimensional Hilbert space is defined as

\[
|\Phi^{+}_{d}\rangle = \frac{1}{\sqrt{d}} \sum_{j} |jj\rangle.
\]  

(31)

From equation (15) we can immediately infer the relation to the SWAP operator

\[
d|\Phi_{d}^{+}\rangle \langle \Phi_{d}^{+}| = \sum_{jk} |jj\rangle \langle kk| = \text{SWAP}_{T_{2}},
\]

(32)

where \(T_{2}\) denotes the partial transposition on the second party of the two-party SWAP. Therefore, the matrix decomposition of the Bell state in the basis \(\{g_{lm}\}\) takes the form

\[
|\Phi_{d}^{+}\rangle \langle \Phi_{d}^{+}| = \frac{1}{d} \sum_{jk} g_{jk} \otimes g_{jk}^{*},
\]

(33)

which again is diagonal in the matrix indices. Obviously the partial transposition could be done as well on the first party, so that the single term in the sum would read \(g_{lm}^{T} \otimes g_{lm}^{*}\), and also the other combination of transposition and Hermitian adjoint (or only complex conjugation) is possible.

We mention the interesting special case of equation (33) when the operator basis consists of two subsets of matrices, one with strictly real and the other with strictly imaginary coefficients. This holds for the Gell-Mann basis, equation (8). Here, the complex conjugation in equation (33) only changes the sign of the terms of the imaginary matrices, so that

\[
|\Phi_{d}^{+}\rangle \langle \Phi_{d}^{+}| = \frac{1}{d} \sum_{j<k} [x_{jk} \otimes x_{jk} - y_{jk} \otimes y_{jk}] + \frac{1}{d} \sum_{j} z_{jk} \otimes z_{jk},
\]

(34)

where \(z_{0}\) is the identity.

We can now derive additional matrix relations in analogy with section 3.1. We have the identity

\[
|\Phi_{d}^{+}\rangle \langle \Phi_{d}^{+}| \cdot |\Phi_{d}^{+}\rangle \langle \Phi_{d}^{+}| = |\Phi_{d}^{+}\rangle \langle \Phi_{d}^{+}|,
\]

and together with equation (33),

\[
|\Phi_{d}^{+}\rangle \langle \Phi_{d}^{+}| = \frac{1}{d} \sum_{j<k} g_{ab} \cdot g_{jk} \otimes (g_{ab} \cdot g_{jk})^{*},
\]

(35)

where again there are several possibilities to place the complex conjugation. Also this equation is remarkable, because it has the same structure as equation (33), while the products \(g_{ab} \cdot g_{jk}\) do not necessarily form a basis.

Taking the partial trace gives

\[
d^{1} 1_{d} = \sum_{j<k} \text{Tr} (g_{ab} \cdot g_{jk}) (g_{ab} \cdot g_{jk})^{*},
\]

(36)

while tracing out both parties leads to

\[
d^{4} = \sum_{j<k} |\text{Tr} (g_{ab} \cdot g_{jk})|^{2} .
\]

(37)

3.4. Combining SWAP and Bell state

The Bell state is invariant under the permutation of its two parties, hence

\[
\text{SWAP} \cdot |\Phi_{d}^{+}\rangle \langle \Phi_{d}^{+}| = |\Phi_{d}^{+}\rangle \langle \Phi_{d}^{+}| \cdot \text{SWAP} = |\Phi_{d}^{+}\rangle \langle \Phi_{d}^{+}|.
\]

(38)

First, this gives another relation analogous to equation (35),

\[
|\Phi_{d}^{+}\rangle \langle \Phi_{d}^{+}| = \frac{1}{d} \sum_{j<k} g_{ab} \cdot g_{jk}^{*} \otimes g_{ab}^{*} \cdot g_{jk}^{*},
\]

(39)

From this, we obtain by tracing out the second party

\[
d^{1} 1_{d} = \sum_{j<k} g_{jk} \cdot g_{jk}^{*}.
\]

(40)
By using equation (25) we find two more equalities containing four-matrix products,

\[ I_d = \frac{1}{d^2} \sum_{j,k} \text{Tr}[g_{jk} \otimes (g_{jk}^* \cdot g_{jk})] = \frac{1}{d^2} \sum_{j,k} g_{jk} \cdot g_{jk}^* \cdot g_{jk} \cdot g_{jk}^* \],

and

\[ I_d = \frac{1}{d^2} \sum_{j,k} \text{Tr}[g_{jk}^* \otimes (g_{jk}^* \cdot g_{jk})] = \frac{1}{d^2} \sum_{j,k} g_{jk}^* \cdot g_{jk}^* \cdot g_{jk} \cdot g_{jk}^* \].

