Higher-Order-Schmidt-Representations and their Relevance for the Basis-Ambiguity

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Abstract

With the help of a useful mathematical tool, the polar decomposition of closed operators, and a simple observation, i.e. the unique relation between tensor-product states and compact operators, we manage to give a compact and coherent account of the various properties of higher-order-Schmidt-representations.
1 Introduction

In the *environment-induced decoherence* approach to the quantum measurement problem (just to mention a few sources from the huge field of published literature, see e.g. [1],[2],[3]), an important role is played by the *Schmidt-representation* in the tensor-product of two Hilbert spaces, here the Hilbert space of the quantum system, $\mathcal{H}_s$, and the Hilbert space of the measuring apparatus (or rather of the *pointer*), $\mathcal{H}_A$. It is argued that the transition

$$\left(\sum_i c_i \psi_i \right) \otimes \Phi_0 \rightarrow \sum_i c_i \psi_i \otimes \Phi_i$$

with

$$\sum_i c_i \psi_i \in \mathcal{H}_s \ , \ \Phi_0, \Phi_i \in \mathcal{H}_A$$

is not yet a measurement of a quantum property of some micro object observable but only a so-called *premeasurement*. As such this statement is quite uncontroversial as long as the pointer system is also not of a macroscopic size. One can, on the other hand, question the above description of the first stage of the measurement process if the $\Phi_i$ (as is usually actually the case) belong to a macroscopic subsystem of the measurement instrument (we will discuss this problem elsewhere [4]).

It is then argued that $\sum c_i \psi_i \otimes \Phi_i$ cannot be associated with the following mixed state of the quantum system

$$\sum |c_i|^2 |\psi_i><\psi_i|$$

because of the well-known *basis non-uniqueness* problem. To reach a unique representation an entanglement of the pointer states with the environment is invoked, i.e.

$$\sum c_i \psi_i \otimes \Phi_i \rightarrow \sum c_i \psi_i \otimes \Phi_i \otimes \epsilon_i$$

with $\epsilon_i$ in the ideal case an orthonormal basis of the environment. It is then argued that this second process of correlation makes the above representation unique.

We do not know how long this result was actually known in full generality in the scientific community before the rigorous proofs provided in [5] and [6]. One finds for example sometimes statements like

$$\sum c_i \psi_i \Phi_i = \sum c'_j \psi'_j \Phi'_j$$
suggesting that it may happen that the sets \( \{ c_i \} \) and \( \{ c'_j \} \) could be really different (which can in fact not! happen as we will show below). Be that as it may, we will in the following present a very brief, mathematically concise and transparent deduction of results being of relevance in this context. The whole line of reasoning can essentially be based on a single observation and one mathematical conceptual tool.

## 2 The Mathematical Tool

The mathematical tool we are employing is the very useful concept of polar decomposition of operators.

**Theorem 2.1** A closable operator from \( \mathcal{H}_1 \) to \( \mathcal{H}_2 \) admits a polar decomposition of the form

\[
A = U \circ |A|
\]

which is essentially unique. \( |A| \) is the positive (s.a.) operator

\[
(A^+A)^{1/2} : \mathcal{H}_1 \to \mathcal{H}_1
\]

and \( U \) is a partial isometry

\[
U : |A| \circ \mathcal{H}_1 \to A \circ \mathcal{H}_1
\]

Remark: As far as we know, the polar decomposition in its general form was introduced by v.Neumann (based on earlier work of E.Schmidt, [7]). See also [8] or [9].

**Theorem 2.2 (Canonical Representation of a Compact Operator)**

With \( A : \mathcal{H}_1 \to \mathcal{H}_2 \) compact, we have

\[
A = \sum_\nu \lambda_\nu |\phi_\nu \rangle \langle \psi_\nu|
\]

All \( \lambda_\nu \neq 0 \) are only finitely degenerated and can be chosen positive (note that phase factors can be absorbed in the ON-bases \( \phi_\nu, \psi_\nu \)). The possible zero-eigenspace may be infinitely degenerated.

