

Local unitary equivalence and entanglement of multipartite pure states

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The necessary and sufficient conditions for the equivalence of arbitrary n -qubit pure quantum states under local unitary (LU) operations derived in [B. Kraus, *Phys. Rev. Lett.* **104**, 020504 (2010)] are used to determine the different LU-equivalence classes of up to five-qubit states. Due to this classification new parameters characterizing multipartite entanglement are found and their physical interpretation is given. Moreover, the method is used to derive examples of two n -qubit states (with $n > 2$ arbitrary) which have the properties that all the entropies of any subsystem coincide; however, the states are neither LU equivalent nor can be mapped into each other by general local operations and classical communication.

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I. INTRODUCTION

The subtle properties of multipartite entangled states allow for many fascinating applications of quantum information, such as one-way quantum computing, quantum error correction, and quantum secret sharing [1,2]. The theory of many-body states also plays an important role in other fields of physics which deal with many-body systems [3]. Thus, the investigation of the nonlocal properties of quantum states is at the heart of quantum information theory. Compared to the bipartite case, which is well understood, the multipartite case is much more complex due to the exponential growth in the dimension of the Hilbert space. Despite its relevance and the enormous effort of theorists, many problems regarding multipartite entanglement are still unsolved [4]. Several entanglement measures for multipartite states, such as the tangle [5], the Schmidt measure [6], the localizable entanglement [7], and geometric measure of entanglement [8] have been introduced. Moreover, different classes of entangled states have been identified [9], and a normal form of multipartite states has been presented [10]. However, even for the simplest case of three qubits the entanglement properties are still not completely understood. One of the main reasons for the lack of knowledge is, arguably, that for many-body entangled states we do have only few applications [4]. This results in the existence of few known operational entanglement measures.

One approach to gaining insight into the complicated structure of multipartite states is to consider a restricted class of states, such as stabilizer states [1], matrix-product states [11], projected entangled pair states [12], locally maximally entangleable states (LMESs) [13], or Gaussian state [14]. Considering a restricted set of states enabled researchers to gain a lot of intuition about the usefulness and manipulation of them. This knowledge in turn led to many of the fascinating applications of multipartite states.

Another way to gain insight into the entanglement properties of quantum states is to consider their interconvertibility. That is, given two states $|\Psi\rangle, |\Phi\rangle$ the question is whether $|\Psi\rangle$ can be transformed into $|\Phi\rangle$ by local operations [4]. One particularly interesting case is the LU equivalence of multipartite states. We say that a n -partite state, $|\Psi\rangle$, is LU equivalent to $|\Phi\rangle$ ($|\Psi\rangle \simeq_{\text{LU}} |\Phi\rangle$) if there exist local unitary operators, U_1, \dots, U_n , such that $|\Psi\rangle = U_1 \otimes \dots \otimes U_n |\Phi\rangle$. Note that two states which are LU equivalent are equally

useful for any kind of application and they possess precisely the same amount of entanglement. Another insight is gained by considering more general operations, such as (deterministic) local operations and classical communication (LOCC). Since entanglement cannot increase under LOCC, a state, $|\Psi\rangle$, which can be mapped into the state $|\Phi\rangle$ by LOCC is necessarily at least as entangled as $|\Phi\rangle$. Thus, all these investigations of convertibility led to a new insight into the general problem of characterizing the different types of entangled quantum states.

In this article we mainly focus on the LU equivalence of multipartite states. Local polynomial invariants have been introduced to distinguish the different LU equivalence classes [15]. However, even though it is known that it is sufficient to consider only a finite set of them, this complete finite set is known only for very few simple cases. In [16] a method for solving the LU-equivalence problem for arbitrary n -qubit states has been presented. There an algorithm which determines the local unitaries, which map the states into each other (if they exist) has been derived. Within this algorithm, different classes of states, which are easily characterized, are distinguished. It has been shown that two states which are within two different classes cannot have the same entanglement.

Here, we use the algorithm presented in [16] in order to investigate the nonlocal properties of multipartite states. We present the LU-equivalence classes of few-body systems and obtain a new insight into multipartite entanglement. The main results derived here are summarized in Sec. II.

The remainder of the article is organized as follows. After presenting the main results of this article (Sec. II), we review the necessary and sufficient conditions for LU equivalence derived in [16]. In Sec. IV we derive some additional methods to determine the local unitaries (if they exist) which interconvert the two states. In Sec. V we characterize the LU-equivalence classes of up to four qubits. For five-qubit states we consider the most challenging class (for using the algorithm) and show how the local unitaries can be determined then. For an arbitrary n (with $n > 2$), the existence of n -qubit states, $|\Psi\rangle$, which are not LU equivalent to their complex conjugate are shown by presenting examples in Sec. VI. In Sec. VII it is shown how the algorithm can be employed to solve the LU-equivalence problem for certain mixed states and also states which describe d -level systems. The new

insight gained into multipartite entanglement is discussed in Sec. VIII.

Throughout this article the following notation is used. The Pauli operators are mainly denoted by X , Y , and Z . Whenever we need the whole set of Pauli operators, we use the notation $\Sigma_1 = X$, $\Sigma_2 = Y$, and $\Sigma_3 = Z$ and H denotes the Hadamard transformation. Otherwise, the subscript of an operator always denotes the system it is acting on or the system it is describing. The reduced states of system i_1, \dots, i_k of $|\Psi\rangle$ ($|\Phi\rangle$) are always be denoted by ρ_{i_1, \dots, i_k} (σ_{i_1, \dots, i_k}) respectively; that is, $\rho_{i_1, \dots, i_k} = \text{tr}_{\neg i_1, \dots, \neg i_k}(|\Psi\rangle\langle\Psi|)$. We denote by \mathbf{i} the classical bit string (i_1, \dots, i_n) , with $i_k \in \{0, 1\} \forall k \in \{1, \dots, n\}$, and $|\mathbf{i}\rangle \equiv |i_1, \dots, i_n\rangle$ denotes the computational basis. Normalization factors as well as the tensor product symbol is omitted whenever it does not cause any confusion and $\mathbb{1}$ denotes the normalized identity operator. The eigenvalues of some matrix M are denoted by $\text{eig}(M)$. For a subsystem A we denote by $E_A(|\Psi\rangle)$ the bipartite entanglement between A and the remaining systems measured with the Von Neumann entropy of the reduced state, ρ_A . For instance, $E_i(|\Psi\rangle) = S(\rho_i)$ denotes the entanglement between qubit i and the remaining $n - 1$ qubits. As commonly used, the states $|\Phi^\pm\rangle = |00\rangle \pm |11\rangle$, $|\Psi^\pm\rangle = |01\rangle \pm |10\rangle$ denote the Bell basis. The state $|\Psi^*\rangle$ denotes the complex conjugate of the state $|\Psi\rangle$ in the computational basis and M^T denotes the transpose of an operator M in the computational basis. Moreover, the matrix $R_w(\alpha)$ with $w \in x, y, z$ denotes the rotation around the w axis with rotation angle α .

II. MAIN RESULTS

On the one hand, the criterion for LU equivalence [16] is used to characterize the LU-equivalence classes for few-body states. On the other hand, it will be employed to shed new light on multipartite entanglement. Furthermore, the criterion will be generalized to certain mixed states and also states which describe d -level systems. The main results derived here can be summarized as follows.

(i) Characterization of LU-equivalence classes: The LU-equivalence classes of quantum states describing up to five qubits are characterized. For two-, three-, and four-qubit states, all the classes are explicitly derived. For five-qubit states, whose classification would work analogously, only the most challenging subset of states are considered. It is explicitly shown how the algorithm can be used to determine the local unitaries (if they exist) which transform one state to the other.

(ii) New insight into multipartite entanglement:

(a) The algorithm presented in [16] distinguishes between different classes of states, such as the class of states with $\rho_{12} = \rho_1 \otimes \mathbb{1}_2$ and the one with $\rho_{12} \neq \rho_1 \otimes \mathbb{1}_2$. It is shown how this classification enables us to gain a new insight into multipartite entanglement. For instance, one class would be the one where one of the two-qubit reduced states is completely mixed. For four-qubit states it is shown that this class is completely characterized by only three nonlocal parameters. Moreover, it is proven that two states within this class are LU equivalent if and only if (iff) the corresponding sets of three parameters coincide. Naturally, all the entanglement contained in a state within this class is also determined by those three parameters to which the

following operational meaning can be given. Recall that the completely positive map (CPM), \mathcal{E}_Ψ , corresponding to a state $|\Psi\rangle$ via the Choi-Jamiołkowski isomorphism [17] can be implemented using a system prepared in the state $|\Psi\rangle$ and local operations. It is shown that the nonlocal content of the CPM, \mathcal{E}_Ψ , is characterized by the three parameters mentioned earlier and vice versa. This leads to the new approach to characterizing the entanglement of a multipartite state by the entangling capability of the operation which can be implemented using the state as the only nonlocal resource.

This suggests a new method of characterizing the entanglement contained in an arbitrary multipartite state: First, divide the Hilbert space into the entanglement classes resulting from the algorithm in [16]. Note that these classes can be easily characterized. Then the entanglement of a state within a certain class should be qualified and quantified. Probably, the different classes might also lead to different applications. For instance, for error correction, one-way quantum computing, and quantum secret sharing, we have that all the employed states have the property that all single-qubit reduced states are completely mixed.

