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SCHMIDT-CORRELATED STATES, WEAK SCHMIDT DECOMPOSITION AND GENERALIZED BELL BASES RELATED TO HADAMARD MATRICES

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Abstract. We study the mathematical structures and relations among some quantities in the theory of quantum entanglement, such as separability, weak Schmidt decompositions, Hadamard matrices etc.. We provide an operational method to identify the Schmidt-correlated states by using weak Schmidt decomposition. We show that a mixed state is Schmidt-correlated if and only if its spectral decomposition consists of a set of pure eigenstates which can be simultaneously diagonalized in weak Schmidt decomposition, i.e. allowing for complex-valued diagonal entries. For such states, the separability is reduced to the orthogonality conditions of the vectors consisting of diagonal entries associated to the eigenstates; moreover, for a special subclass of these states this is surprisingly related to the so-called complex Hadamard matrices. Using the Hadamard matrices, we provide a variety of generalized maximal entangled Bell bases.

Keywords: quantum entanglement, Schmidt-correlated states, weak Schmidt decompositions, complex-valued simultaneous diagonalization, Hadamard matrices, generalized Bell bases.

1. Introduction

As one of the most striking features of quantum systems, quantum entanglement [1] plays crucial roles in quantum information processing [2] such as quantum computation, quantum teleportation, dense coding, quantum cryptographic schemes, quantum radar, entanglement swapping and remote states preparation. Nevertheless, many significant open problems in characterizing the entanglement of quantum systems still remain open.

Let $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B \simeq \mathbb{C}^n \otimes \mathbb{C}^n$ be a bipartite composite system. The mathematical problem consists in deriving separability criteria of mixed quantum states, and more generally, in quantifying their degree of entanglement. Such basic problems in the theory of quantum entanglement turn out to be surprisingly difficult, see e.g. [3] for a monographic treatment. Reasons for the difficulty are that the representations of a mixed state ρ as a (statistical) ensemble of pure states are not unique, and that the pure states in a representation in general cannot be simultaneously diagonalized in terms of suitable bases of $\mathcal{H}_A$ and $\mathcal{H}_B$ (Schmidt decomposition).

One of the main idea of the paper is that one can weaken the requirement of simultaneous Schmidt diagonalization to a more general complex version, that is, the generalized Schmidt coefficients are allowed to be complex-valued, see Section 2. We call it the *weak Schmidt decomposition*. It was first introduced by [4] to study quantum states. In our applications, this concept will invoke the Hadamard matrices, a class of matrices that already have received considerable mathematical attention, though some basic problems still remain unresolved, see [5] for a survey.

We first recall some basic concepts in the theory of quantum entanglement. The entanglement of formation [6–9] and concurrence [10–13] are among the important measures to quantify the entanglement. However, due to the extremizations involved in the computation, only a few analytic formulae have been obtained for states like two-qubit ones [10, 14], isotropic states [15] and Werner states [16]. Instead of analytic formulas, some progress has been made toward the lower and upper bounds [17–26].

A mixed state ρ is called *Schmidt-correlated*, or *maximally correlated* [4, 27, 28], if there exists an orthonormal basis, $\{|e_j f_l\rangle\}_{j,l=1}^{n}$, of $\mathcal{H}$ such that

$$\rho = \sum_{j,l=1}^{n} C_{jl} \, |e_j f_j\rangle \, \langle e_l f_l| \, . \tag{1}$$

It is called maximally correlated since for any classical measurement on $\mathcal{H}_A$ or $\mathcal{H}_B$, Alice and Bob will always obtain the same result. One readily sees that Schmidt-correlated states are at most of rank n. It turns out that this class of states exhibits many excellent properties [4, 27, 29–33]. However, given a general state ρ written in the computational basis, any operational method to decide whether it is Schmidt-correlated is still missing in the literature. In this paper, we show that to find out whether a state is Schmidt-correlated it suffices to check whether its spectral decomposition consists of pure eigenstates which can be simultaneously diagonalized in weak Schmidt decomposition, see Theorem 3.1. Although the spectral decomposition may not be unique in the case that it possesses eigenvalues of high multiplicity and it is very possible that the property of simultaneously diagonalization in weak Schmidt decomposition strongly depends on the choice of the ensembles (or eigenstates), our theorem indicates that it is sufficient to check only one of the ensembles. In fact, one can derive that all ensembles of a mixed state can be simultaneously diagonalized in weak Schmidt decomposition if and only if one of them can be, for which we present a direct proof by the Schrödinger's mixture theorem (Theorem 8.2 in [3]), see [33] for an alternative proof. The criteria for this simultaneous diagonalization then are expressed in terms of standard matrix theory, see [4, 34, 35]. In this way, we provide an operational method to solve the problem.

Generally, it is of significance to find a complete basis of maximal entanglement, e.g. the Bell states for qubits. In this paper, we use complex

Hadamard matrices to introduce a wide class of bases consisting of generalized Bell states of maximal entanglement, which contains the well-known Weyl operator basis [4, 36–41] as a special case.