**Observation 2.3** With the help of the polar decomposition we can conclude

\[
A = U \circ |A| \quad , \quad |A| \circ \psi_\nu = \lambda_\nu \psi_\nu \quad , \quad U \circ \psi_\nu = \phi_\nu
\]

i.e.

\[
|A| = \sum_\nu \lambda_\nu |\psi_\nu \rangle \langle \psi_\nu|
\]

that is, the \( \lambda_\nu, \psi_\nu \) are the eigenvalues and eigenvectors of \( |A| \).
3 The Schmidt-Representation

From the above polar decomposition of a compact and, in particular, Hilbert-Schmidt operator the Schmidt-representation follows immediately.

**Observation 3.1** A vector $\Psi$ in $H_1 \otimes H_2$,

$$\Psi = \sum c_{ij} e_i \otimes f_j$$  \hspace{1cm} (12)

$\{e_i \otimes f_j\}$ an orthonormal basis in $H_1 \otimes H_2$, can be uniquely associated with an operator from $H_1 \rightarrow H_2$ or vice versa, i.e. with

$$A := \sum c_{ij} |e_i><f_j| : H_2 \rightarrow H_1$$  \hspace{1cm} (13)

With $\Psi$ normalisable, $A$ is Hilbert-Schmidt, hence compact. It follows $A = U \circ |A|$ with $|A|$ having the spectral representation

$$|A| = \sum \lambda_i |\phi_i><\phi_i| , \phi_i \in H_2$$  \hspace{1cm} (14)

and

$$U \circ \Phi_i = \psi_i \in H_1$$  \hspace{1cm} (15)

thus

$$A = \sum \lambda_i |\psi_i><\phi_i|$$  \hspace{1cm} (16)

and

$$\Psi = \sum \lambda_i \cdot \psi_i \otimes \phi_i$$  \hspace{1cm} (17)

the latter being the Schmidt-representation.

Remark: without mentioning it always, the eigenbasis of $|A|$ comprises also the subspace belonging to the eigenvalue zero, which, on the other hand, does not show up in the representation of $\Psi$.

Before we proceed, we want to employ the above representation to derive a few other results which are useful in the study of e.g. entanglement-entropy etc.

**Observation 3.2** With

$$A : H_2 \rightarrow H_1 , \quad A = \sum c_{ij} |e_i><f_j|$$  \hspace{1cm} (18)

we have

$$A^+ = \sum \overline{c_{ij}} |f_j><e_i|$$  \hspace{1cm} (19)
and
\[ A^+A = \sum c_{ij} \overline{c}_{ij} |f_j><f_j| \quad (20) \]
\[ AA^+ = \sum c_{i'j} \overline{c}_{ij} |e_i><e_i| \quad (21) \]

Furthermore we have

**Observation 3.3** \( A^+A \) is the reduced density matrix of \( P_\Psi \) in \( \mathcal{H}_2 \).

Proof: We have
\[ (\Psi|1 \otimes B|\Psi) = \sum |\lambda_i|^2 (\phi_i|B|\phi_i) = \text{Tr} ((A^+A)B) \quad (22) \]

4 The Uniqueness-Question for \( \mathcal{H}_1 \otimes \mathcal{H}_2 \)

If all \( \lambda_i \neq 0 \) are different, the spectral representation in the above form of \( |A| \) is unique apart from the possibly degenerated zero-eigenspace. If some \( \lambda_i \neq 0 \) are degenerate, for example, \( \lambda := \lambda_1 = \lambda_2 = \cdots = \lambda_k \), we can choose in the \( k \)-dimensional subspace \( \mathcal{H}_\lambda \) arbitrarily many different ON-bases, connected with each other by unitary transformations
\[ \{\phi_1, \phi_2, \ldots, \phi_k\} \rightarrow \{\phi'_1, \phi'_2, \ldots, \phi'_k\}, \quad \phi'_i = V \circ \phi_1 \quad (23) \]
with \( V \) unitary in \( \mathcal{H}_\lambda \).