(b) The other new insight into multipartite entanglement which we derive here using the LU-equivalence criterion is the following. For any $n > 2$ examples of n -qubit states, $|\Psi\rangle$ and $|\Phi\rangle$, which have the properties that for any subsystem A , composed of arbitrary many qubits, the eigenvalues of the reduced states, $\rho_A = \text{tr}_{\neg A}(|\Psi\rangle\langle\Psi|)$ and $\sigma_A = \text{tr}_{\neg A}(|\Phi\rangle\langle\Phi|)$ coincide, are presented. Therefore, all the bipartite entanglement in those two states, measured with the von Neumann entropy of the reduced states, coincide. It is shown, however, that the states are neither LU equivalent nor LOCC comparable. Therefore, neither $|\Psi\rangle$ can be mapped into $|\Phi\rangle$ by LOCC nor vice versa. Surprisingly, in those examples we have $|\Phi\rangle = |\Psi^*\rangle$, where $|\Psi^*\rangle$ denotes the complex conjugate of $|\Psi\rangle$ in the computational basis. The fact that $|\Psi\rangle$ and $|\Psi^*\rangle$ can have so different nonlocal properties does not seem very physical. As a consequence of the existence of these states it is suggested to divide the Hilbert space into two subsets, in case $|\Psi\rangle$ is not LU equivalent to $|\Psi^*\rangle$: one which corresponds to $|\Psi\rangle$ and one which corresponds to its complex conjugate. The nonlocal properties should then be investigated within one of the subsets since there will not be a physical measure which will distinguish between $|\Psi\rangle$ and $|\Psi^*\rangle$.

(iii) Generalization of LU-equivalence criterion: It is demonstrated how the solution of the LU equivalence for pure n -qubit states can be generalized to mixed states and also to d -level systems.

III. LU EQUIVALENCE OF MULTIPARTITE STATES

Here we briefly summarize the necessary and sufficient conditions for the existence of LU operations which transform two n -qubit states to each other [16]. We first review a standard form for multipartite states (see also [18] and [13]) and provide some examples of states in their standard form. It has been shown that two generic multipartite states, that is, states where none of the single-qubit reduced states is proportional to the

identity, are, such as in the bipartite case, LU equivalent iff their standard forms coincide [16]. For nongeneric states the systematic method of determining the local unitaries (if they exist) which interconvert two arbitrary states is reviewed.

A. Standard form of multipartite states

Let us first recall the definition of the standard form for multipartite states. Any decomposition of a multipartite state which has the property that the single-qubit reduced states are all diagonal in the computational basis is called trace decomposition. It is obtained by applying local unitary transformations, U_i^1 , which diagonalize the single-qubit reduced states, ρ_i ; that is, $U_i^1 \rho_i (U_i^1)^\dagger = D_i \equiv \text{diag}(\lambda_i^1, \lambda_i^2)$. A sorted trace decomposition, which we denote by $|\Psi_{\text{st}}\rangle$ in the following, is then defined as a trace decomposition with $\lambda_i^1 \geq \lambda_i^2$. The sorted trace decomposition of a generic state, $|\Psi\rangle$ with $\rho_i \neq \mathbb{1} \forall i$ is unique up to local phase gates. That is $U_1, \dots, U_n |\Psi_{\text{st}}\rangle$ is a sorted trace decomposition of a generic state, $|\Psi\rangle$, iff (up to a global phase, α_0) $U_i = Z_i(\alpha_i) \equiv \text{diag}(1, e^{i\alpha_i})$. It is straightforward to impose certain conditions on the phases $\alpha_i, i \in \{0, \dots, n\}$ in order to make the sorted trace decomposition of generic states unique [16]. We call this unique sorted trace decomposition the standard form of the multipartite state. Note that any state can be transformed into its standard form by local unitary operations.

Let us now also recall how the standard form can be defined for states with $\rho_i = \mathbb{1}$, for some system i [13]. In this case the standard form can be chosen to be $\lim_{\epsilon \rightarrow 0} |\Psi(\epsilon)\rangle$, where $|\Psi(\epsilon)\rangle$ denotes the unique standard form of $\sqrt{1-\epsilon}|\Psi\rangle + \sqrt{\epsilon}|\mathbf{0}\rangle$, where the phase gates are fixed by the same conditions as for generic states [13]. It should be noted here that for nongeneric states the standard form is not unique, as can be seen by the following simple example of a three-qubit states. Both the GHZ state $|\Psi\rangle = |000\rangle + |111\rangle$ and $HHH|\Psi\rangle$ are standard forms of the state $|\Psi\rangle$; however, they do not coincide.

Let us now derive the standard form for some examples. For two-qubit states the standard form coincides with the Schmidt decomposition [19]. In [20] the standard form of three-qubit states has been derived. In order to present the standard forms of certain n -partite states we recall here the notion of the so-called LMESs [13]. LMESs have been introduced as a new, physically motivated classification of pure quantum states describing n qubits. A state is called LMES if local auxiliary qubits can be attached to the system qubits in such a way that the resulting state is maximally entangled in the bipartite splitting system qubits versus auxiliary qubits. To be more precise, a state $|\Psi\rangle$ is a LMES if there exist local control operations $C_i = |0\rangle\langle 0| \otimes U_i^0 + |1\rangle\langle 1| \otimes U_i^1$, with $U_i^{0,1}$ single-qubit unitary operators acting on the system qubit i such that the $2n$ -qubit state $C_1 \otimes C_2 \otimes \dots \otimes C_n |\Psi\rangle |+\rangle^{\otimes n}$, with $|+\rangle = 1/\sqrt{2}(|0\rangle + |1\rangle)$, is a maximally entangled state between the system and the auxiliary systems. This set of states coincides with the set of states which can be used to encode locally the maximum amount of n independent bits. Prominent examples of these states are the stabilizer states, which are used for quantum error correction and one-way quantum computing. In [13] it has been shown that a state is

LME iff it is LU equivalent to a state of the form

$$|\Psi\rangle = \sqrt{\frac{1}{2^n}} \sum_{\mathbf{i}} e^{i\alpha_{\mathbf{i}}} |\mathbf{i}\rangle \equiv U_{ph}^\Psi |+\rangle^{\otimes n}, \tag{1}$$

where $\alpha_{\mathbf{i}} \in \mathcal{R}$ and U_{ph}^Ψ denotes the diagonal unitary operator with entries $e^{i\alpha_{\mathbf{i}}}$. Thus, a state is LME iff there exists a product basis such that all the coefficients of the state in this basis are phases.

Note that all those states can be easily transformed into their trace decomposition by applying the local unitary operations HU_i , where $U_i = \text{diag}(e^{i\phi_i}, 1)$, with $\cot(\phi_i) = \frac{\langle X_i \rangle}{\langle Y_i \rangle}$ if $\langle Y_i \rangle \neq 0$ and $\phi_i = 0$ else. To derive the trace decomposition from the standard form one simply has to impose the conditions on the local phase gates, as mentioned earlier.

B. Criterion for LU equivalence

Since the standard form is unique for generic states we have, similarly to the bipartite case, that two generic states are LU equivalent iff their standard forms are equivalent.

Let us now turn to the more complicated case of nongeneric states. First, the condition of LU equivalence for generic states is rewritten in the following way. It can be easily seen that the standard forms of two generic states, $|\Psi\rangle$ and $|\Phi\rangle$, are equivalent iff there exists a bit string $\mathbf{k} = (k_1, \dots, k_n)$, local phase gates $Z_i(\alpha_i)$, and a global phase α_0 such that

$$e^{i\alpha_0} \bigotimes_i Z_i(\alpha_i) X_i^{k_i} W_i |\Psi\rangle = \bigotimes_i V_i |\Phi\rangle, \tag{2}$$

where W_i and V_i are local unitaries which diagonalize ρ_i (σ_i). That is, $\bigotimes_i W_i |\Psi\rangle$ and $\bigotimes_i V_i |\Phi\rangle$ are trace decompositions of $|\Psi\rangle$ and $|\Phi\rangle$, respectively. For generic states, k_i is chosen such that the order of the eigenvalues of the single-qubit reduced states of $\bigotimes_i X_i^{k_i} W_i |\Psi\rangle$ and $\bigotimes_i V_i |\Phi\rangle$ coincides and the phases α_i are chosen to fulfill the conditions mentioned earlier [16]. Note that the reason for the freedom of the phase gates in Eq. (2) is simply due to the fact that we have been considering only single-qubit reduced states to define the trace decomposition of multipartite states.

Obviously, two arbitrary states $|\Psi\rangle$ and $|\Phi\rangle$ are LU equivalent iff there exist local unitaries V_i and W_i and a bit string $\mathbf{k} = (k_1, \dots, k_n)$ and phases α_i such that Eq. (2) is fulfilled. For nongeneric states, a constructive method of determining the unitaries V_i and W_i in Eq. (2) has been presented in [16]. Once those unitaries are fixed it is then easy to decide whether there exist local phase gates for a certain bit string \mathbf{k} such that Eq. (2) is fulfilled (see Lemma 1).