The paper is organized as follows. In section 2, we introduce the main concept of the paper, simultaneous diagonalizations in weak singular value decomposition (weak Schmidt decomposition). In Section 3, we prove our main result, Theorem 3.1, and use it to identify all Schmidt-correlated states. Section 4 is devoted to the separability criteria of Schmidt-correlated states. In section 6, we explore the deep connections among the separability criterion, Hadamard matrices and generalized Bell bases. Conclusion and remarks are given in the last section.

2. Weak Schmidt decomposition

Let $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B \simeq \mathbb{C}^n \otimes \mathbb{C}^n$ be a bipartite composite system and $\{|jl\rangle\}_{j,l=1}^n$ the computational basis of $\mathcal{H}$. In this basis, any pure state can be written as $|\psi\rangle = \sum_{j,l=1}^n a_{jl} |jl\rangle$ which associates with a matrix $A = (a_{jl})_{n\times n}$. The Schmidt decomposition asserts that there exists an orthonormal basis of $\mathcal{H}$, $\{|e_j f_l\rangle\}_{j,l=1}^n$, such that $|\psi\rangle = \sum_{j=1}^n \sqrt{\lambda_j}\, |e_j\rangle |f_j\rangle$ where $\lambda_j \geq 0$ and $\sum_{j=1}^n \lambda_j = 1$. This follows from the singular value decomposition, SVD in short, of the matrix A, i.e. there exist $n \times n$ unitary matrices U and V such that

$$UAV^t = \begin{pmatrix} \sqrt{\lambda_1} & & & \\ & \sqrt{\lambda_2} & & \\ & & \ddots & \\ & & & \sqrt{\lambda_n} \end{pmatrix}_{n\times n},$$

where t denotes the transpose.

A pure state $|\psi\rangle$ is called *separable* if it is a product state, i.e. $|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle\,,\ |\psi_1\rangle \in \mathcal{H}_A,\ |\psi_2\rangle \in \mathcal{H}_B$. A *mixed state* ρ is a statistical ensemble of pure states, denoted by $\{p_k, |\psi_k\rangle\}_{i=1}^K$ with $p_k > 0$ and $\sum_{k=1}^K p_k = 1$, that is,

$$\rho := \sum_{k=1}^K p_k \, |\psi_k\rangle \langle\psi_k| \, . \tag{2}$$

A mixed state ρ is *separable* if it can be expressed as a convex combination of separable pure states, i.e., there exists an ensemble of separable pure states, otherwise it is called entangled [42]. In general, it is difficult to decide whether a given mixed state is separable or not, because the ensembles of a mixed state are generically non-unique. There are neither operational sufficient and necessary criteria for judging the separability in general, nor analytical formulae for entanglement of formation or concurrence for arbitrary mixed states. However, if one could carry out the Schmidt decomposition simultaneously for all the pure states in an ensemble of a mixed state, then the calculation would be much easier. Therefore the question is under which conditions one can diagonalize a set of pure states in SVD simultaneously.

This is answered by Wiegmann's theorem [34]: A set of matrices $\{A_k\}_{k=1}^K$ can be simultaneously diagonalized in SVD iff for any $1 \le i, j \le K$

$$A_i A_j^\dagger = A_j A_i^\dagger \text{ and } A_i^\dagger A_j = A_j^\dagger A_i.$$

However, this demand is too strong for our purposes, as is already evident from the following example,

$$|\psi_1\rangle \sim A_1 = \begin{pmatrix} 1 & & \\ & \omega & \\ & & \omega^2 \end{pmatrix}, \qquad |\psi_2\rangle \sim A_2 = \begin{pmatrix} 1 & & \\ & \omega^2 & \\ & & \omega \end{pmatrix},$$

where $\omega = \frac{1}{2} + i\frac{\sqrt{3}}{2}$. Direct calculation shows that A_1 and A_2 cannot be transformed to SVD simultaneously, although they are already in complex diagonal form.

Our idea is to investigate when the pure states of an ensemble of a mixed state can be simultaneously diagonalized in complex-valued form. Namely, we consider the case that is more general than SVD in which we allow complex-valued entries for the diagonal matrices. We say that $\{|\psi_k\rangle\}_{k=1}^K$ can be *simultaneously diagonalized in weak SVD* if there exist $n \times n$ unitary matrices U and V such that UA_kV^t $(1 \le k \le K)$ are complex-valued diagonal matrices, where A_k are the matrix representations of $|\psi_k\rangle$. This kind of diagonalization can be regarded as a "*weak Schmidt decomposition*." A mixed state ρ is called *simultaneously diagonalizable in weak SVD* if there exists an ensemble $\{p_i, |\psi_i\rangle\}$ of ρ such that $\{|\psi_i\rangle\}$ can be simultaneously diagonalized in weak SVD. The previous example shows that this simultaneous diagonalization is really weaker than classical simultaneous diagonalization in SVD.