In this situation we have
\[ A = \sum \lambda_i |\psi_i><\phi_i| = \sum \lambda_i |\psi'_i><\phi'_i|, \quad \psi'_i = U \circ \phi'_i \quad (24) \]

**Observation 4.1** In the case of a degeneracy the \( \{\psi_i, \phi_i\} \) may be replaced by \( \{\psi'_i, \phi'_i\} \) but the weights \( \lambda_i \) remain the same. They represent the unique eigenvalues of \( |A| \). That is, we have by the same token
\[ \Psi = \sum \lambda_i \psi_{i,\nu} \otimes \phi_{i,\nu} = \sum \lambda_i \psi'_{i,\nu} \otimes \phi'_{i,\nu} \quad (25) \]
with \( \nu \) denoting the possible degeneration in the subspaces \( \mathcal{H}_\lambda \).
5 The Schmidt-Representation for three and more Hilbert-Spaces

Let $\Psi$ be a vector in $H_1 \otimes H_2 \otimes H_3$, i.e.

$$\Psi = \sum c_{ijk} \psi_i^1 \otimes \psi_j^2 \otimes \psi_k^3$$  \hspace{1cm} (26)$$

**Assumption 5.1** It exists a Schmidt-representation for $\Psi$, i.e.

$$\Psi = \sum \lambda_i \Phi_i^1 \otimes \Phi_i^2 \otimes \Phi_i^3$$  \hspace{1cm} (27)$$

with $\lambda_i$ positive and $\{\Phi_i^\nu\}$ (parts of) ON-bases in $H_\nu$.

**Observation 5.2** We associate the operator

$$A : H_1 \otimes H_2 \rightarrow H_3 \hspace{1cm} A := \sum c_{ijk} |\psi_k^3> <\psi_i^1 \otimes \psi_j^2|$$  \hspace{1cm} (28)$$

with $\Psi$, so that again the $\lambda_i$ are the eigenvalues of the operator

$$|A| : H_1 \otimes H_2 \rightarrow H_1 \otimes H_2 \hspace{1cm} |A| = \sum \lambda_i |\Phi_i^1 \otimes \Phi_i^2 > <\Phi_i^1 \otimes \Phi_i^2|$$  \hspace{1cm} (29)$$

and $A$ can be written as

$$A = U \circ |A| = \sum \lambda_i |\Phi_i^3> <\Phi_i^1 \otimes \Phi_i^2|$$  \hspace{1cm} (30)$$

**Proposition 5.3** The Schmidt-representation (if it exists!) is unique even if some $\lambda_i$ are degenerate.

Proof: We learned above that even if we assume that two different representations do exist, i.e.

$$\Psi = \sum \lambda_i \Phi_i^1 \otimes \Phi_i^2 \otimes \Phi_i^3 = \sum \lambda'_i (\Phi'_i)^1 \otimes (\Phi'_i)^2 \otimes (\Phi'_i)^3$$  \hspace{1cm} (31)$$

the sets $\{\lambda_i\}$ and $\{\lambda'_i\}$ are necessarily the same as both represent the unique set of eigenvalues of $|A|$. Hence it remains only the possibility

$$\Psi = \sum_{i,\nu} \lambda_i \Phi_{i,\nu}^1 \otimes \Phi_{i,\nu}^2 \otimes \Phi_{i,\nu}^3 = \sum \lambda_i (\Phi'_{i,\nu})^1 \otimes (\Phi'_{i,\nu})^2 \otimes (\Phi'_{i,\nu})^3$$  \hspace{1cm} (32)$$

where $\nu$ denote the possible degeneration of the eigenvalues $\lambda_i$. $\Phi_{i,\nu}^1 \otimes \Phi_{i,\nu}^2$ are elements in the eigenspace of $\lambda_{i_0}$ (belonging to $|A|$) while $U$ maps them onto $\Phi_{i,\nu}^3$. The same holds for the rhs of the equation.
Assume now that e.g. \( \lambda_{i_0} > 0 \) is degenerate. Then we have for the corresponding part of \( \Psi \):

\[
\Psi_{\lambda_{i_0}} = \lambda_{i_0} \cdot \sum_{\nu=1}^{N} \Phi_{1,i,\nu}^{1} \otimes \Phi_{1,i,\nu}^{2} \otimes \Phi_{1,i,\nu}^{3} = \lambda_{i_0} \cdot \sum_{\nu=1}^{N} \Phi'_{i,\nu}^{1} \otimes (\Phi'_{i,\nu})^{2} \otimes (\Phi'_{i,\nu})^{3}
\] (33)

Note that in contrast to the two-Hilbert space case, the existence of an eigenbase for \( \lambda_{i_0} \) of the above homogeneous form is rather special. We show that only one homogeneous eigenbase can exist in the case of three or more Hilbert spaces.