Since we are going to determine the local unitaries which transform two states into each other in Sec. V we review here the constructive method to compute the unitaries V_k and W_k . First of all, it is easy to see that if $|\Psi\rangle$ is such that there exists some system i such that $\rho_i \neq \mathbb{1}$, the unitaries V_i and W_i can be determined by considering the necessary condition for LU equivalence, $\rho_i = U_i \sigma_i U_i^\dagger$. Analogously to the generic case, the equation $D_i = \text{diag}(\lambda_1^i, \lambda_2^i) = W_i \rho_i W_i^\dagger = V_i \sigma_i V_i^\dagger$ determines W_i and V_i (and $k_i = 0$) uniquely up to a phase gate. Thus, for this case we have that $|\Psi\rangle \simeq_{\text{LU}} |\Phi\rangle$ iff

there exist two phases, α_i and α_0 , and local unitaries U_j such that

$${}_i\langle l|W_i\Psi_s\rangle = e^{i(\alpha_0+\alpha_i l)} \bigotimes_{j \neq i} U_{ji} \langle l|V_i\Phi_s\rangle \quad \text{for } l \in \{0,1\}, \quad (3)$$

where W_i and V_i are chosen such that $D_i = \text{diag}(\lambda_1^i, \lambda_2^i) = W_i \rho_i W_i^\dagger = V_i \sigma_i V_i^\dagger$. Hence, if there is one system where the reduced state is not completely mixed, then the problem of LU equivalence of n -qubit states can be reduced to the one of $(n-1)$ -qubit states. This statement can be easily generalized to the case where more than one single-qubit reduced state is not completely mixed.

Let us now turn to the remaining case where $\rho_i = \mathbb{1} \forall i$. Instead of considering the necessary conditions $\rho_i = U_i \sigma_i U_i^\dagger$, one considers the necessary conditions $\rho_{n_1, \dots, n_l, k} = U_{n_1} \dots U_{n_l} U_k \sigma_{n_1, \dots, n_l, k} U_{n_1}^\dagger \dots U_{n_l}^\dagger U_k^\dagger$, for some appropriately chosen set $\{n_1, \dots, n_l, k\}$ and computes U_k as a function of U_{n_1}, \dots, U_{n_l} . More precisely, it has been shown that if $|\Psi\rangle = U_1, \dots, U_n |\Phi\rangle$ and if there exist systems n_1, \dots, n_l and k such that $\rho_{n_1, \dots, n_l, k} \neq \rho_{n_1, \dots, n_l} \otimes \mathbb{1}_k$, then V_k in Eq. (2) can be determined from the state $|\Phi\rangle$ and W_k can be determined as a function of the unitaries U_{n_1}, \dots, U_{n_l} . To be more specific, we assume without loss of generality that $n_1 = 1, \dots, n_l = l$. Due to the condition $\rho_{1, \dots, l, k} \neq \rho_{1, \dots, l} \otimes \mathbb{1}_k$ it can be shown that there exist at least two tuples $\mathbf{i} = (i_1, \dots, i_l)$ and $\mathbf{j} = (j_1, \dots, j_l)$ such that at least one of the Hermitian 2×2 matrices $B_{\mathbf{i}}^\dagger = A_{\mathbf{i}}^\dagger + (A_{\mathbf{j}}^\dagger)^\dagger$ and $C_{\mathbf{i}}^\dagger = i A_{\mathbf{i}}^\dagger - i (A_{\mathbf{j}}^\dagger)^\dagger$, where $A_{\mathbf{i}}^\dagger \equiv \text{tr}_{-k}[(|\mathbf{i}\rangle\langle \mathbf{j}| + \text{H.c.})|\Phi\rangle\langle \Phi|]$ is not proportional to the identity. Without loss of generality, we assume that $\mathbb{1} \not\propto B_{\mathbf{i}}^\dagger = \text{tr}_{-k}[(|\mathbf{i}\rangle\langle \mathbf{j}| + \text{H.c.})|\Phi\rangle\langle \Phi|]$. Using that $|\Psi\rangle = U_1, \dots, U_n |\Phi\rangle$, we have

$$U_k B_{\mathbf{i}}^\dagger U_k^\dagger = \text{tr}_{-k}[(|\mathbf{i}\rangle\langle \mathbf{j}| + \text{H.c.})U_1^\dagger, \dots, U_l^\dagger |\Psi\rangle\langle \Psi| U_1, \dots, U_l]. \quad (4)$$

Since $B_{\mathbf{i}}^\dagger$ is Hermitian we can diagonalize it as well as the right-hand side of Eq. (4). It can then be shown that $|\Psi\rangle = U_1, \dots, U_n |\Phi\rangle$ iff there exists $i_k \in \{0,1\}$ and α_0 and α_k such that $e^{i\alpha_0} X^{i_k} U(\alpha_k) W_k(U_1, \dots, U_l) |\Psi\rangle = U_1, \dots, V_k, \dots, U_n |\Phi\rangle$, where V_k is the unitary which diagonalizes $B_{\mathbf{i}}^\dagger$ and can therefore be determined directly from the state $|\Phi\rangle$ and $W_k(U_1, \dots, U_l)$ diagonalizes the right-hand side of Eq. (4).

Note that this constructive method of computing V_k and W_k is based on the necessary condition for LU equivalence given in Eq. (4) for any l -tuples \mathbf{i}, \mathbf{j} . Since the 2×2 matrices occurring in this equation are Hermitian, one can, similarly to the previous cases, determine the unitaries V_k and W_k by diagonalizing these matrices. In contrast to before, we find here that W_k might depend on U_1, \dots, U_l . Again, since those unitaries are obtained by diagonalizing a 2×2 matrix the phase gate occurring in Eq. (2) cannot be determined like that. This is the reason why the condition of LU equivalence has been rewritten in the seemingly more complicated form presented in Eq. (2).

In order to check then whether or not there exist phases α_i such that Eq. (2) is satisfied, the following lemma [16], which is proven here, has been used. We consider four n -qubit systems which are denoted by A, B, C , and D , respectively. The i th qubit of system A is denoted by A_i , etc. Furthermore,

we use the notation $|\chi\rangle_i = (|0110\rangle - |1001\rangle)_{A_i, B_i, C_i, D_i}$ and $P_{AC}^i = \sum_{\mathbf{k}} |\mathbf{k}\rangle\langle \mathbf{k}|_{A_1, C_1, \dots, A_{i-1}, C_{i-1}, A_{i+1}, C_{i+1}, \dots, A_n, C_n}$. Similarly, we define P_{BD}^i for systems B, D . For a state $|\Psi\rangle$ we define $K_\Psi \equiv \{\mathbf{k}$ such that $\langle \mathbf{k}|\Psi\rangle = 0\}$ and $|\Psi_{\{\bar{\alpha}_i\}}\rangle = |\Psi\rangle + 2e^{-i\bar{\alpha}_0} \sum_{\mathbf{k} \in K_\Psi} e^{-i \sum_{i=1}^n \bar{\alpha}_i k_i} |\mathbf{k}\rangle$ for some phases $\bar{\alpha}_i$ and $|\Psi_0\rangle = |\Psi\rangle + 2 \sum_{\mathbf{k} \in K_\Psi} |\mathbf{k}\rangle$.

Lemma 1. Let $|\Psi\rangle, |\Phi\rangle$ be n -qubit states. Then there exist local phase gates $Z_i(\alpha_i)$ and a phase α_0 such that $|\Psi\rangle = e^{i\alpha_0} \bigotimes_{i=1}^n Z_i(\alpha_i) |\Phi\rangle$ iff there exist phases $\{\bar{\alpha}_i\}_{i=0}^n$ such that (i) $|\langle \mathbf{i}|\Psi_0\rangle| = |\langle \mathbf{i}|\Phi_{\{\bar{\alpha}_i\}}\rangle| \forall \mathbf{i}$ and (ii) $\langle \chi|_i P_{AC}^i P_{BD}^i |\Psi_0\rangle_A |\Psi_0\rangle_B |\Phi_{\{\bar{\alpha}_i\}}\rangle_C |\Phi_{\{\bar{\alpha}_i\}}\rangle_D = 0 \forall i \in \{1, \dots, n\}$.

Condition (ii) can be interpreted as follows. Taking two copies of the state $|\Psi_0\rangle$ and two copies of the state $|\Phi_{\{\bar{\alpha}_i\}}\rangle$ and projecting the four qubits, A_i, B_i, C_i , and D_i onto the state $|\chi\rangle_i$ leads to a $4(n-1)$ -qubit state, which is in the kernel of $P_{AC}^i P_{BD}^i$ for any system i . Before proving Lemma 1, we introduce here another lemma, which will be required for the proof. Using the same notation as before, we have the following.

Lemma 2. $|\Psi\rangle$ can be converted into $|\Phi\rangle$ by local unitary phase gates iff there exist phases $\{\bar{\alpha}_i\}_{i=0}^n$ such that $|\Psi_0\rangle$ is converted into $|\Phi_{\{\bar{\alpha}_i\}}\rangle$ by local unitary phase gates.

Proof. If $|\Psi\rangle = e^{i\alpha_0} \bigotimes_{i=1}^n Z_i(\alpha_i) |\Phi\rangle$, for some phases $\{\alpha_i\}$, then $K_\Psi = K_\Phi$ and choosing $\bar{\alpha}_i = \alpha_i$ for $i \in \{0, \dots, n\}$ fulfills the condition. To prove the inverse direction, we assume that there exist phases $\{\bar{\alpha}_i\}_{i=0}^n$ such that $|\Psi_0\rangle = e^{i\alpha_0} \bigotimes_{i=1}^n Z_i(\alpha_i) |\Phi_{\{\bar{\alpha}_i\}}\rangle$ for some phases $\{\alpha_i\}$. Due to the factor 2 in the definition of $|\Psi_0\rangle$ and $|\Phi_{\{\bar{\alpha}_i\}}\rangle$, this implies $K_\Psi = K_\Phi$. Defining the projector $P = \sum_{\mathbf{k} \notin K_\Psi} |\mathbf{k}\rangle\langle \mathbf{k}|$ we have $P|\Psi_0\rangle = |\Psi\rangle$ and $P e^{i\alpha_0} \bigotimes_{i=1}^n Z_i(\alpha_i) |\Phi_{\{\bar{\alpha}_i\}}\rangle = e^{i\alpha_0} \bigotimes_{i=1}^n Z_i(\alpha_i) P|\Phi_{\{\bar{\alpha}_i\}}\rangle$ and therefore $|\Psi\rangle = e^{i\alpha_0} \bigotimes_{i=1}^n Z_i(\alpha_i) |\Phi\rangle$. ■

The reason for introducing this lemma is that it implies that if one wants to decide whether two states are up to local phase-gate equivalent, one only needs to consider states where none of the coefficients in the computational basis vanish. Let us now use the lemma above to prove Lemma 1.