By matrix theory, see Wiegmann [34] and Gibson [35], the set of matrices $\{A_k\}_{k=1}^K$ can be simultaneously diagonalized in weak SVD if and only if

$$A_j A_k^\dagger A_l = A_l A_k^\dagger A_j, \qquad \forall 1 \le j, k, l \le K, \tag{3}$$

or if and only if $A_k^\dagger A_l$ is normal and

$$A_j A_k^\dagger A_k A_l^\dagger = A_k A_l^\dagger A_j A_k^\dagger, \qquad \forall 1 \le j, k, l \le K. \tag{4}$$

This simultaneous diagonalization was first introduced to study quantum states by [4].

The following example (whose general nature will become apparent in Section 6) shows the advantage of this generalized diagonalization. Consider a 3×3 mixed state,

$$\rho := \sum_{k=1}^{3} p_k |\psi_k\rangle \langle\psi_k|,$$

where

$$|\psi_1\rangle = \frac{1}{3}(1, 1, 1|1, \omega, \omega^2|1, \omega^2, \omega)^t,$$
$$|\psi_2\rangle = \frac{1}{3}(1, \omega, \omega^2|1, \omega^2, \omega|1, 1, 1)^t$$

and

$$|\psi_3\rangle = \frac{1}{3}(1, \omega^2, \omega|1, 1, 1|1, \omega, \omega^2)^t,$$

$p_k > 0$, $1 \le k \le 3$ and $\sum_{k=1}^3 p_k = 1$. While $\{|\psi_i\rangle\}_{i=1}^3$ have the same singular values, they cannot be simultaneously diagonalized in SVD in the classical sense. However, they can be simultaneously diagonalized in weak SVD through

$$U = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 1 & 1 \\ 1 & \omega & \omega^2 \\ 1 & \omega^2 & \omega \end{pmatrix}^\dagger, \qquad V = I,$$

where I stands for the identity matrix. Corresponding to this simultaneous diagonalization, one has

$$\rho := \sum_{k=1}^{3} p_k \left|\phi_k\right\rangle \left\langle\phi_k\right|,$$

where

$$|\phi_1\rangle = \frac{1}{\sqrt{3}}(1, 0, 0|0, 1, 0|0, 0, 1)^t,$$

$$|\phi_2\rangle = \frac{1}{\sqrt{3}}(1, 0, 0|0, \omega, 0|0, 0, \omega^2)^t,$$

$$|\phi_3\rangle = \frac{1}{\sqrt{3}}(1, 0, 0|0, \omega^2, 0|0, 0, \omega)^t.$$

Obviously this ensemble has a much clearer internal structure than the previous one. We shall discuss such states in detail in next sections.

3. Schmidt-correlated states and simultaneous diagonalization in weak SVD

Schmidt-correlated states have proven to be quite useful, see [4, 27, 29–33]. However, given a general state ρ written in the computational basis $\{|jl\rangle\}_{1\le j,l\le n}$,

$$\rho = \sum_{i,j,k,l} \rho_{ij,kl} \left|ij\right\rangle \left\langle kl\right|,$$

it is a hard problem to decide whether it is Schmidt-correlated. In this section, we provide an operational method to solve this problem.

Theorem 3.1. *For a mixed state ρ, the following are equivalent:*

(a) ρ is Schmidt-correlated.

(b) ρ is simultaneously diagonalizable in weak SVD, i.e. there exists an ensemble of ρ, $\{p_k, |\psi_k\rangle\}_{k=1}^K$, such that $\{|\psi_k\rangle\}$ is simultaneously diagonalized in weak SVD.

(c) For all ensembles of ρ, $\{q_s, |\phi_s\rangle\}_{s=1}^S$, $\{|\phi_s\rangle\}$ are simultaneously diagonalized in weak SVD.

Proof. $(a) \Longrightarrow (b)$: Let ρ be of the form (1). One can show that the matrix $C = (C_{jl})_{n\times n}$ is positive semidefinite and has trace 1. Hence the spectral theorem implies that

$$C_{jl} = \sum_{k=1}^{n} \lambda_k v_k^j (v_k^l)^*, \qquad 1 \le j, l \le n,$$

where λ_k are the eigenvalues of C satisfying $\lambda_k \ge 0$ and $\sum_{k=1}^n \lambda_k = 1$, and $(v_k^1, v_k^2, \cdots, v_k^n)^t$ are the normalized eigenvectors pertaining to λ_k. This yields

$$\rho = \sum_{k=1}^{n} \lambda_k \left(\sum_{j=1}^{n} v_k^j \left| e_j f_j \right\rangle \right) \left(\sum_{l=1}^{n} (v_k^l)^* \left\langle e_l f_l \right| \right).$$

By setting $p_k = \lambda_k$ and $|\psi_k\rangle = \sum_{j=1}^n v_k^j \left| e_j f_j \right\rangle$, we prove (b).

$(b) \Longrightarrow (a)$: This follows from direct computation.

$(c) \Longrightarrow (b)$: This is trivial.