In the eigenspace \( \mathcal{H}_{\lambda_{i_0}} \) with the assumed two homogeneous bases \( \Phi_{1,i,\nu}^{1} \otimes \Phi_{1,i,\nu}^{2} \) and \( (\Phi'_{i,\nu})^{1} \otimes (\Phi'_{i,\nu})^{2} \) we can write

\[
\Phi_{1,i,\nu}^{1} \otimes \Phi_{1,i,\nu}^{2} = \sum_{\mu=1}^{N} c_{\nu\mu} (\Phi'_{i,\mu})^{1} \otimes (\Phi'_{i,\mu})^{2}
\] (34)

Take now an operator \( B \) in \( \mathcal{H}_1 \) and hence \( B \otimes 1 \) in \( \mathcal{H}_1 \otimes \mathcal{H}_2 \). It follows

\[
(\Phi_{1,i,\nu}^{1} \otimes \Phi_{1,i,\nu}^{2} | B \otimes 1 | \Phi_{1,i,\nu}^{1} \otimes \Phi_{1,i,\nu}^{2}) = (\Phi_{1,i,\nu}^{1} | B | \Phi_{1,i,\nu}^{1}) = \sum_{\mu=1}^{N} |c_{\nu\mu}|^2 ((\Phi'_{i,\mu})^{1} | B | (\Phi'_{i,\mu})^{1})
\] (35)

with \( \sum |c_{\nu\mu}| = 1 \) and \( N > 1 \) (degeneracy).

**Observation 5.4** As a consequence of our assumption a pure state on \( \mathcal{B}(\mathcal{H}_1) \) equals a mixture. This is not! possible (see the appendix for a proof of this well-known result).

We hence arrive at a contradiction and the proposition is proved.

Another question which was for example addressed by Peres (6) is, how special such a homogeneous Schmidt-representation is for more than two Hilbert spaces. A simple counting analysis suggests, that it is in fact quite special. In our framework we can give a complete and general answer. We exemplify the analysis for the case of three Hilbert spaces and make the necessary generalisations afterwards.

Take a general vector state in \( \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3 \),

\[
\Psi = \sum c_{ijk} e_i \otimes f_j \otimes g_k
\] (36)

with bases \( e_i, f_j, g_k \) in \( \mathcal{H}_1, \mathcal{H}_2, \mathcal{H}_3 \). Under what conditions can \( \Psi \) be represented as

\[
\Psi = \sum \lambda_i \cdot \Phi_{1,i}^{1} \otimes \Phi_{1,i}^{2} \otimes \Phi_{1,i}^{3}
\] (37)
with (partial) bases $\Phi^1_i, \Phi^2_i, \Phi^3_i$ in $H_1, H_2, H_3$.

We learned above that the possibility of such a representation is associated with operators $A, U, |A|$ so that $\Phi^1_i \otimes \Phi^2_i$ can be extended to an eigenbasis of $|A|$ with the above $\Phi^1_i \otimes \Phi^2_i$ belonging to the set of non-zero eigenvalues, $A_\pm$, of $|A|$.

Remark: Note that the basis vectors, belonging to $\lambda_0 = 0$ need not! be of such a diagonal form.