Proof. As mentioned earlier, due to Lemma 2 it remains to show that for any state $|\psi\rangle$ with $\langle \mathbf{k}|\psi\rangle \neq 0 \forall \mathbf{k}$ we have that $|\psi\rangle = e^{i\alpha_0} \bigotimes_{i=1}^n Z_i(\alpha_i) |\phi\rangle$ for some phases $\{\alpha_i\}$ iff condition (i) and (ii) in Lemma 1 are satisfied. Note that condition (ii) is equivalent to $\langle 0\mathbf{k}|\psi\rangle \langle 1\mathbf{l}|\psi\rangle \langle 1\mathbf{k}|\phi\rangle \langle 0\mathbf{l}|\phi\rangle = \langle 1\mathbf{k}|\psi\rangle \langle 0\mathbf{l}|\psi\rangle \langle 0\mathbf{k}|\phi\rangle \langle 1\mathbf{l}|\phi\rangle$, where 0,1 act on system i and \mathbf{k}, \mathbf{l} denote the computational basis states of the remaining $n-1$ qubits.

Let us now prove the *only if* part: If $|\psi\rangle = e^{i\alpha_0} \bigotimes_{i=1}^n Z_i(\alpha_i) |\phi\rangle$ for some phases $\{\alpha_i\}$, then $\langle \mathbf{i}|\psi\rangle = e^{i\phi_i} \langle \mathbf{i}|\phi\rangle$, with $\phi_i = \alpha_0 + \sum_k \alpha_k i_k$, which implies (i). Condition (ii) (for $i=1$) is then equivalent to $e^{i(\phi_{0\mathbf{k}} + \phi_{1\mathbf{l}})} x_{\mathbf{k}\mathbf{l}} = e^{i(\phi_{1\mathbf{k}} + \phi_{0\mathbf{l}})} x_{\mathbf{k}\mathbf{l}}$, where $x_{\mathbf{k}\mathbf{l}} = \langle 0\mathbf{k}|\phi\rangle \langle 1\mathbf{l}|\phi\rangle \langle 1\mathbf{k}|\phi\rangle \langle 0\mathbf{l}|\phi\rangle$. It is easy to see that this condition is fulfilled since $e^{i(\phi_{0\mathbf{k}} - \phi_{1\mathbf{k}})} = e^{-i\alpha_1} \forall \mathbf{k}$. In the same way, one can show that the conditions for $i \neq 1$ are fulfilled.

To prove the *if* part, we first note that condition (i) implies that $\langle \mathbf{i}|\Psi\rangle = e^{i\phi_i} \langle \mathbf{i}|\Phi\rangle$ for some phases ϕ_i . Condition (ii) (for $i=1$) implies then that $e^{i(\phi_{0\mathbf{k}} - \phi_{1\mathbf{k}})} = e^{i(\phi_{0\mathbf{l}} - \phi_{1\mathbf{l}})} \forall \mathbf{k}, \mathbf{l}$, since $x_{\mathbf{k}\mathbf{l}} = \langle 0\mathbf{k}|\phi\rangle \langle 1\mathbf{l}|\phi\rangle \langle 1\mathbf{k}|\phi\rangle \langle 0\mathbf{l}|\phi\rangle \neq 0 \forall \mathbf{k}, \mathbf{l}$. Thus, $e^{i(\phi_{0\mathbf{k}} - \phi_{1\mathbf{k}})}$ must be independent of \mathbf{k} and, therefore, we have $e^{i(\phi_{0\mathbf{k}} - \phi_{1\mathbf{k}})} = e^{-i\alpha_1}$, for some phase α_1 . Equivalently, we have

$e^{i\phi_{k_1, k}} = e^{i(\alpha_1^{(k_1)} + \phi_{1k})}$, where $\alpha_1^{(0)} = -\alpha_1$ and $\alpha_1^{(1)} = 0$. Similarly, we obtain $e^{i(\phi_{k_1 0 k_3, \dots, k_n} - \phi_{k_1 1 k_3, \dots, k_n})} = e^{-i\alpha_2}$ and therefore $e^{i\phi_{k_1, k_2, k_3, \dots, k_n}} = e^{i(\alpha_1^{(k_1)} + \alpha_2^{(k_2)} + \phi_{11k_3, \dots, k_n})}$. Continuing in this way we find $e^{i\phi_{k_1, \dots, k_n}} = e^{i\alpha_0} e^{i \sum_j \alpha_j k_j}$, where $\alpha_0 = \phi_{1, \dots, 1} - \sum \alpha_i$. Thus, we have $|\psi\rangle = e^{i\alpha_0} \bigotimes_{i=1}^n Z_i(\alpha_i) |\phi\rangle$. ■

It is important to note here that the state on the right-hand side of Eq. (2) is completely determined using the method summarized previously. Thus, the set K_ψ in Lemma 1 can be determined and therefore this lemma can be applied. The states are LU equivalent iff the conditions in Lemma 1 are fulfilled for some bit string \mathbf{k} . The unitaries which interconvert the states are, up to the symmetry of the states, uniquely determined and are given by $U_i = W_i^\dagger Z_i(\alpha_i) X^{k_i} V_i$ (up to a global phase).¹

In summary, the LU-equivalence problem has been solved by presenting a systematic method to determine the local unitaries (if they exist) which interconvert the states. This has been achieved by determining V_i and W_i in Eq. (2) by imposing necessary conditions of LU equivalence, such as $\rho_i = U_i \sigma_i U_i^\dagger$ and Eq. (4). Once all the unitaries V_i and W_i are determined (even as functions of some others), the states are LU equivalent iff there exist local phase gates which interconvert the transformed states (after applying $\bigotimes_i V_i$, $\bigotimes_i W_i$ to $|\Phi\rangle, |\Psi\rangle$, respectively). This can then be easily decided by employing Lemma 1.

Before ending this section let us present here another way of checking whether two states are interconvertible by local phase gates. Due to Lemma 2 we only need to consider states $|\Psi\rangle, |\Phi\rangle$ with $K_\psi = K_\phi = \emptyset$. Here and in the following we denote by \odot the Hadamard product, that is, the componentwise product, and by $/$ we denote the inverse operation, that is, the componentwise division. For instance, if $|\Psi\rangle = \sum_i a_i |\mathbf{i}\rangle$ and $|\Phi\rangle = \sum_i b_i |\mathbf{i}\rangle$, with $b_i \neq 0 \forall \mathbf{i}$, then $|\Psi\rangle / |\Phi\rangle = \sum_i a_i / b_i |\mathbf{i}\rangle$.

Lemma 3. Let $|\Psi\rangle$ and $|\Phi\rangle$ be n -qubit states with $K_\psi = K_\phi = \emptyset$. Then there exist phases $\{\alpha_i\}$ such that $|\Psi\rangle = e^{i\alpha_0} \bigotimes_i Z(\alpha_i) |\Phi\rangle$ iff (i) $|\langle \mathbf{i} | \Psi \rangle| = |\langle \mathbf{i} | \Phi \rangle|$ and (ii) $|\Psi\rangle / |\Phi\rangle$ is a product state.

Proof. (Only if): If $|\Psi\rangle = e^{i\alpha_0} \bigotimes_i Z(\alpha_i) |\Phi\rangle$, condition (i) is obviously fulfilled. In order to show that condition (ii) is fulfilled we use that $e^{i\alpha_0} \bigotimes_i Z(\alpha_i) |\Phi\rangle = e^{i\alpha_0} \bigotimes_i Z(\alpha_i) |+\rangle^{\otimes n} \odot |\Phi\rangle$. Thus, $|\Psi\rangle / |\Phi\rangle = e^{i\alpha_0} \bigotimes_i Z(\alpha_i) |+\rangle^{\otimes n}$, which is a product state.