$(a) \Longrightarrow (c)$: This follows directly from Schrödinger's mixture theorem, Theorem 8.2 in [3]. (One can also show this by an argument in [33].) By "$(a) \Longrightarrow (b)$" above, the ensemble of eigenstates of $\rho = \sum_{k=1}^n \lambda_k |\psi_k\rangle \langle\psi_k|$ is simultaneously diagonalizable. Schrödinger's mixture theorem implies that for any ensemble of ρ, $\{q_s, |\phi_s\rangle\}_{s=1}^S$, there exists an $S \times S$ unitary matrix U such that

$$|\phi_s\rangle = \frac{1}{\sqrt{q_s}} \sum_{k=1}^{n} U_{sk} \sqrt{\lambda_k} \, |\psi_k\rangle .$$

Since $\{|\psi_k\rangle\}_{k=1}^n$ is simultaneously diagonalizable, so is $\{|\phi_s\rangle\}_{s=1}^S$. □

This theorem suggests an operational method to check whether a mixed state ρ is Schmidt-correlated. First at all, we write ρ in the spectral decomposition, i.e. $\rho = \sum_{k=1}^K \lambda_k |\psi_k\rangle \langle\psi_k|$ where $\{\lambda_k\}_{k=1}^K$, are eigenvalues of ρ and $\{|\psi_k\rangle\}_{k=1}^K$ are the corresponding eigenstates. Although the spectral decomposition may not be unique, e.g. the eigenvalues has high multiplicity, by our result it suffices to check whether a particular ensemble $\{|\psi_k\rangle\}$ is simultaneously diagonalized in weak SVD. As we know, this reduces to the criteria of the simultaneous diagonalization in weak SVD by Wiegmann [34] and Gibson [35], see (3) or (4). Furthermore, one can use the process of simultaneous diagonalization to calculate the basis $\{|e_j f_l\rangle\}$ which diagonalizes $\{|\psi_k\rangle\}$.

Remark 3.1. Of course, since finding the eigenvalue decomposition of a general state involves finding the root of polynomial, this cannot be explicitly carried out in general for dimension higher than four (in practice higher than two), and it is therefore not computationally operational, but only numerical with finite accuracy. More precisely, any ensemble is valid for checking the Schmidt-correlated property, and the operational method to decompose a density matrix into a sum of projectors consists in decomposing it into the projector onto the first column and the reminder, and to iterate this. This works by polynomial formulas and together with Wiegmann's theorem it is then operational to check the property of being Schmidt correlated.

4. Separability of Schmidt-correlated states

While the problem of separability of a general mixed state is hard, for Schmidt-correlated states, i.e. simultaneously diagonalizable in weak SVD states, the criteria of separability is quite simple once we know the basis $\{|e_j f_l\rangle\}$ which diagonalizes the state. Let ρ be a mixed state of ensemble $\{p_k, |\psi_k\rangle\}_{k=1}^K$,

$$\rho := \sum_{k=1}^{K} p_k \left|\psi_k\right\rangle \left\langle\psi_k\right| , \tag{5}$$

where $\{|\psi_k\rangle\}_{k=1}^K$ can be simultaneously diagonalized in a new orthonormal basis $\{|e_j f_l\rangle\}_{1\le j,l\le n}$ such that

$$|\psi_k\rangle := \sum_{j=1}^{n} \alpha_{j,k} \left|e_j f_j\right\rangle \sim A_k = \begin{pmatrix} \alpha_{1,k} & & & \\ & \alpha_{2,k} & & \\ & & \ddots & \\ & & & \alpha_{n,k} \end{pmatrix}_{n\times n}$$

with diagonal entries $\alpha_{j,k} \in \mathbb{C}$ and $\sum_{j=1}^n |\alpha_{j,k}|^2 = 1$. The following theorem gives a necessary and sufficient condition for the separability of ρ.

Theorem 4.1. *Let ρ be a Schmidt-correlated state written in the orthonormal basis $\{|e_j f_l\rangle\}$*

$$\rho = \sum_{j,l=1}^{n} C_{jl} \left|e_j f_j\right\rangle \left\langle e_l f_l\right| .$$

Then the following are equivalent:

(a) ρ is separable.
(b) ρ is PPT (positive partial transposition).
(c) $C_{jl} = 0, \quad \forall j \neq l$.
(d) For any ensemble $\{p_k, |\psi_k\rangle\}_{k=1}^K$ of ρ, denoted by $|\psi_k\rangle := \sum_{j=1}^n \alpha_{j,k} |e_j f_j\rangle$, we have

$$\sum_{k=1}^{K} p_k \alpha_{j,k} \alpha_{l,k}^{*} = 0 \tag{6}$$

for all $j \neq l,\ 1 \le j, l \le n$, where $*$ denotes complex conjugate.
(e) For any ensemble of ρ, (6) holds.

Remark 4.1. For states of rank at most n, the separability is equivalent to the PPT property which has been obtained by Horodecki-Lewenstein-Vidal-Cirac [43]. For special Schmidt-correlated states, we give a simple proof here by direct calculation.

Proof. Direct computation shows that $(c), (d), (e)$ are equivalent.

$(a) \Longrightarrow (b)$: This follows from a theorem of Peres [44].