We infer from the analysis of the Schmidt-representation of the twofold tensor product that the operator $A$, induced by $\Psi$, has always a representation

$$A = \sum_l |U \circ u_l > < u_l|$$

(38)

$u_l$ being the eigenvectors of $|A| : H_1 \otimes H_2 \rightarrow H_1 \otimes H_2$. However, in general the $u_l$ are not of product form! The general representation reads

$$u_l = a^{ij}_l \cdot e_i \otimes f_j \quad (\text{summation convention})$$

(39)

In the following we can restrict our analysis to the subspace, $V$, being spanned by the eigenbasis belonging to the positive eigenvalues. If a Schmidt-representation exists, $V$ is spanned by an eigenbasis of the form $\{\Phi^1_i \otimes \Phi^2_i\}$. For $l$ fixed we then have

$$\Phi^1_l = x^i e_i, \quad \Phi^2_l = y^j f_j$$

(40)

and

$$\Phi^1_l \otimes \Phi^2_l = x^i y^j e_i \otimes f_j$$

(41)

The matrix $(x^i y^j)$ has the following form. Take e.g. a $n \times n$ submatrix

$$\begin{pmatrix}
  x^1 y^1 & \cdots & x^1 y^n \\
  \vdots & \ddots & \vdots \\
  x^n y^1 & \cdots & x^n y^n
\end{pmatrix}$$

(42)

All rows are proportional to each other, e.g.

$$x^i y^1 = y^1 / y^2 \cdot (x^i y^2) \quad \text{etc.} \quad (43)$$

We hence have

**Observation 5.5** The rank of the matrix $(x^i y^j)$ is one.
Conclusion 5.6 In case of a generic $\Psi$, the respective eigenvectors $u_i = a_i^j e_i \otimes f_j$ have matrices $(a_i^j)$ (l fixed) with a rank which is generically of the order $O(\min(\dim \mathcal{H}_1, \dim \mathcal{H}_2))$, i.e., the probability of having such a particular Schmidt-basis is very small in general.

For the tensor product of more than three spaces, we can put the question in the following form. We ask for the probability that an arbitrary vector can be represented as a product, that is

$$c_{ijk...n} e_i \otimes f_j \otimes \cdots \otimes r_n = (a^1 e_i) \otimes (b^1 f_j) \otimes \cdots \otimes (q^n r_n) \quad (44)$$

For reasons of simplicity we assume that all Hilbert spaces have the same dimension $N$. On the rhs we have $N \cdot n$ unknowns $a^1, \ldots, q^n$. The different $c_{ijk...n}$ yield $N^n$ equations.

Conclusion 5.7 i) In the generic case the system of equations is strongly overdetermined as $N^n > N \cdot n$ for $N \geq 2$ and $n \geq 3$.

ii) On the other hand, for $N = n = 2$ we have $N^n = N \cdot n$. However, this does guarantee that the system has a solution (see the following example).

Take e.g. the former singulett state

$$\Psi = (\uparrow\downarrow - \downarrow\uparrow) \quad (45)$$

It is entangled, hence cannot be written as a product. The above system of equations would yield:

$$0 = a^1 b^1 , \quad 0 = a^2 b^2 , \quad 1 = a^1 b^2 , \quad -1 = a^2 b^1 \quad (46)$$

which is contradictory. This is possible since the equations are non-linear!

6 Appendix

The relation

$$(\psi|B|\psi) = \sum_{1}^{N} \lambda_i (\phi_i|B|\phi_i) \quad (47)$$

with $|\psi|^2 = 1$, $\phi_i$ being orthonormal and $0 < \lambda_i < 1$ for $N > 1$ because of $\sum_{1}^{N} \lambda_i = 1$, which is assumed to hold for the full algebra $B(\mathcal{H})$, implies the identity

$$P_{\psi} = \sum_{1}^{N} \lambda_i \cdot P_{\phi_i} \quad (48)$$
We hence have
\[ 1 = (\psi | P_\psi | \psi) = \sum_{i=1}^{N} \lambda_i \cdot |(\psi | \phi_i)|^2 \]  
(49)
with \(0 < \lambda_i < 1\), \(|(\psi | \phi_i)|^2 \leq 1\) and \(|(\psi | \phi_i)|^2 = 1\) only if \(\psi = e^{i\alpha} \cdot \phi_i\). I.e., there exists at least one term for which holds \(|(\psi | \phi_i)|^2 < 1\). This implies
\[ 1 = \sum_{i=1}^{N} \lambda_i \cdot |(\psi | \phi_i)|^2 < 1 \]  
(50)
which is a contradiction.

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