(If): Due to condition (i) we have that $|\Psi\rangle / |\Phi\rangle = \sum e^{i\alpha_i} |\mathbf{i}\rangle$ for some phases α_i . That is, $|\Psi\rangle / |\Phi\rangle$ is a LME state. Due to condition (ii) this LME state must be a product state; that is, $\sum e^{i\alpha_i} |\mathbf{i}\rangle = \bigotimes_i |\phi_i\rangle$, where $|\phi_i\rangle = e^{i\Phi_0^i} (\lambda_0^i |0\rangle + e^{i\Phi_1^i} \lambda_1^i |1\rangle)$, with $\lambda_k^i \geq 0$. This implies that $e^{i\alpha_i} = e^{i(\Phi_0 + \sum_k \Phi_k^i)}$, where $\Phi_0 = \sum_k \Phi_0^k$. Thus, the LME state is a product state iff it is equivalent to $e^{i\alpha_0} \bigotimes_i Z(\alpha_i) |+\rangle^{\otimes n}$ for some phases $\{\alpha_i\}$ and therefore $|\Psi\rangle = e^{i\alpha_0} \bigotimes_i Z(\alpha_i) |\Phi\rangle$. ■

As mentioned earlier, Lemma 2 can be used to generalize Lemma 1 to states $|\Psi\rangle$ for which $K_\psi \neq \emptyset$. Note that condition (ii) has a physical interpretation. The Hadamard product of two states $|\psi\rangle, |\phi\rangle$ corresponds to the state one would get by the following procedure. Let $|\psi\rangle$ ($|\phi\rangle$) describe the system $1_1, \dots, n_1$ ($1_2, \dots, n_2$), respectively, and consider n pairs

of maximally entangled two-qubit states, $|\Phi^+\rangle = \sum_{i=0}^1 |ii\rangle$, describing systems $1_3, 1_4, \dots, n_3, n_4$. Then, $|\phi\rangle \odot |\psi\rangle = \bigotimes_{i=1}^n \langle \Psi_{i_1, i_2, i_3}^0 | \psi \rangle_{1_1, \dots, n_1} |\phi\rangle_{1_2, \dots, n_2} \bigotimes_{i=1}^n |\Phi^+\rangle_{i_3, i_4}$, where $|\Psi^0\rangle$ denotes the GHZ states here. This resembles the procedure of gate teleportation [21]. Note that condition (ii) is fulfilled iff there exists a product state, $\bigotimes_i |\phi_i\rangle$ such that $|\Psi_0\rangle = |\Phi_{\bar{\alpha}_i}\rangle \odot \bigotimes_i |\phi_i\rangle$.

IV. ADDITIONAL METHODS FOR COMPUTING THE LOCAL UNITARIES

We have seen before how the local unitaries which occur in Eq. (2) can be determined by imposing certain necessary conditions of LU equivalence [see Eq. (4)]. One might also use other necessary conditions for LU equivalence to determine those local unitaries. For instance, if $|\Psi\rangle = U_1, \dots, U_n |\Phi\rangle$ then $\text{tr}_1(\rho_1 \otimes \mathbb{1}_2 \rho_{12}) = U_2 \text{tr}_1(\sigma_1 \otimes \mathbb{1}_2 \sigma_{12}) U_2^\dagger$ and $\text{tr}_{23}(\rho_{123} \otimes \mathbb{1}_1 \rho_{1'2'3} \otimes \mathbb{1}_1) = U_1 \otimes U_1' \text{tr}_{23}(\sigma_{123} \otimes \mathbb{1}_1 \sigma_{1'2'3} \otimes \mathbb{1}_1) U_1^\dagger \otimes U_1'^\dagger$. Of course, any generalization of these equations must be fulfilled too. Here we will use those and other necessary conditions for LU equivalence to derive some additional methods to compute the unitaries in Eq. (2) for certain multipartite states. Depending on the properties of the states of interest, one method or the other might be better suited. In Sec. V we use the various methods to compute the local unitaries directly, that is, not as a function of other unitaries. This makes the characterization of LU-equivalence classes easier.

Here we first consider the LU equivalence of two-qubit mixed states. Then we focus on those states for which there exists at least one system i with $\rho_i \neq \mathbb{1}$ and derive a simple way to determine the unitaries in Eq. (2).

A. Two-qubit mixed states

For two-qubit mixed states ρ, σ , necessary and sufficient conditions for LU equivalence have been derived in [22]. However, if $\rho = \rho_{ij}$ ($\sigma = \sigma_{ij}$) denotes the reduced state of some systems i, j of a multipartite state, $|\Psi\rangle$ ($|\Phi\rangle$), respectively, and the aim is to investigate the LU equivalence of $|\Psi\rangle$ and $|\Phi\rangle$, then one must determine all local unitaries, U_i, U_j , which fulfill $\rho_{ij} = U_i U_j \sigma_{ij} U_i^\dagger U_j^\dagger$ and then check if there exists one of them, which transforms the multipartite states into each other. We show here how to achieve this task.

We have seen earlier that if there exists some system i such that $\rho_i \neq \mathbb{1}$, then V_i, W_i , and k_i in Eq. (2) can be determined by imposing the necessary condition $\rho_i = U_i \sigma_i U_i^\dagger$. Thus, it remains to consider the case where both reduced states are proportional to the identity which implies that $\rho = \mathbb{1} + \sum_{k,l} \Lambda_{k,l} \Sigma_k \otimes \Sigma_l$, where $\Lambda = \sum_{kl} \lambda_{kl} |k\rangle \langle l|$ is real. Applying the local unitary operation $U_1 \otimes U_2$ to the state, ρ leads to $U_1 \otimes U_2 \rho U_1^\dagger \otimes U_2^\dagger = \mathbb{1} + \sum_{k,l} \Lambda'_{k,l} \Sigma_k \otimes \Sigma_l$, with $\Lambda' = O_1 \Lambda O_2^T$. Here, O_1, O_2 are real orthogonal matrices which are defined via the equation $U_i (\vec{n} \vec{\sigma}) U_i^\dagger = (O_i \vec{n} \vec{\sigma})$ for $i = 1, 2$. Using the singular value decomposition of the real matrix Λ , $\Lambda = O_1 D O_2^T$, where D is a diagonal matrix and $O_{1,2}$ are real and orthogonal, and the fact that the state $\mathbb{1} + \sum_{k,l} D_{k,k} \Sigma_k \otimes \Sigma_k$, is Bell diagonal shows that the

¹Note that the phases α_i can be easily computed.

eigenbasis of any two-qubit density matrix with completely mixed reduced states is maximally entangled.

In order to show now under which conditions two two-qubit states are LU equivalent we recall the following lemma which was proven in [23].

Lemma 4. Any two maximally entangled basis of two qubits can be mapped to each other using local unitary operations [23]. That is, if $\{|\Psi_i\rangle\}_{i=1}^4$ and $\{|\Phi_i\rangle\}_{i=1}^4$ denote two maximally entangled bases, then there exist four phases γ_i , and local unitaries U_1, U_2 such that $|\Psi_i\rangle = e^{i\gamma_i} U_1 \otimes U_2 |\Phi_i\rangle \forall i \in \{1, 2, 3, 4\}$.

This lemma, together with the fact that the eigenbasis of any two-qubit density matrix with completely mixed reduced states is maximally entangled, implies the following corollary.

Corollary 1. Let ρ and σ be two-qubit density matrices with completely mixed reduced states. Then $\rho \simeq_{\text{LU}} \sigma$ iff $\text{eig}(\rho) = \text{eig}(\sigma)$.

Let us now consider two LU-equivalent states, ρ, σ with $\rho_i = \sigma_i = \mathbb{1}$ for $i = 1, 2$ and derive some conditions on the local unitary operations, which transform σ to ρ . First we apply local unitaries V_i and W_i such that $\bar{\rho} = W_1 W_2 \rho W_1^\dagger W_2^\dagger = \mathbb{1} + \sum_i (D_\rho)_i \Sigma_i \Sigma_i$ and $\bar{\sigma} = V_1 V_2 \sigma V_1^\dagger V_2^\dagger = \mathbb{1} + \sum_i (D_\sigma)_i \Sigma_i \Sigma_i$, with $D_\rho = D_\sigma = \text{diag}(\lambda_1, \lambda_2, \lambda_3)$. We choose, without loss of generality, the order of λ_i such that if there is no degeneracy $\lambda_1 > \lambda_2 > \lambda_3$; otherwise, $\lambda_1 = \lambda_2$. If D_ρ is not proportional to the identity, it is easy to see that $\bar{\rho} = \bar{U}_1 \bar{U}_2 \bar{\sigma} \bar{U}_1^\dagger \bar{U}_2^\dagger$ implies that \bar{U}_i is of the form $Z(\alpha_i) X^{k_i}$, for some phase α_i and $k_i \in \{0, 1\}$.² Thus, if ρ and σ denote for instance the reduced state of system 1 and 2 of some multipartite state, $|\Psi\rangle, |\Phi\rangle$, respectively, then $|\Psi\rangle \simeq_{\text{LU}} |\Phi\rangle$ iff Eq. (2) is fulfilled for V_1, V_2 and W_1, W_2 such that $W_1 W_2 \rho W_1^\dagger W_2^\dagger = \bar{\sigma} = V_1 V_2 \sigma V_1^\dagger V_2^\dagger = \mathbb{1} + \sum_i (D_\rho)_i \Sigma_i \Sigma_i$, where $D_\rho = \text{diag}(\lambda_1, \lambda_2, \lambda_3)$ with λ_i sorted as mentioned earlier.