$(b) \Longrightarrow (c)$: We use a contradiction argument. Suppose there exist $1 \leq j_0 < l_0 \leq n$ such that $C_{j_0 l_0} \neq 0$, then we will show that ρ is NPPT (non-positive partial transposition). In fact, taking the partial transpose of the second subsystem of ρ yields

$$\rho^{T_B} = \sum_{1 \leq j,l \leq n} C_{jl} \left| e_j f_l \right\rangle \left\langle e_l f_j \right|.$$

Since one of the principal minors of order two of ρ^{T_B} reads as

$$\begin{vmatrix} (\rho^{T_B})_{j_0 l_0, j_0 l_0} & (\rho^{T_B})_{j_0 l_0, l_0 j_0} \\ (\rho^{T_B})_{l_0 j_0, j_0 l_0} & (\rho^{T_B})_{l_0 j_0, l_0 j_0} \end{vmatrix} = -\left| C_{j_0 l_0} \right|^2 < 0,$$

we have $\rho^{T_B} \ngeq 0$. Hence, ρ is NPPT.

$(c) \Longrightarrow (a)$: Obviously, $\rho = \sum_j C_{jj} \left| e_j f_j \right\rangle \left\langle e_j f_j \right|$ is separable. $\square$

5. Entanglement of Schmidt-correlated states

The states we are considering provide us more information about the entanglement. Let us first consider a 2×2 pure entangled state

$$|\psi\rangle = \alpha \left|00\right\rangle + \beta \left|11\right\rangle \ \in \mathcal{H} = \mathcal{H}_A^2 \times \mathcal{H}_B^2,$$

where $|\alpha|^2 + |\beta|^2 = 1$. It yields the density matrix

$$\rho = |\psi\rangle \langle\psi| = \left(\begin{array}{cc:cc} |\alpha|^2 & 0 & 0 & \alpha\bar{\beta} \\ 0 & 0 & 0 & 0 \\ \hdashline 0 & 0 & 0 & 0 \\ \bar{\alpha}\beta & 0 & 0 & |\beta|^2 \end{array}\right).$$

It is entangled if $\alpha, \beta \neq 0$. Defined by the von Neumann entropy of the reduced density matrices, the entanglement of formation is given by

$$E(|\psi\rangle) = -|\alpha|^2 \log |\alpha|^2 - |\beta|^2 \log |\beta|^2. \tag{7}$$

Consider a mixed state,

$$\rho = p \left|\psi\right\rangle \left\langle\psi\right| + p' \left|\psi'\right\rangle \left\langle\psi'\right| = \left(\begin{array}{cc:cc} p|\alpha|^2 + p'|\alpha'|^2 & 0 & 0 & p\alpha\bar{\beta} + p'\alpha'\bar{\beta}' \\ 0 & 0 & 0 & 0 \\ \hdashline 0 & 0 & 0 & 0 \\ p\bar{\alpha}\beta + p'\bar{\alpha'}\beta' & 0 & 0 & p|\beta|^2 + p'|\beta'|^2 \end{array}\right).$$

where $p, p' \geq 0$, $p + p' = 1$, $|\psi\rangle = (\alpha, 0|0, \beta)^t$ and $|\psi'\rangle = (\alpha', 0|0, \beta')^t$ with $\alpha, \beta, \alpha', \beta' \in \mathbb{C}$ and $|\alpha|^2 + |\beta|^2 = 1$, $|\alpha'|^2 + |\beta'|^2 = 1$. Then ρ is separable if and only if $p\alpha\bar{\beta} + p'\alpha'\bar{\beta}' = 0$. In fact, the concurrence of ρ is given by

$$C(\rho) = 2|p\alpha\bar{\beta} + p'\alpha'\bar{\beta}'|. \tag{8}$$

From (7) and (8) it is clear that, for a pure state the entanglement is given by the diagonal elements in the Schmidt form. Nevertheless, for mixed states, the diagonal elements do not play such "important roles".

Now we turn to the 3×3 case. Let $|\psi\rangle = (\alpha, 0, 0|0, \beta, 0|0, 0, \gamma)^t$. Then

$$\rho = |\psi\rangle \langle\psi| = \left(\begin{array}{ccc:ccc:ccc} |\alpha|^2 & 0 & 0 & 0 & \alpha\bar{\beta} & 0 & 0 & 0 & \alpha\bar{\gamma} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hdashline 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \bar{\alpha}\beta & 0 & 0 & 0 & |\beta|^2 & 0 & 0 & 0 & \beta\bar{\gamma} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hdashline 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \bar{\alpha}\gamma & 0 & 0 & 0 & \bar{\beta}\gamma & 0 & 0 & 0 & |\gamma|^2 \end{array}\right).$$

ρ is entangled if at least one of the terms $\alpha\bar{\beta}, \alpha\bar{\gamma}, \beta\bar{\gamma}$ is nonvanishing.

