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# Decomposition of pure states of quantum register

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**Abstract.** The generalization of Schmidt decomposition due to Cartelet-Higuchi-Sudbery applied to quantum register (a system of $N$ qubits) is shown to acquire direct geometrical meaning: any pure state is canonically associated with a chain of a simplicial complex. A leading vector method is presented to calculate the values of the coefficients of appropriate chain.

**PACS.** 03.67.-a Quantum information – 03.65.Ud Entanglement and quantum nonlocality (e.g. EPR paradox, Bell's inequalities, GHZ states, etc. – 03.65.Fd Algebraic methods

**QICS.** 31.40.+d Multiparty entanglement distribution

Many problems arising in quantum information processing require quantifiable description of equivalence classes of states of multipartite quantum system where two states are treated equivalent if they can be interconverted by a local unitary transformation (see, e.g. [1] for a review).

For pure bipartite states such a canonical form is given by the Schmidt decomposition

$$|\Psi\rangle \;=\; \sum c_i|\psi_i\rangle|\psi_i'\rangle$$

where $|\psi_i\rangle$ (resp., $|\psi_i'\rangle$) are sets of mutually orthogonal states in the first (second, resp.) subsystem. This canonical form was generalized for pure $N$-partite states: the CHS (Carteret–Higuchi–Sudbery) decomposition [2] was obtained

$$|\Psi\rangle \;=\; \sum_{i_1\cdots i_N} c_{i_1\cdots i_N}|\psi_{i_1}^{(1)}\rangle\cdots|\psi_{i_N}^{(N)}\rangle \qquad (1)$$

with the coefficients $c_{i_1\cdots i_N}$ having the following properties:

(i) $c_{jii\cdots i} = c_{iji\cdots i} = \ldots = c_{ii\cdots ij} = 0$ if $1 \le i < j \le d$;
(ii) $c_{i_1\cdots i_N}$ is real and non-negative if at most one of the $i_r$ differs from $d$;
(iii) $|c_{ii\ldots ii}| \ge |c_{j_1\ldots j_N}|$ if $i \le j_r$ for $r = 1,\ldots,N$.

Recently a combinatorial, quantitative *non-numeric* characteristics of multipartite (generally, mixed) quantum states was suggested [5] where any multipartite state was characterized by its separability polytope which remains unchanged under local transformations. These two approaches may be combined.

In our paper we dwell on special class of multipartite systems, such that each subsystem is a qubit, such systems are called *quantum registers*. The state space $\mathcal{H}$ of a quantum register is a tensor product of two-dimensional Hilbert spaces:

$$\mathcal{H} = \mathcal{B}\otimes\mathcal{B}\otimes\cdots\otimes\mathcal{B} = \mathbf{C}^{2^N}.$$

Then all the indices in (1) take two values — 0 and 1 and the above conditions for the coefficients $c_{i_1\cdots i_N}$ read:

(i) $c_{100\cdots 0} = c_{010\cdots 0} = \ldots = c_{00\cdots 01} = 0$;
(ii) the coefficients $c_{11\ldots 11}$ and $c_{1\ldots 101\ldots 1}$ are real and non-negative;
(iii) the coefficient $c_{00\ldots 00}$ has the greatest absolute value among others.

The main idea of the paper is the following. Each coefficient $c_{1\ldots 101\ldots 1}$ is labelled by a sequence of 0-s and 1-s. On the other hand, with each such sequence a subset of a set of cardinality $d$ can be associated, and vice versa. That is why we may say that the coefficients of the CHS decomposition of a register are labelled by subsets of a set. For this, we introduce a geometric interpretation. For the sake of self-consistence, introduce necessary definitions. A state $h \in \mathcal{H}$ is said to be a PRODUCT STATE if it can be

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decomposed into a product:

$$h = h_1 \otimes h_2 \otimes \cdots \otimes h_N.$$

Fix a basis $\{|0\rangle, |1\rangle\}$ in $\mathcal{B}$, then any basis vector in the product space can be encoded as a binary string of $N$ components, and $h \in \mathcal{H}$ can be decomposed as:

$$h = h^{00\ldots0}|0\rangle|0\rangle\cdots|0\rangle + h^{10\ldots0}|1\rangle|0\rangle\cdots|0\rangle + \cdots + \cdots + h^{11\ldots1}|1\rangle|1\rangle\cdots|1\rangle. \quad (2)$$