Otherwise, if D_ρ is proportional to the identity and $\rho \neq \mathbb{1}$, we apply the local unitaries V_i and W_i defined earlier and denote the resulting states again by ρ, σ , respectively. In this case we find $\rho = \sigma = \mathbb{1} - \lambda |\Psi^-\rangle \langle \Psi^-|$ for some $\lambda \neq 0$. Then any pair of unitaries U_1, U_2 which transforms σ to ρ must fulfill that $U_2 = U_1$. Hence, in this case we have that if ρ and σ denote, for instance, the reduced state of system 1 and 2 of some multipartite state, $|\Psi\rangle, |\Phi\rangle$, respectively, then $|\Psi\rangle \simeq_{\text{LU}} |\Phi\rangle$ iff Eq. (2) is fulfilled for $V_1 = V_2 = \mathbb{1}$, $k_1 = k_2 = 0$, $\alpha_1 = \alpha_2$, and $W_1 = W_2 = e^{i\beta_1 X_i} e^{i\gamma_1 Z_i}$, for some phases β_1, γ_1 . Note that if $\rho_{12} = \mathbb{1} - \lambda |\Psi^-\rangle \langle \Psi^-|$ with $\lambda \neq 1$, then $|\Psi\rangle \simeq_{\text{LU}} |\Phi\rangle$ implies that ${}_{12}\langle \Psi^- | \Psi \rangle \simeq_{\text{LU}} {}_{12}\langle \Psi^- | \Phi \rangle$ since $U \otimes U |\Psi^-\rangle = |\Psi^-\rangle$ for any unitary U . Thus, similar to the case where $\rho_i \neq \mathbb{1}$, one would simply measure those systems where the reduced state is a full-rank Werner state [24].

In the remaining case, that is, if $\rho = \mathbb{1}$, it is clear that considering the two-qubit reduced state will not help us to find any condition on the local unitaries.

So far we have seen that whenever there exist two systems i, j such that ρ_{ij} is not LU equivalent to $\mathbb{1} + \lambda \sum_i \Sigma_i \otimes \Sigma_i$, then the unitaries V_i, V_j, W_i, W_j and k_i, k_j in Eq. (2) can be

easily determined. We are going to show next that in this case also other unitaries, V_l and W_l , for $l \notin \{i, j\}$ can be easily computed. As before we consider the case where $\rho_i = \mathbb{1} \forall i$. In the following lemma we say that the unitaries can be determined by considering a certain operator if they can be determined using the fact that the operator for the state $|\Psi\rangle$ and the one for the state $|\Phi\rangle$ must be LU equivalent if $|\Psi\rangle \simeq_{\text{LU}} |\Phi\rangle$.

Lemma 5. If there exist systems i, j such that ρ_{ij} is not LU equivalent to $\mathbb{1} + \lambda \sum_i \Sigma_i \otimes \Sigma_i$ for any $\lambda \in \mathbf{R}$, then, for any system l for which either $\rho_{il} \neq \mathbb{1}$ or $\rho_{jl} \neq \mathbb{1}$, V_l, W_l , and k_l can be determined by either considering ρ_{il} or ρ_{jl} or by considering $\text{tr}_i(\rho_{ij} \rho_{il})$ or $\text{tr}_j(\rho_{ij} \rho_{jl})$.

Proof. If ρ_{il} or ρ_{jl} is not LU equivalent to $\mathbb{1} + \lambda \sum_i \Sigma_i \otimes \Sigma_i$, for some λ , then V_l, W_l , and k_l can be determined as shown previously. Otherwise, we assume, without loss of generality, that $\rho_{il} \neq \mathbb{1}$. Then we have that $\rho_{il} = \mathbb{1} + \sum_{i_1, i_2=1}^3 \Lambda_{i_1 i_2} \Sigma_{i_1} \otimes \Sigma_{i_2}$ with Λ proportional to a real orthogonal matrix and $\rho_{ij} = \mathbb{1} + \sum_i \tilde{\Lambda}_{i i_2} \Sigma_{i_2} \otimes \Sigma_{i_2}$ with $\tilde{\Lambda}$ not proportional to a real orthogonal matrix. Then, we find $\text{tr}_i(\rho_{ij} \rho_{il}) = \mathbb{1} + \sum_{i_1, i_2} \tilde{\Lambda}_{i_1 i_2} \Lambda_{i_1 i_2} \Sigma_{i_2} \Sigma_{i_2}$, where the matrix $(\tilde{\Lambda})^T \Lambda$ is not orthogonal. Since the unitaries V_i and W_i are already fixed, the equation $W_j W_l \text{tr}_i(\rho_{ij} \rho_{il}) W_j^\dagger W_l^\dagger = V_j V_l \text{tr}_i(\sigma_{ij} \sigma_{il}) V_j^\dagger V_l^\dagger$ determines V_l, W_l , and $k_l = 0$. ■

B. States where there exists a system i with $\rho_i \neq \mathbb{1}$

Let us now turn to the case where there exists at least one system i such that its reduced state is not completely mixed. Without loss of generality, we chose $i = 1$. Let us assume that the states of interest, $|\Psi\rangle$ and $|\Phi\rangle$, do have sorted trace decomposition. That is, in particular, the unitaries V_i and W_i which make ρ_i and σ_i diagonal in the computational basis [see Eq. (2)] have already been applied. Then we know that $U_1 = Z(\alpha_1)$ for some phase α_1 . We present now several methods to determine the unitaries V_i and W_i of Eq. (2). As in [16], the idea is to construct out of the states $|\Psi\rangle$ and $|\Phi\rangle$ nondegenerate 2×2 matrices which must be LU equivalent in case $|\Psi\rangle$ and $|\Phi\rangle$ are, for example, $U \rho_i U^\dagger = \sigma_i$ or $\text{tr}_1[(\rho_1 \otimes \mathbb{1}_i) \rho_{1i}] = U_i \text{tr}_1[(\sigma_1 \otimes \mathbb{1}_i) \sigma_{1i}] U_i^\dagger$. Those necessary conditions of LU equivalence can then be used to fix W_i, V_i , and k_i in Eq. (2). The local phase gates, which cannot be fixed in this way, must be determined at the end using one of the lemmas in Sec. III.

Since the states $|\Psi\rangle$ and $|\Phi\rangle$ have sorted trace decomposition, we have $|\Psi\rangle = \sqrt{p_1} |0\rangle |\Psi_0\rangle + \sqrt{1-p_1} |1\rangle |\Psi_1\rangle$, with $\langle \Psi_i | \Psi_j \rangle = \delta_{i,j}$ and $p_1 > 1/2$ and $|\Phi\rangle = \sqrt{p_2} |0\rangle |\Phi_0\rangle + \sqrt{1-p_2} |1\rangle |\Phi_1\rangle$ with $\langle \Phi_i | \Phi_j \rangle = \delta_{i,j}$ and $p_2 > 1/2$, which is just the Schmidt decomposition for the bipartite splitting, system 1 versus the rest. Then we have that the states are LU equivalent iff (1) $p_1 = p_2$ and (2) there exist phases ϕ, α_1 and unitaries U_j such that

$$\begin{aligned} |\Psi_0\rangle &= e^{i\gamma_1} \bigotimes_{j \neq 1} U_j |\Phi_0\rangle, \\ |\Psi_1\rangle &= e^{i\gamma_2} \bigotimes_{j \neq 1} U_j |\Phi_1\rangle, \end{aligned} \quad (5)$$

where $\gamma_1 = \phi + \alpha_1$ and $\gamma_2 = \phi - \alpha_1$ [see Eq. (3)]. Note that the last two conditions are fulfilled iff

²This can be easily seen by noting that the condition $O_i D_\rho O_i^T = D_\rho$ implies that $O_i D^2 O_i^T = D^2$, for $i = 1, 2$, which defines O_i uniquely up to $R_z(\alpha) R_x(\pi)^k$, for $k = 0, 1$.

$$\beta_1|\Psi_0\rangle\langle\Psi_0| + \beta_2|\Psi_1\rangle\langle\Psi_1| = \bigotimes_{j \neq 1} U_j(\beta_1|\Phi_0\rangle\langle\Phi_0| + \beta_2|\Phi_1\rangle\langle\Phi_1|) \bigotimes_{j \neq 1} U_j^\dagger$$

for all values of β_1, β_2 .

There are several ways now to compute the unitaries V_i and W_i in Eq. (2). First of all, if $\rho_i \neq \mathbb{1}$, then $U_i = Z(\alpha_i)$ for some phase α_i . Let us now consider the case where $\rho_i = \mathbb{1}$. If $\rho_{1i} \neq \rho_1 \otimes \mathbb{1}$, Eq. (4) can be used to compute V_i , W_i , and k_i . In particular, we would consider one of the matrices $B_{l,m} \equiv \text{tr}_{\neq i}(|\Psi_l\rangle\langle\Psi_m| + \text{H.c.})$ or $C_{l,m} \equiv \text{tr}_{\neq i}(i|\Psi_l\rangle\langle\Psi_m| + \text{H.c.})$ for some l, m and diagonalize this matrix in order to compute W_i , V_i , and k_i .

It is the aim of this section to derive some other methods too determining those unitaries. First, we use the fact that Eq. (4) must be fulfilled for any values of l, m if the states are LU equivalent. Considering certain combinations of those equations will lead to other approaches to determine the unitaries V_i and W_i and the bit value k_i . In the second part of this section we show how a combination of the Eqs. (5) can be used to compute those unitaries.