Similarly for a 3×3 mixed state $\rho = p\,|\psi\rangle\langle\psi| + p'\,|\psi'\rangle\langle\psi'| + p''\,|\psi''\rangle\langle\psi''|$ with $p, p', p'' \geq 0$, $p + p' + p'' = 1$,

$$\begin{aligned} |\psi\rangle &= (\alpha, 0, 0|0, \beta, 0|0, 0, \gamma)^t, \\ |\psi'\rangle &= (\alpha', 0, 0|0, \beta', 0|0, 0, \gamma')^t, \\ |\psi''\rangle &= (\alpha'', 0, 0|0, \beta'', 0|0, 0, \gamma'')^t, \end{aligned}$$

where $\alpha, \beta, \gamma, \alpha', \beta', \gamma', \alpha'', \beta'', \gamma'' \in \mathbb{C}$, $|\alpha|^2 + |\beta|^2 + |\gamma|^2 = 1$, $|\alpha'|^2 + |\beta'|^2 + |\gamma'|^2 = 1$ and $|\alpha''|^2 + |\beta''|^2 + |\gamma''|^2 = 1$. The corresponding density matrix ρ is

$$\left(\begin{array}{ccc:ccc:ccc} p|\alpha|^2 + p'|\alpha'|^2 + p''|\alpha''|^2 & 0 & 0 & 0 & p\alpha\bar{\beta} + p'\alpha'\bar{\beta}' + p''\alpha''\bar{\beta}'' & 0 & 0 & 0 & p\alpha\bar{\gamma} + p'\alpha'\bar{\gamma}' + p''\alpha''\bar{\gamma}'' \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hdashline 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ p\bar{\alpha}\beta + p'\bar{\alpha}'\beta' + p''\bar{\alpha}''\beta'' & 0 & 0 & 0 & p|\beta|^2 + p'|\beta'|^2 + p''|\beta''|^2 & 0 & 0 & 0 & p\beta\bar{\gamma} + p'\beta'\bar{\gamma}' + p''\beta''\bar{\gamma}'' \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hdashline 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ p\bar{\alpha}\gamma + p'\bar{\alpha}'\gamma' + p''\bar{\alpha}''\gamma'' & 0 & 0 & 0 & p\bar{\beta}\gamma + p'\bar{\beta}'\gamma' + p''\bar{\beta}''\gamma'' & 0 & 0 & 0 & p|\gamma|^2 + p'|\gamma'|^2 + p''|\gamma''|^2 \end{array}\right).$$

The three key entries in ρ are $T_{1,2} := p\alpha\bar{\beta} + p'\alpha'\bar{\beta}' + p''\alpha''\bar{\beta}''$, $T_{1,3} := p\alpha\bar{\gamma} + p'\alpha'\bar{\gamma}' + p''\alpha''\bar{\gamma}''$ and $T_{2,3} := p\beta\bar{\gamma} + p'\beta'\bar{\gamma}' + p''\beta''\bar{\gamma}''$. The mixed state ρ is entangled if and only if at least one of the terms $T_{1,2}, T_{1,3}$ and $T_{2,3}$ is nonzero. These three quantities provide more detailed information about the entanglement. In fact, one can somehow quantify the entanglement of the state by the vector $(T_{1,2}, T_{1,3}, T_{2,3})$.

Obviously, the previous discussions apply to any $n \times n$ bipartite system for such special states.

6. Generalized Bell bases and complex Hadamard matrices

In this section, we introduce generalized Bell bases and explore their connections with Hadamard matrices and the separability criterion. This is motivated by the fact that the computational basis $|jl\rangle$, while usually used when investigating entanglement, is not always the most suitable one for our purposes. In particular, mixed states that have ensembles of pure states which can be simultaneously diagonalized should rather be investigated in that diagonalized form as this involves the least number of parameters. As the separability concerns the question to what extent a state behaves like a product state, the non-separability is however quantified by entanglement. Hence one should look at the length of the projection of a given state onto the maximally entangled states. Therefore we introduce a new kind of bases consisting of maximal entangled states, called generalized Bell bases (see (9) below), which contains the specific Bell-states for the case of qubit pairs.

First we want to find nontrivial solutions of the system of equations (6). We restrict to the following class of states.

Assumption 6.1. *The Schmidt-correlated state ρ written in* (5) *satisfies*
(a) $K = n$,
(b) $|\alpha_{j,k}| = a_j \neq 0$ *for any* $1 \leq j, k \leq n$,
(c) $p_k = 1/n$ *for all* $1 \leq k \leq n$.

The normalization conditions require that $\sum_{j=1}^{n} a_j^2 = 1$. In polar coordinates, one can write $\alpha_{j,k} = a_j e^{i\theta_{j,k}}$. In fact, we will figure out soon that only the phases $(e^{\theta_{j,k}})$ matter for the separability of ρ in this case. In characterizing all the solutions of (6), the key observation is that the orthogonality conditions of Theorem 4.1 translates into the conditions for a complex Hadamard matrix. Here, an $n \times n$ complex matrix H is called a *complex Hadamard matrix*, see [5, 45, 46], if $|H_{j,k}| = 1$ for all $1 \leq j, k \leq n$ and $HH^{\dagger} = nI$. Equivalently, $\frac{1}{\sqrt{n}} H$ is a unitary matrix.