We will see below that these identities are closely related to those in equations (20) and (29).

3.5. The fully coherent state

For the sake of completeness we mention here also a link between matrix bases to the fully coherent state in \( \mathcal{H}_d \),

\[ |+\rangle_d = \frac{1}{\sqrt{d}} \sum_j |j\rangle \].

In the standard basis we see that

\[ d |+\rangle_d (+| = \sum_{j,k} |j\rangle \langle k|, \]

so that, by virtue of equation (13),

\[ \sqrt{d}^3 \ |+\rangle_d (+| = \sum_{j,k} U_{lmjk}^* g_{lm}. \]

The components of the unitary \( U \) appear explicitly because there is no double occurrence of matrix index pairs.

3.6. Collecting the results

Let us briefly summarize the main results we have obtained so far. Starting from the decompositions of SWAP and the Bell state, we found a number of relations that contain products of two matrices,

\[ \text{SWAP} = \frac{1}{d} \sum_{j,k} g_{jk} \otimes g_{jk}^*, \]

\[ d^2 I_d = \sum_{j,k} g_{jk} \cdot g_{jk}^*, \]

\[ d I_d = \sum_{j,k} \text{Tr}(g_{jk}) \cdot g_{jk}^*, \]

\[ d^2 I_d = \sum_{j,k} |\text{Tr}(g_{jk})|^2, \]

and

\[ |\Phi_j^+\rangle \langle \Phi_j^+| = \frac{1}{d^2} \sum_{j,k} g_{jk} \otimes g_{jk}^*, \]

\[ d I_d = \sum_{j,k} g_{jk}^* \cdot g_{jk}, \]

\[ d I_d = \sum_{j,k} \text{Tr}(g_{jk}) \cdot g_{jk}^*, \]

\[ d^2 I_d = \sum_{j,k} |\text{Tr}(g_{jk})|^2, \]

Moreover, there are several identities with products of four matrices

\[ I_d \otimes I_d = \frac{1}{d^2} \sum_{j,k,l,m} g_{jk} \otimes g_{jk}^* \cdot g_{lm} \cdot g_{lm}^*, \]

\[ d^2 I_d = \sum_{j,k,l,m} g_{jk}^* \cdot g_{jk} \cdot g_{lm} \cdot g_{lm}^*, \]

\[ d^3 I_d = \sum_{j,k,l,m} g_{jk} \cdot g_{jk}^* \cdot g_{lm} \cdot g_{lm}^*, \]

\[ |\Phi_j^+\rangle \langle \Phi_j^+| = \frac{1}{d^3} \sum_{j,k,l,m} g_{jk} \otimes g_{jk}^* \otimes g_{lm} \cdot g_{lm}^*, \]

\[ = \frac{1}{d^3} \sum_{j,k,l,m} g_{jk} \cdot g_{jk}^* \otimes (g_{lm} \cdot g_{lm}^*)^*, \]

\[ d^2 I_d = \sum_{j,k,l,m} g_{jk} \cdot g_{jk}^* \cdot g_{lm} \cdot g_{lm}^*, \]

\[ d^4 I_d = \sum_{j,k,l,m} |\text{Tr}(g_{jk} \cdot g_{lm})|^2. \]
As discussed before, it is possible to re-assign conjugations, daggers and transpositions to other factors in most of the relations.

4. Decompositions of the trace and other maps

Matrix expansions are relevant not only for operators like SWAP, but also for quantum channels and other maps, as indicated already in the preceding section. Here we provide some explicit examples that are particularly useful in calculations using the Bloch representation.

4.1. The trace

The trace maps an operator into the complex numbers, but instead one may consider the map to another operator \( \text{Tr} d r \rightarrow r \). There is a well-known matrix expansion for this map (cf., e.g., [3]). Consider an operator \( A \in \mathcal{B}(\mathcal{H}_d) \). Then

\[
\text{Tr}(A) I_d = \frac{1}{d} \sum_{lm} g_{lm} \cdot A \cdot g_{lm}^\dagger,
\]

which at first glance looks remarkable—how can this work for any matrix basis \( \{g_{jk}\} \)? Applying our method from the previous sections, we start by reading this relation in the standard matrix basis. We find that here it is rather evident,

\[
\text{Tr}(A) I_d = \sum_{jk} \langle j| A|k\rangle \otimes I_d
\]

As before, we notice the double occurrence of the basis indices, therefore we know that substituting the transformation equation (13) straightforwardly leads to the result,

\[
\text{Tr}(A) I_d = \frac{1}{d} \sum_{jk} \sum_{lm} \sum_{lmm} g_{lm} \cdot A \cdot g_{lm}^\dagger \cdot U_{jk,lm}^\dagger U_{jk,lm}
\]

which leads to

\[
\text{Tr}(A) I_d = \frac{1}{d} \sum_{lm} g_{lm} \cdot A \cdot g_{lm}^\dagger,
\]

After all, equation (46) confirms what was to be expected from equation (29) in section 3.2: The depolarization channel can be realized by using the elements of a matrix basis as Kraus operators. With this expansion of the trace map it becomes obvious that equation (42) can be read as a version of equation (20) [the same holds for equation (30)].