If $\rho_{1i} \neq \rho_1 \otimes \mathbb{1}$, then V_i and W_i can be easily computed as follows. First of all, it is clear that if $\rho_1 \neq \sigma_1$, then the states are not LU equivalent. Thus, we assume that $\rho_1 = \sigma_1$. The fact that $\rho_1 \neq \mathbb{1}$ and $\rho_i = \mathbb{1}$ implies that $\rho_{1i} = \mathbb{1} + aZ\mathbb{1} + \sum_{j_1, j_2=1}^3 \Lambda_{j_1 j_2} \Sigma_{j_1} \otimes \Sigma_{j_2}$ for some $a \in \mathbb{R}$ and where $\Lambda \neq 0$ since $\rho_{1i} \neq \rho_1 \otimes \mathbb{1}$. Similarly, we have $\sigma_{1i} = \mathbb{1} + aZ\mathbb{1} + \sum_{j_1, j_2=1}^3 \Gamma_{j_1 j_2} \Sigma_{j_1} \otimes \Sigma_{j_2}$. As mentioned before, the two states are LU equivalent; that is, $\rho_{1i} = U_1 U_i \sigma_{1i} U_1^\dagger U_i^\dagger$ iff there exists a real orthogonal matrix O_i and a phase α_1 such that $\Lambda = O_1 \Gamma O_1^T$, where $O_1 = R_z(\alpha_1)$. As explained in Sec. II A, if Λ is not orthogonal, then the unitaries V_i and W_i can be easily computed. Otherwise, we use the following necessary condition for LU equivalence: $(\rho_1 \otimes \mathbb{1}_i) \rho_{1i} = U_1 U_i [(\sigma_1 \otimes \mathbb{1}_i) \sigma_{1i}] U_1^\dagger U_i^\dagger$ and therefore $\text{tr}_i[(\rho_1 \otimes \mathbb{1}_i) \rho_{1i}] = U_i \text{tr}_i[(\sigma_1 \otimes \mathbb{1}_i) \sigma_{1i}] U_i^\dagger$. Since $\text{tr}_i[(\rho_1 \otimes \mathbb{1}_i) \rho_{1i}] = \mathbb{1} + a \sum_j \lambda_{3j} \Sigma_j$, the preceding equation can be used to determine V_i and W_i (and $k_i = 0$) as those operators which diagonalize $\text{tr}_i[(\rho_1 \otimes \mathbb{1}_i) \rho_{1i}]$ and $\text{tr}_i[(\sigma_1 \otimes \mathbb{1}_i) \sigma_{1i}]$, respectively. That is, unless $\Lambda_{3j} = 0 \forall j$, V_i and W_i are defined by the equation $V_i \text{tr}_i[(\rho_1 \otimes \mathbb{1}_i) \rho_{1i}] V_i^\dagger = W_i \text{tr}_i[(\sigma_1 \otimes \mathbb{1}_i) \sigma_{1i}] W_i^\dagger = \text{diag}(\gamma_1, \gamma_2)$ for some γ_i . If $\Lambda_{3i} = 0 \forall i$, Λ cannot be orthogonal and therefore the unitaries can be determined as explained in Sec. IV A. Thus, if $\rho_{1i} = U_1 U_i \sigma_{1i} U_1^\dagger U_i^\dagger$ the methods described previously will lead to the unitaries V_i and W_i in Eq. (2) unless $\rho_{1i} = \rho_1 \otimes \mathbb{1}$.

Another method of computing the unitaries is the following. Instead of considering the single equation $|\Psi\rangle = U_1, \dots, U_n |\Phi\rangle$, we use the fact that the basis for the first system has been fixed. Therefore, we can use both equations given in Eq. (5). Note that the states $|\Psi_0\rangle, |\Psi_1\rangle$ and the states $|\Phi_0\rangle, |\Phi_1\rangle$ are orthogonal, respectively. In [25] it has been shown that two orthogonal multipartite pure states can be perfectly distinguished using local operations. We are going to use this result now in order to determine the unitaries V_i and W_i . It is easy to see that for any pair of orthogonal states, $|\Psi_0\rangle, |\Psi_1\rangle$, there exist local unitaries, W_i such that [25]

$$M_i \equiv \text{tr}_{-i}(|\Psi_0\rangle\langle\Psi_1|) = W_i N_i W_i^\dagger, \quad (6)$$

where N_i is an off-diagonal matrix with $(N_i)_{1,2} = a_i$, $(N_i)_{2,1} = b_i$, for some complex numbers a_i, b_i . If $|a_i| \neq |b_i|$, that is, if $N_i N_i^\dagger \not\propto \mathbb{1}$, it is easy to see that by imposing

the condition that $|a_i| > |b_i|$, this equation determines W_i uniquely (up to a phase gate). If $|a_i| = |b_i| \neq 0$, M_i is, up to a global phase, a Hermitian traceless matrix. Thus, in this case we would choose W_i such that $M_i = e^{i\bar{\alpha}} W_i^\dagger D_i W_i$ for some phase $\bar{\alpha}$ and D_i diagonal. Defining V_i in the same way for the state $|\Phi\rangle$ we have that $|\Psi\rangle \simeq_{\text{LU}} |\Phi\rangle$ iff Eq. (2) has a solution for the so chosen matrices V_i and W_i .³

Before concluding this section we mention another method of computing the unitaries in Eq. (5) for a general state with $\rho_i \neq \mathbb{1}$. It is based on the following observation. Let us denote by $|\Psi_0\rangle$ ($|\Psi_1\rangle$) a (un-normalized) state describing systems $2, \dots, n$ ($2', \dots, n'$), respectively. Then $\langle\Psi^-|_{ii'} \Psi_0, \Psi_1\rangle = 0$ iff the state $|\Psi\rangle = |0\rangle|\Psi_0\rangle + |1\rangle|\Psi_1\rangle$ is either a product state in the bipartite splitting system 1 versus the rest or system i versus the rest. This can be easily verified as follows. We write $|\Psi_k\rangle = |0\rangle_i |\Psi_{k0}\rangle + |1\rangle_i |\Psi_{k1}\rangle$ for $k \in \{0, 1\}$. Then $\langle\Psi^-|_{ii'} \Psi_0, \Psi_1\rangle = 0$ iff either (a) $|\Psi_{00}\rangle|\Psi_{11}\rangle = 0$ and $|\Psi_{01}\rangle|\Psi_{10}\rangle = 0$, which implies that either $|\Psi\rangle = |k\rangle_i |\Psi_k\rangle$ or $|\Psi\rangle = |k\rangle_i (\sqrt{p}|0\rangle_i |\Psi_{0k}\rangle + \sqrt{1-p}|1\rangle_i |\Psi_{1k}\rangle)$ for $k \in \{0, 1\}$, or (b) $|\Psi_{00}\rangle = a|\Psi_{01}\rangle$ and $|\Psi_{10}\rangle = a|\Psi_{11}\rangle$, for some a . In this case we find $|\Psi\rangle = (a|0\rangle + |1\rangle)_i \otimes (\sqrt{p}|0\rangle|\Psi_{01}\rangle + \sqrt{1-p}|1\rangle|\Psi_{11}\rangle)$. Note that if $|\Psi\rangle$ is a product state in any bipartite splitting, system i versus the rest, then the unitaries V_i and W_i and the bit value k_i in Eq. (2) can obviously be easily determined. If $|\Psi\rangle$ is not a product state in this splitting, then we can combine the two equations in Eq. (5) to

$$\langle\Psi^-|_{ii'} \Psi_0, \Psi_1\rangle = e^{i(\gamma_1 + \gamma_2)} \bigotimes_{j \neq i, 1} U_j \bigotimes_{j' \neq i', 1'} U_{j'} \langle\Psi^-|_{ii'} \Phi_0, \Phi_1\rangle, \quad (7)$$

where we used that $|\Psi^- \rangle = U \otimes U |\Psi^- \rangle$ for any unitary U . This approach will be useful if there are only a few unitaries not determined, for instance, if $|\Psi\rangle$ is a three-qubit state. Choosing, without loss of generality, $i = 2$, we have $\langle\Psi^-|_{22'} \Psi_0, \Psi_1\rangle = e^{i(\gamma_1 + \gamma_2)} U_3 U_{3'} \langle\Psi^-|_{22'} \Phi_0, \Phi_1\rangle$, which can then be used to determine U_3 , or equivalently V_3, W_3 , and k_3 . Of course, the projection onto the singlet state can also be performed on more systems.

In summary, in this subsection we have explained some simple ways to compute V_i, W_i , and k_i for states which have the properties that $\rho_i = \mathbb{1}$ and that there exists some system j such that $\rho_{ji} \neq \rho_j \otimes \mathbb{1}$. For states with $\rho_{ji} \neq \rho_j \otimes \mathbb{1}$, the unitaries can be easily computed using either that $(\rho_1 \otimes \mathbb{1}) \rho_{1i} \simeq_{\text{LU}} (\sigma_1 \otimes \mathbb{1}) \sigma_{1i}$ is a necessary condition for LU equivalence or that the states $|\Psi_0\rangle$ and $|\Psi_1\rangle$ in Eq. (5) are orthogonal. For general states (not requiring that $\rho_{ji} \neq \rho_j \otimes \mathbb{1}$) where there exists a system j with $\rho_j \neq \mathbb{1}$, Eq. (7) (and its generalizations) can be used to find new conditions on the unitaries. Note that if $\rho_1 \neq \mathbb{1}$ and $\rho_{12} = \rho_1 \otimes \mathbb{1}$, then we have

$$|\Psi\rangle = \sqrt{p}|0\rangle(|0\rangle|\Psi_{00}\rangle + |1\rangle|\Psi_{01}\rangle) + \sqrt{1-p}|1\rangle(|0\rangle|\Psi_{10}\rangle + |1\rangle|\Psi_{11}\rangle), \quad (8)$$

³Note that if $\rho_{1i} = \rho_1 \otimes \mathbb{1}$, the condition that $\text{tr}_{-i}(|\Psi_0\rangle\langle\Psi_1|) \propto \langle 0|_i \rho_{1i} |1\rangle_i$ is local unitarily equivalent to $\text{tr}_{-i}(|\Phi_0\rangle\langle\Phi_1|)$ cannot, like any other necessary condition of LU equivalence considering just ρ_{1i} , enable us to determine the unitaries V_i and W_i . In fact, in this case we find $M_i = 0$.

with $\langle \Psi_{ij} | \Psi_{kl} \rangle = 1/2 \delta_{ik} \delta_{jl}$, where p and $1-p$ denote the eigenvalues of ρ_1 .