Theorem 6.1. *Let ρ be a Schmidt-correlated state which is an ensemble of $\{p_k, |\psi_k\rangle\}_{k=1}^{K}$ with $|\psi_k\rangle = \sum_{j=1}^{K} \alpha_{j,k} |e_j f_j\rangle$ for an orthonormal basis $|e_j f_l\rangle$ satisfying Assumption 6.1. Then ρ is separable if and only if $(e^{i\theta_{j,k}})_{n\times n}$ is a complex Hadamard matrix, where $e^{i\theta_{j,k}}$ is the phase factor of $\alpha_{j,k}$.*

Proof. It follows from Theorem 4.1 that the separability is equivalent to the equations (6). It is obvious that $|e^{i\theta_{j,k}}| = 1$ for all $1 \leq j, k \leq n$. By Assumption 6.1, $p_k = 1/n, \alpha_{j,k} = a_j e^{i\theta_{j,k}}$, we have

$$
\begin{aligned}
(6) \quad &\Longleftrightarrow \quad \frac{1}{n} a_j a_k \sum_{k=1}^{n} e^{i\theta_{j,k}} (e^{i\theta_{l,k}})^* = 0 \quad (j \neq l), \\
&\Longleftrightarrow \quad \sum_{k=1}^{n} e^{i\theta_{j,k}} (e^{i\theta_{l,k}})^* = 0 \quad (j \neq l).
\end{aligned}
$$

This is equivalent to the property that $(e^{i\theta_{j,k}})_{n\times n}$ is a complex Hadamard matrix. $\square$

Remark 6.1. The moduli of the diagonal entries, a_j, in Assumption 6.1 can be chosen arbitrarily (as long as the normalization condition $\sum_{j=1}^{n} a_j^2 = 1$

holds). This theorem indicates that when the phase factors $(e^{i\theta_{j,k}})$ constitute a complex Hadamard matrix, no matter what a_j are, the state ρ becomes separable.

By the theory of complex Hadamard matrices, there always exists a solution to (6) for any $n \in \mathbb{N}$ under Assumption 6.1. For instance, for any n the Fourier matrix $F_n := (H_{j,k})_{n\times n} := (e^{i(j-1)(k-1)\frac{2\pi}{n}})_{n\times n}$ is an Hadamard matrix. Two Hadamard matrices, H_1 and H_2, are called equivalent if there exist diagonal unitary matrices D_1 and D_2 and permutation matrices P_1 and P_2 such that

$$H_1 = D_1 P_1 H_2 P_2 D_2.$$

For the classification up to this equivalence of Hadamard matrices for $n \le 5$, see e.g. Tadej and Zyczkowski [5]. For instance, the Fourier matrix is the only Hadamard matrix for $n = 3$ and $n = 5$. For $n = 4$, there is a continuous non-equivalent family of Hadamard matrices. For $n \ge 6$, things become more complicated. In particular, a complete classification of Hadamard matrices of order 6 is still unknown.

For $n = 3$, $\rho = 1/n \sum_{k=1}^{n} |\psi_k\rangle\langle\psi_k|$ is then separable if and only if, up to the equivalence of Hadamard matrices,

$$(e^{i\theta_{j,k}})_{3\times 3} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & \omega & \omega^2 \\ 1 & \omega^2 & \omega \end{pmatrix},$$

where $\omega = \frac{1}{2} + i\frac{\sqrt{3}}{2}$, i.e.,

$$|\psi_1\rangle \sim \begin{pmatrix} a_1 & & \\ & a_2 & \\ & & a_3 \end{pmatrix}, \quad |\psi_2\rangle \sim \begin{pmatrix} a_1 & & \\ & a_2\omega & \\ & & a_3\omega^2 \end{pmatrix}, \quad |\psi_3\rangle \sim \begin{pmatrix} a_1 & & \\ & a_2\omega^2 & \\ & & a_3\omega \end{pmatrix}.$$

In higher dimensions, there are more freedom for the existence of Hadamard matrices and the corresponding constructions of separable states. Our result connnects the separability problem to the study of Hadamard matrices.

We now construct generalized Bell bases for $\mathcal{H}_A^n \times \mathcal{H}_B^n$ by Hadamard matrices. Let

$$\begin{aligned} |\psi_l^1\rangle &= \frac{1}{\sqrt{n}} \sum_{j=1}^{n} e^{i\phi_{j,l}^1} |j, j\rangle, \\ |\psi_l^2\rangle &= \frac{1}{\sqrt{n}} \sum_{j=1}^{n} e^{i\phi_{j,l}^2} |j, j+1\rangle, \qquad (9) \\ &\cdots\cdots \\ |\psi_l^n\rangle &= \frac{1}{\sqrt{n}} \sum_{j=1}^{n} e^{i\phi_{j,l}^n} |j, j+n-1\rangle, \end{aligned}$$

where we count $j + n - 1 \pmod n$, $1 \le l \le n$, and $(e^{i\phi_{j,l}^s})_{j,l}$ is a Hadamard matrix for any fixed $1 \le s \le n$. One finds that $\{|\psi_l^k\rangle\}_{1\le l,k\le n}$ constitute an orthonormal basis of $\mathcal{H}_A^n \times \mathcal{H}_B^n$. By using Hadamard matrices, we know that $|\psi_l^k\rangle$, $1 \leq l, k \leq n$, is maximally entangled. Therefore, any mixed state ρ can be written as

$$\rho = \sum_{1 \leq l,k,m,j \leq n} \rho_{lk,mj} \left|\psi_l^k\right\rangle \left\langle\psi_m^j\right| .$$