Any such string can be, in turn, associated with a subset of the set $\mathcal{V} = \{1,\ldots,N\}$. In particular, the vector $|0\ldots0\rangle$ stands for empty set $\emptyset$. Given a subset $\mathbf{s} \subseteq \{1,\ldots,N\}$ we denote

$$|\mathbf{s}\rangle \;=\; |\sigma^1\rangle \otimes \cdots \otimes |\sigma^N\rangle.$$

so that

$$|\sigma^i\rangle \;=\; \begin{cases} 1, & i \in \mathbf{s} \\ 0 & \text{otherwise.} \end{cases}$$

In terms of decomposition (2), the CHS decomposition of a quantum register of length $N$ takes the form

$$h = h^{\emptyset}|\emptyset\rangle + \sum_{2\le|\mathbf{s}|\le N-2} h^{\mathbf{s}}|\mathbf{s}\rangle + \sum_{|\mathbf{s}|\ge N-1} h^{\mathbf{s}}|\mathbf{s}\rangle \quad (3)$$

where $|\mathbf{s}|$ stands for the cardinality of $\mathbf{s}$. Let us calculate the number of independent real parameters in the decomposition (3). The number of nonzero summands of (3) in generic case is $2^N - N$, then the number of real parameters describing them is $2(2^N - N)$. But the summands in the third term of (3) are real, and the numbers of real parameters reduces to $2(2^N - N) - (N - 1)$. Since $h$ is a normalized vector, we have to subtract one more real parameter, so we are left with

$$2(2^N - N) - (N - 1) - 1 = 2^{N+1} - 3N$$

real parameters describing this decomposition in generic case. This is an analog of Schmidt decomposition, and the number of independent real parameters $2^{N+1} - 3N$ can not be reduced in generic case.

## 1 Simplicial complexes and chains

In our paper the decomposition (3) is given a geometrical meaning. Begin with necessary definitions. Let $\mathcal{V} = \{1,\ldots,N\}$ be a non-empty finite set, call the elements of $\mathcal{V}$ VERTICES.

**Definition 1.** *A collection $\mathcal{K}$ of non-empty subsets of $\mathcal{V}$ is called (abstract)* SIMPLICIAL COMPLEX *with the set of vertices $\mathcal{V}$ whenever*

- $\forall v \in \mathcal{V} \quad \{v\} \in \mathcal{K}$,
- $\forall \mathbf{s} \in \mathcal{K}, \forall \mathbf{t} \subseteq \mathcal{V} \quad \mathbf{t} \subseteq \mathbf{s} \Rightarrow \mathbf{t} \in \mathcal{K}$.

*The elements $\mathbf{s} \in \mathcal{K}$ are called* SIMPLICES. *If $\mathbf{t} \subseteq \mathbf{s}$, then $\mathbf{t}$ is said to be a* SUB-SIMPLEX *of $\mathbf{s}$.*

Suppose we have enumerated the vertices of $\mathcal{K}$, then any simplex of $\mathcal{K}$ can be encoded as a binary string. Conversely, any binary string corresponds to a subset of vertices. As an example, consider the special case which we shall need in the sequel, when $\mathcal{K}$ is the complex of all sub-simplices of a simplex $S$. In this case there is 1–1 correspondence between all binary strings and simplices of $\mathcal{K}$. The zero string $00,\ldots,0$ is associated with the empty simplex $\emptyset$.