Evidently, in the multipartite case equation (46) can be applied as partial trace operation to any subset of parties.

4.2. The identity map

In analogy with section 3.1 a small detour has to be taken in order to represent the identity map in terms of a matrix basis, \( \text{Id}(A) = I_d A \). This is because the two indices do not belong to a single matrix basis. We can achieve this by writing

\[
\sum_{jk} \langle j| A|k\rangle \otimes |m\rangle \cdot |l\rangle
\]

which leads to

\[
\text{Id}(A) = \frac{1}{d^2} \sum_{jk} \sum_{lm} g_{jk} \cdot g_{lm}^\dagger \cdot A \cdot g_{jk} \cdot g_{lm},
\]

equation (30) may be viewed, for example, as the normalization condition for the map in equation (47). In fact, we could have directly used equation (23) and the SWAP relation (25) to derive this result.

4.3. General linear maps

Extending the results of the preceding paragraphs we may analyze the matrix expansion of general linear maps \( \mathcal{L}(A), A \in \mathcal{B}(\mathcal{H}_d) \) (also referred to as superoperators). It is natural to study a linear map via the action on a basis of the Hilbert-Schmidt space. Here, this means to analyze, e.g., the Bloch representation of \( A \),
The action of \( \mathcal{L}(-) \) on the matrix basis \( \{ g_{jk} \} \) is simple. For example, it is easy to recognize the result for the identity map.

It is worthwhile mentioning here also the Choi-Jamiolkowski representation [36, 40, 41] of the map \( \mathcal{L}(-) \), because it is obtained via a similar reasoning. The Choi state \( C_C \) is defined as

\[
C_C = \mathcal{L} \otimes \text{Id}[\Phi^+_{j,k}] = \frac{1}{d^2} \sum_{jk} \mathcal{L}(g_{jk}) \otimes g_{jk}^*.
\]

Then the map \( \mathcal{L}(A) \) can be represented as

\[
d \text{Tr}_2[C_C \cdot (I_d \otimes A^T)] = \frac{1}{d} \sum_{jk} \mathcal{L}(g_{jk}) \text{Tr}(g_{jk}^* A^T)
\]

\[
= \mathcal{L} \left( \frac{1}{d} \sum_{jk} g_{jk} \text{Tr}[g_{jk}^* A] \right)
\]

\[
= \mathcal{L}(A).
\]

### 4.4. The transposition

The examples in the previous paragraphs indicate that along these lines it is possible to derive other results. The first is an explicit decomposition of the transposition map. Taking into account the expansion of an operator \( A \) in the standard basis, \( A = \sum_{jk} a_{jk} \langle j|k \rangle \langle k| \), we find [42]

\[
A^T = \sum_{jk} a_{kj} \langle k|j \rangle \langle j|k \rangle
\]

\[
= \sum_{jklm} a_{kl} \langle k|m \rangle \langle m|l \rangle \langle l|k \rangle \langle k|j \rangle.
\]

If we want to apply the transformation equation (13), we have to take one of the basis matrices in the decomposition with a complex conjugation,

\[
A^T = \frac{1}{d} \sum_{jk,lm} a_{kl} U_{jk,lm}^* g_{lm}^* \cdot A \cdot g_{pq}^* U_{jk,pq}
\]

\[
= \frac{1}{d} \sum_{jklm} g_{lm}^* \cdot A \cdot g_{jm}^*.
\]

We notice that this identity provides the link between the four-operator product in equation (41) and equation (29).

### 4.5. Partial transpose and reshuffling operation

Transposition has several generalizations if one considers multi-party operators [36, 43–45]. The first of them is partial transposition, for example, on the second party. Consider the two-party operator \( B \in \mathcal{B}(\mathcal{H}_d \otimes \mathcal{H}_d) \), that is,

\[
B = \sum_{jklm} B_{jklm} \langle j|k \rangle \langle k|lm \rangle.
\]

Then partial transposition on the second party exchanges the second indices in both groups,

\[
B_T^2 = \sum_{jklm} B_{jm,kl} \langle j|k \rangle \langle k|lm \rangle,
\]

while the first party remains unaffected. By using the results of the previous section we can give a matrix expansion for this map,

\[
B_T^2 = \frac{1}{d} \sum_{jk} (I_d \otimes g_{jk}) \cdot B \cdot (I_d \otimes g_{jk}^*).
\]