When we choose $(e^{\phi_{j,l}^s})_{n\times n} = F_n$ in (9) for $1 \leq s \leq n$, where F_n is the Fourier matrix of order n, we recover the well-known Weyl operator basis. The Weyl operators have been introduced in the context of quantum teleportation [36] and investigated thoroughly in the literature (see e.g. [37–40]). Note that our generalized Bell bases possess more freedom, as we may choose any complex Hadamard matrices. In higher dimensions, there exist plenty of complex Hadamard matrices, offering a potential for new applications. Let us consider an example:

Example 6.1. *For $n = 4$, besides the Weyl basis there exist many other Bell bases. Let*

$$(e^{\phi_{j,l}^s})_{4\times 4} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & ie^{ia_s} & -1 & -ie^{ia_s} \\ 1 & -1 & 1 & -1 \\ 1 & -ie^{ia_s} & -1 & ie^{ia_s} \end{pmatrix},$$

where $1 \leq s \leq 4$ and $a_s \in \mathbb{R}$. These are Hadamard matrices, see (65) in Section 5.4 [5]. Then for any $a_s \in \mathbb{R}$, $1 \leq s \leq 4$, we have the following Bell basis:

$$\begin{pmatrix} 1 &&& \\ & 1 && \\ && 1 & \\ &&& 1 \end{pmatrix}, \begin{pmatrix} 1 &&& \\ & ie^{ia_1} && \\ && -1 & \\ &&& -ie^{ia_1} \end{pmatrix}, \begin{pmatrix} 1 &&& \\ & -1 && \\ && 1 & \\ &&& -1 \end{pmatrix}, \begin{pmatrix} 1 &&& \\ & -ie^{ia_1} && \\ && -1 & \\ &&& ie^{ia_1} \end{pmatrix};$$

$$\begin{pmatrix} & 1 && \\ && 1 & \\ &&& 1 \\ 1 &&& \end{pmatrix}, \begin{pmatrix} & 1 && \\ && ie^{ia_2} & \\ &&& -1 \\ -ie^{ia_2} &&& \end{pmatrix}, \begin{pmatrix} & 1 && \\ && -1 & \\ &&& 1 \\ -1 &&& \end{pmatrix}, \begin{pmatrix} & 1 && \\ && -ie^{ia_2} & \\ &&& -1 \\ ie^{ia_2} &&& \end{pmatrix};$$

$$\begin{pmatrix} && 1 & \\ &&& 1 \\ 1 &&& \\ & 1 && \end{pmatrix}, \begin{pmatrix} && 1 & \\ &&& ie^{ia_3} \\ -1 &&& \\ & -ie^{ia_3} && \end{pmatrix}, \begin{pmatrix} && 1 & \\ &&& -1 \\ 1 &&& \\ & -1 && \end{pmatrix}, \begin{pmatrix} && 1 & \\ &&& -ie^{ia_3} \\ -1 &&& \\ & ie^{ia_3} && \end{pmatrix};$$

$$\begin{pmatrix} &&& 1 \\ 1 &&& \\ & 1 && \\ && 1 & \end{pmatrix}, \begin{pmatrix} &&& 1 \\ ie^{ia_4} &&& \\ & -1 && \\ && -ie^{ia_4} & \end{pmatrix}, \begin{pmatrix} &&& 1 \\ -1 &&& \\ & 1 && \\ && -1 & \end{pmatrix}, \begin{pmatrix} &&& 1 \\ -ie^{ia_4} &&& \\ & -1 && \\ && ie^{ia_4} & \end{pmatrix}.$$

In [47] the case of

$$\rho = \sum_{1 \leq j,l \leq n} \rho_{jl,jl} \left|\psi_l^j\right\rangle \left\langle\psi_l^j\right|$$

for $n = 3$ has been investigated. In the present paper, we have studied in detail the mixed state

$$\rho = \sum_{1 \leq l \leq n} \rho_{jl,jl} \left| \psi_l^j \right\rangle \left\langle \psi_l^j \right| \tag{10}$$

for fixed j, $1 \leq j \leq n$, and arbitrary dimension $n \geq 2$.

7. Conclusion and remarks

We have studied the weak Schmidt decomposition of quantum states in which the generalized Schmidt coefficients are allowed to be complex-valued. Using this concept, we can identify all so-called Schmidt-correlated states by verifying the spectral decomposition of the states, hence provide an operational method to the identification of Schmidt-correlated states. The separability of such states has been translated into the orthogonality condition of the diagonal entries of eigenstates of any ensemble. Moreover, we have introduced generalized Bell bases and presented their connections with Hadamard matrices and separability criteria. Our construction of generalized Bell bases includes the well-known Weyl operator basis as a special case. These mathematical structures and relations among the separability, weak Schmidt decompositions, Hadamard matrices, generalized Bell bases etc. may help in the further characterization of quantum entanglement.

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