### Chains

The DIMENSION of a simplex $\mathbf{s}$ is the number of its vertices minus one:

$$\dim \mathbf{s} = \operatorname{card} \mathbf{s} - 1 \quad (4)$$

denote by $\mathcal{K}^m$ the $m$-skeleton of the complex $\mathcal{K}$ — the set of its simplices of dimension $m$

$$\mathcal{K}^m = \{\mathbf{s} \in \mathcal{K} :\; \dim \mathbf{s} = m\}$$

and consider the linear spans

$$\mathcal{H}^m = \operatorname{span} \mathcal{K}^m = \left\{ \sum_{\mathbf{s}\in\mathcal{K}^m} c_{\mathbf{s}} \cdot |\mathbf{s}\rangle \right\}.$$

The elements of $\mathcal{H}^m$ are called CHAINS of dimension $m$. The direct sum

$$\mathcal{H} = \bigoplus_{m=0}^{N} \mathcal{H}^m \quad (5)$$

is called the COMPLEX OF CHAINS of $\mathcal{K}$. The decomposition (5) endows $\mathcal{H}$ with the structure of graded linear space.

### Simplicial representation of the register space

We shall represent the states of the $N$-bit register by chains of the appropriate simplicial complex. Consider a simplex $S$ whose vertices are in 1–1 correspondence with the bits of the register, and let $\mathcal{K}$ be the complex of all sub-simplices of $S$, including the empty one. Consider the decomposition (2) of an arbitrary state of the register. We see that the basic elements are in 1–1 correspondence with the simplices of $\mathcal{K}$, that is, we can consider the vectors of the register's state space as chains of the complex $\mathcal{H}$ and write down (2) as the following sum

$$h = \sum_{\mathbf{s}\in\mathcal{K}} h^{\mathbf{s}}|\mathbf{s}\rangle. \quad (6)$$

**Definition 2.** *Let $\mathbf{s}, \mathbf{t}$ be two simplices, $\mathbf{s} \neq \emptyset$, $\mathbf{t} \neq S$ and $v$ be a vertex of $S$ such that $v \in \mathbf{s}$ and $v \notin \mathbf{t}$. The following expression will be called* EXCHANGEABILITY CONDITION *of a chain $h$:*

$$h^{\mathbf{s}} h^{\mathbf{t}} \;=\; h^{\mathbf{s}\setminus v} h^{\mathbf{t}\cup v}. \quad (7)$$

The following lemma gives us a necessary and sufficient condition for $h$ to be a product vector.

**Lemma 1.** *Whatever be a product basis in $\mathcal{H}$, a vector $h \in \mathcal{H}$ is product if and only if for any $\mathbf{s} \neq \emptyset$ and any $\mathbf{t} \neq S$ the exchangeability condition (7) holds.*

Begin with the case $h^{\emptyset} = 0$. If $h$ is product, then it has the form $h = h^{11\ldots1}|11\ldots1\rangle$ and (7) trivially holds. Vice versa, if (7) holds, then, putting $\mathbf{t} = \emptyset$ in (7), we get $h^{\mathbf{s}\setminus v}h^{v} = 0$ for any $\mathbf{s}$ and any $v \in \mathbf{s}$, in particular, when $\mathbf{s} = S$, the set of all vertices, $h^{S\setminus v}h^{v} = 0$ for any $v$.

Now assume that $h^{\emptyset} \neq 0$. This can always be achieved by appropriate swapping of labeling basis vectors by 0 and 1. To be more precise, suppose that $h^{\emptyset} = 0$. Since the vector $h$ is nonzero, in any basis it has at least one nonzero component. This component is labeled by a string like $\mathbf{s} = 00\ldots101\ldots10$. Relabel the computational basis in those qubits which correspond to the entries of 1 into the string $\mathbf{s}$, then in the new basis the non-zero component of $h^{\mathbf{s}'}$ will have the label $\mathbf{s}' = 00\ldots00$, that is, be $h^{\emptyset}$.