Alternatively, one can apply the reshuffling map to \( B \) that exchanges the second index in the first with the first index in the second group,

\[
B_R = \sum_{jklm} B_{jkm} \langle j|k \rangle \langle k|lm \rangle.
\]
In full analogy with what was said before we have

\[ B^\otimes = \frac{1}{d} \sum_{j,k} (1_d \otimes g_{j,k}) \cdot B \cdot (g_{j,k}^* \otimes 1_d). \]  

(55)

This is readily extended to the case of more than two parties, where any subset of indices in the first group can be exchanged with another subset of the same size in the second group.

4.6. The universal state inversion

For completeness, we include the universal state inversion map here, because it provides an example where a specific choice of matrix basis leads to an interesting expansion. Universal state inversion is a relevant map that applied to physical states helps to explore the boundary of the state space and is therefore also useful in entanglement detection [37, 42, 46–48].

Consider first a Hermitian single-party operator \( A \), i.e., \( A \in \mathcal{B}(\mathcal{H}_d) \) and \( A = A^\dagger \). Universal state inversion is defined as

\[ \mathcal{S}(A) = \text{Tr}(A) 1_d - \text{Id}(A). \]  

(56)

Because of the hermiticity of \( A \) we can write \( A = (A^*)^\dagger \). By using the results for the trace and the transposition maps we can rewrite the definition

\[ \mathcal{S}(A) = \frac{1}{d} \sum_{j,k} g_{j,k} \cdot A^* \cdot g_{j,k}^* - \frac{1}{d} \sum_{l,m} g_{l,m} \cdot A^* \cdot g_{l,m}^* \]

\[ = \frac{1}{d} \sum_{j,k} g_{j,k} \cdot A^* \cdot (g_{j,k}^* - g_{j,k}^*). \]  

(57)

For the Gell-Mann basis we have the special situation that the matrices are Hermitian and have either only real elements, or only imaginary ones. That is, the parenthesis in equation (57) is non-zero only for the imaginary Gell-Mann matrices \( \Lambda_{d}^{(i)} \equiv y_{ij} \), cf. Eq. (8b). Therefore

\[ \mathcal{S}(A) = \frac{2}{d} \sum_{j<k} y_{j,k} \cdot A^* \cdot y_{j,k}. \]  

(58)

This result is readily generalized to multi-party operators. In order to present the idea it suffices to consider the case of two parties, i.e., Hermitian operators \( B \in \mathcal{B}(\mathcal{H}_d \otimes \mathcal{H}_d) \). Then

\[ \mathcal{S}(B) = [\text{Tr}_{12}(\cdot) \otimes 1_d - \text{Id}] \cdot [\text{Tr}_{12}(\cdot) \otimes 1_d - \text{Id}] B \]

\[ = \text{Tr}_{12}(B) 1_d^2 - \text{Tr}_{12}(B) \otimes 1_d - 1_d \otimes \text{Tr}_{12}(B) + B. \]  

(59)

By applying the same steps as in the single-party case we arrive at

\[ \mathcal{S}(B) = \frac{4}{d^2} \sum_{j<k<l<m} (y_{j,k} \otimes y_{l,m}) \cdot B^* \cdot (y_{j,k} \otimes y_{l,m}). \]  

(60)

We note that this is reminiscent of Wootters’ \( R \) matrix for two qubits [49], in fact, it is the higher-dimensional generalization of that definition [42, 46]. For pure states \( B = |\psi\rangle\langle\psi| \) it directly leads to the squared concurrence of \( |\psi\rangle \),

\[ C(\psi)^2 = \text{Tr}[|\psi\rangle\langle\psi| \cdot \mathcal{S}(\psi)|\psi\rangle] \]

\[ = \frac{4}{d^2} \sum_{j<k,l<m} |\langle\psi| y_{j,k} \otimes y_{l,m} \psi^* \rangle|^2. \]  

(61)

5. Conclusion

We have presented a few important definitions regarding orthogonal bases of the Hilbert-Schmidt space and then derived various identities, that is, matrix expansions of relevant operators and maps. We hope this brief account renders the known relations for matrix bases more transparent and makes the derivation of similar identities easier. There are many additional connections between the central equalities derived here, and therefore also alternative ways to obtain them. We have not mentioned all of them in order to avoid excessive cross-referencing and to keep the line of reasoning visible. Finally, we believe that this collection of results may give some intuition for the structure of matrix expansions and for the typical applications where they have proven useful.
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Data availability statement

No new data were created or analysed in this study.

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