Suppose the exchangeability condition (7) holds, we have to prove that $h$ is product. Let us first reconstruct the factors giving the product. The overall phase factor will be the phase factor of $h^{\emptyset}$. Take it out, then $h^{\emptyset}$ becomes a positive real number. Then normalize the vector: $h \mapsto h/||h||$. Reconstruct the parameter $\alpha_1$ from:

$$\tan\alpha_1 = \left|\frac{h^{10\ldots00}}{h^{\emptyset}}\right|.$$

Then, reconstruct the phase $\mathrm{e}^{\mathrm{i}\phi_1}$ setting it equal to that of $h^{10\ldots00}$. And repeat this consecutively for all other vertices (=bits of the register). Finally, we have to prove that the vector

$$V(h) = \otimes_{k=1}^{N}(\cos\alpha_k|0\rangle + \mathrm{e}^{\mathrm{i}\phi_\mathrm{k}}\sin\alpha_\mathrm{k}|1\rangle)$$

is that what we have started with. Denote every simplex $\mathbf{s}$ by $\mathbf{s} = \sigma^1\sigma^2\ldots\sigma^n$, each $\sigma = 0$ or 1. Then calculate

$$V(h)^{\mathbf{s}} = \bigotimes_{k=1}^{N}\left((1-\sigma^k)\cos\alpha_k|0\rangle + \sigma^k\mathrm{e}^{\mathrm{i}\phi_\mathrm{k}}\sin\alpha_\mathrm{k}|1\rangle\right). \tag{8}$$

We have to prove now that $h^{\mathbf{s}} = V(h)^{\mathbf{s}}$ for any simplex $\mathbf{s} \in \mathcal{K}$. For $\mathbf{s}$ whose binary string contains at most one 1, this is so by construction. For $\mathbf{s}$ of dimension 1 (i.e. containing 2 vertices, $\mathbf{s} = \{u, v\}$) it is so due to (7). When we have proved it for for all 1-dimensional simplices, the exchangeability condition (7) allows us to prove it for all 2-dimensional simplices, and so on.

The converse is straightforward. If $h$ is a product vector, then $h = \bigotimes_{k=1}^{N}\left(\cos\alpha_k|0\rangle + \mathrm{e}^{\mathrm{i}\phi_\mathrm{k}}\sin\alpha_\mathrm{k}|1\rangle\right)$. Therefore the product $h^{\mathbf{s}}h^{\mathbf{t}} = \prod_{j\in\mathbf{s}}\mathrm{e}^{\mathrm{i}\phi_\mathrm{j}}\sin\alpha_\mathrm{j}\prod_{\mathrm{k}\in\mathbf{t}}\mathrm{e}^{\mathrm{i}\phi_\mathrm{k}}\sin\alpha_\mathrm{k}$ remains unchanged when the term $\mathrm{e}^{\mathrm{i}\phi_\mathrm{v}}\sin\alpha_\mathrm{v}$ from the first factor is moved to the second one: $h^{\mathbf{s}}h^{\mathbf{t}} = h^{\mathbf{s}\setminus\{v\}}h^{\mathbf{t}\cup\{v\}}$.

## 2 The leading vector method

In this section we present a way to extract the greatest product component from a given vector $h \in \mathcal{H}$. Given a basis $\mathcal{K}$ in $\mathcal{H}$, decompose $h$:

$$h = \sum_{\mathbf{s}\in\mathcal{K}} h^{\mathbf{s}}|\mathbf{s}\rangle$$

and form the vector $V_0h$:

$$V_0h = \otimes_{k=1}^{N}(h^{\emptyset}|0\rangle + h^{\{k\}}|1\rangle).$$

**Lemma 2.** *If $h$ is a product state such that $h^{\emptyset} \neq 0$ then*

$$h = \frac{V_0h}{(h^{\emptyset})^{N-1}}.$$

This follows immediately from (8). Note that the condition $h^{\emptyset} \neq 0$ does not restrict the generality of the result since, as mentioned above, $h^{\emptyset}$ can be always made nonzero by appropriate swapping of the the labeling of vectors of the current product basis.

**Definition 3.** *Let $h$ be a vector in $\mathcal{H}$ such that $h^{\emptyset} \neq 0$ with respect to a given computational basis. Then the vector $V(h)$ is called a* LEADING VECTOR *of $h$:*

$$V(h) = \frac{V_0h}{(h^{\emptyset})^{N-1}} = \frac{1}{(h^{\emptyset})^{N-1}}\otimes_{k=1}^{N}\left(h^{\emptyset}|0\rangle + h^{\{k\}}|1\rangle\right). \tag{9}$$

Note that the mapping $h \mapsto V(h)$ is only uniform

$$V(\lambda h) = \lambda V(h)$$

rather than linear:

$$V(h + h') \neq V(h) + V(h').$$

**Lemma 3.** *Let $h \in \mathcal{H}$ and $h^{\emptyset} \neq 0$ in a given basis $\mathcal{V}$. Then the decomposition of the residual vector $h' = h - V(h)$ with respect to the basis $\mathcal{K}$ (6) contains at most $2^N - N - 1$ nonzero terms.*

The statement of the lemma follows directly from formula (9):

$$\begin{array}{ll}(V(h))^{\emptyset} &= (h)^{\emptyset}\\ (V(h))^{\{k\}} &= (h)^{\{k\}} \quad \text{for any } k = 1,\ldots,N\end{array}$$

therefore the residual vector $h' = h - V(h)$ will contain at least $N+1$ zero terms when decomposed in the basis $\mathcal{K}$.

### The leading vector after local transformations

Suppose we have made a local transformation $h \mapsto U_m h$ in the $m$th bit[1], then the squared norm of the leading vector of the transformed $h$, denote it $\kappa_h(U_m)$, is:

$$\kappa_h(U_m) = ||V(U_m h)||^2 = \\ = \left|\frac{1}{(U_m h^{\emptyset})^{N-1}}\right|^2 \prod_{k=1}^{N}\left(\left|U_m h^{\emptyset}\right|^2 + \left|U_m h^{\{k\}}\right|^2\right). \tag{10}$$

[1] Although, $U_m$ is still a unitary transformation acting in the whole product space, no ambiguity occurs when we write $U_m = \mathbf{1}\otimes\cdots\otimes U_m\otimes\cdots\otimes\mathbf{1}$.

In a similar way we can define the the value $\kappa_h(U) = ||V(Uh)||^2$ for any product of local transformations $U = \otimes_m U_m$. When we fix a vector $h$, the dependence $U \mapsto \kappa_h(U)$ becomes a continuous function on a compact set $\otimes_m SU(2)$, therefore it takes its maximal value for a particular $U = \otimes_m U_m \in \otimes_m SU(2)$. Choose the new basis $\mathcal{K}'$ making transformations in each $m$th bit

$$\begin{pmatrix} |0'\rangle \\ |1'\rangle \end{pmatrix} = U_m \begin{pmatrix} |0\rangle \\ |1\rangle \end{pmatrix}. \tag{11}$$

**Lemma 4.** *In the basis* $\mathcal{K}'$ (11)

$$V(h) = h^{\emptyset}|\emptyset\rangle.$$

For a proof, consider an infinitesimal local transformation $U_m(\tau)$ at $m$-th bit. Due to (10) the norm of the derivative is proportional to the value of $h^{\{m\}}$. Since $\mathcal{K}'$ is chosen so that it is maximal, all the derivatives should be zero, therefore $h^{\{m\}} = 0$ for any $N = 1, \ldots, N$.

Corollary

In the basis $\mathcal{K}'$ (11)

$$V(h) \perp (h - V(h))$$

therefore

$$h = V(h) \oplus (h - V(h)). \tag{12}$$

## Concluding remarks

Let us summarize the result we obtained. The decomposition suggested here is a special case of CHS canonical form [2] for multipartite pure states, when the dimension of the Hilbert space of each subsystem is two. The basic idea is that the coefficients in this case are labeled by 0-1 strings of length $N$ which are, in turn, treated as characteristic function of subsets of an $N$-element set.

This special case is of practical interest, since these system are the one usually dealt in quantum computing. The CHS canonical form contains generically

$$d^N - \frac{1}{2}Nd(d-1)$$

different terms. In our construction according to (3), any pure state of a quantum register of length $N$ is decomposed into a sum of at most $2^N - (1/2)2N(2-1) = 2^N - N$ pure product states. The number of real parameters of CHS decomposition

$$2d^N - N(d^2-1) - 1$$

in our case reduces to

$$2^{N+1} - 3N - 1.$$

The leading vector method presented here reduces the problem of finding this canonical form to finding the maximum of a smooth function on a compact set.

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