V. EXAMPLES

We employ now the algorithm presented in [16] and the results shown in the previous section to characterize the LU-equivalence classes of up to five qubits. We show that in all these cases it is not necessary to determine some unitaries as functions of some others but that it is always possible to determine them directly.

A. Two-qubit states

The standard form of a two-qubit state is $|\Psi\rangle = \lambda_1|00\rangle + \lambda_2|11\rangle$, with $\lambda_1 \geq \lambda_2 \geq 0$, which coincides with the Schmidt decomposition [19]. It is a well-known fact that bipartite states are LU equivalent iff their Schmidt coefficients coincide. Let us now demonstrate how this result can be rederived with the method presented in [16] for two qubits. If $\lambda_1 \neq \lambda_2$, that is, $\rho_i \neq \mathbb{1}$ then, $|\Psi\rangle \simeq_{\text{LU}} |\Phi\rangle$ iff $\text{eig}(\rho_1) = \text{eig}(\sigma_1)$, that is, iff the Schmidt coefficients λ_i are the same. For $\lambda_1 = \lambda_2$ we have that $\rho_1 = \rho_2 = \mathbb{1}$ and therefore the states are LU equivalent iff $\text{eig}(\rho) = \text{eig}(\sigma)$ (Corollary 1), which is obviously the case.

B. Three-qubit states

First we transform both states, $|\Psi\rangle$ and $|\Phi\rangle$, to their sorted trace decomposition. If there exists some i such that $\rho_i \neq \mathbb{1}$, we know that $U_i = Z(\alpha_i)$. Without loss of generality, we assume $i = 1$. Then we have that the states $|\Psi\rangle = \sqrt{p_1}|0\rangle|\Psi_0\rangle + \sqrt{1-p_1}|1\rangle|\Psi_1\rangle$ for some $p_1 > 1/2$ and $\langle \Psi_i | \Psi_j \rangle = \delta_{ij}$ and $|\Phi\rangle = \sqrt{p_2}|0\rangle|\Phi_0\rangle + \sqrt{1-p_2}|1\rangle|\Phi_1\rangle$ for some $p_2 > 1/2$ and $\langle \Phi_i | \Phi_j \rangle = \delta_{ij}$ are LU equivalent iff (1) $\text{eig}(\rho_1) = \text{eig}(\sigma_1)$, that is, iff $p_1 = p_2$, and (2) there exist local unitaries U_2, U_3 and two phases, ϕ and α_1 such that

$$\begin{aligned} |\Psi_0\rangle &= e^{i\gamma_1} U_2 \otimes U_3 |\Phi_0\rangle, \\ |\Psi_1\rangle &= e^{i\gamma_2} U_2 \otimes U_3 |\Phi_1\rangle, \end{aligned} \quad (9)$$

where $\gamma_1 = \phi + \alpha_1$ and $\gamma_2 = \phi - \alpha_1$. Since the states are not LU equivalent if $p_1 \neq p_2$, we assume that $p_1 = p_2$ and show now in detail how the unitaries can be computed. According to the method summarized in Sec. II, we distinguish the two cases (1) $\rho_{12} \neq \rho_1 \otimes \mathbb{1}$ and (2) $\rho_{12} = \rho_1 \otimes \mathbb{1}$. Since the rank of ρ_{12} cannot be larger than 2, the second case is only possible if $p = 1$, that is, the states $|\Psi\rangle$ is a product state. Then, the two states are LU equivalent iff the two-qubit states ${}_1\langle 0|\Psi\rangle$ and ${}_1\langle 0|\Phi\rangle$ are (see Sec. V A). In the first case we have that either (1a) at least one of the two states $|\Psi_i\rangle$ is not maximally entangled or (1b) both are maximally entangled. To investigate the case (1a), we assume, without loss of generality, that $|\Psi_0\rangle$ is not maximally entangled and denote by W_i (V_i) the local unitaries which map $|\Psi_0\rangle$ ($|\Phi_0\rangle$) to its standard form, respectively; that is, $|\Psi_0\rangle = W_1^\dagger W_2^\dagger (\sqrt{q_1}|00\rangle + \sqrt{1-q_1}|11\rangle)$, with $q_1 > 1/2$ [$|\Phi_0\rangle = V_1^\dagger V_2^\dagger (\sqrt{q_2}|00\rangle + \sqrt{1-q_2}|11\rangle)$ with $q_2 > 1/2$]. Obviously, $|\Psi_0\rangle \simeq_{\text{LU}} |\Phi_0\rangle$ iff $q_1 = q_2$. In this case, the most general unitaries which transform $|\Phi_0\rangle$ to $|\Psi_0\rangle$, that is, $|\Psi_0\rangle = e^{i\gamma_1} U_2 \otimes U_3 |\Phi_0\rangle$, are of the form $U_i = W_i Z(\alpha_i) V_i^\dagger$ for some phase α_i . Thus, we have that $|\Psi\rangle \simeq_{\text{LU}} |\Phi\rangle$ iff there exists phases α_i such that Eq. (2) is fulfilled for $k_1 = k_2 = k_3 = 0$,

$V_1 = W_1 = \mathbb{1}$, and V_i and W_i as defined earlier. This condition can then be easily checked using Lemma 1. In case (1b) we have that both $|\Psi_0\rangle$ and $|\Psi_1\rangle$ are maximally entangled and are therefore LU equivalent to $|\Phi^\pm\rangle$. Thus, $|\Psi\rangle$ is LU equivalent to $|\Phi\rangle$ in this case iff ${}_1\langle k|\Phi\rangle$ is maximally entangled for $k = 0, 1$. Since any state in this class is LU equivalent to the state $\sqrt{p_1}|0\rangle|\Phi^+\rangle + \sqrt{1-p_1}|1\rangle|\Phi^-\rangle$, the unitaries which map two states within this class to each other can be easily computed.

Let us now consider the remaining case where all single-qubit reduced states are completely mixed. Since $\rho_1 = \rho_2 = \mathbb{1}$, the eigenbasis of ρ_{12} is maximally entangled and therefore LU equivalent to the Bell basis (see Sec. IV A). Thus, any state with $\rho_i = \mathbb{1} \forall i$ is LU equivalent to $|\Psi\rangle = |\Phi^+\rangle|0\rangle + |\Phi^-\rangle|1\rangle = \mathbb{1} \otimes \mathbb{1} \otimes H|\Psi_0\rangle$, where $|\Psi_0\rangle = 1/\sqrt{2}(|000\rangle + |111\rangle)$ denotes the GHZ state [26].

In summary, we obtained the following necessary and sufficient condition for LU equivalence: The two three-qubit states $|\Psi\rangle$ and $|\Phi\rangle$ are LU equivalent iff one of the following conditions are fulfilled:

- (1) $E_i(|\Psi\rangle) = E_i(|\Phi\rangle) = 1 \forall i$ (i.e., $\rho_i = \mathbb{1} \forall i$).
- (2) There exists some system i such that $E_i(|\Psi\rangle) = E_i(|\Phi\rangle) = 0$ and $E_j(|\Psi\rangle) = E_j(|\Phi\rangle)$ for some system $j \neq i$.
- (3) There exists some system i such that $0 < E_i(|\Psi\rangle) < 1$ and $E_i(|\Psi\rangle) = E_i(|\Phi\rangle)$ and either
 - (3a) $E_j({}_i\langle k|\Psi\rangle) = E_j({}_i\langle k|\Phi\rangle) = 1$ for $k = 0, 1$ for some system $j \neq i$ holds;⁴ or
 - (3b) $E_j({}_i\langle k|\Psi\rangle) = E_j({}_i\langle k|\Phi\rangle) < 1$ for one value of $k \in \{0, 1\}$, and for the unitaries which can be easily and directly determined in this case there exists a bit string \mathbf{k} and local phase gates such that Eq. (2) has a solution.

For three qubits the polynomial invariants which define the different LU-equivalence classes are known [15,27]. In [28] we will compare them to the criterion derived here and investigate the measures of entanglement which are required to identify the different classes.

This completes the solution to the LU-equivalence problem of three-qubit states. However, in order to illustrate the method presented in [16], we apply it to the most complicated case, where $\rho_i = \mathbb{1} \forall i$. We show now that all these states are LU equivalent without using the fact that they are LU equivalent to the GHZ state, $|\Psi_0\rangle$. In other words, we determine now the unitaries $\{U_i\}$ such that $|\Psi\rangle = |\Psi_0\rangle = U_1 U_2 U_3 |\Phi\rangle$, where $|\Phi\rangle = S_1^\dagger S_2^\dagger S_3^\dagger |\Psi\rangle$. Here, S_i are some fixed unitaries. Since the rank of ρ_{12} is 2, we can compute U_2 as a function of U_1 . We find $U_2^\dagger \text{tr}_{-2}(|i\rangle\langle i|_1 |\Psi\rangle\langle \Psi|) U_2 = U_2^\dagger |i\rangle\langle i|_2 U_2 = S_2^\dagger \text{tr}_{/2}(W_1^\dagger |i\rangle\langle i|_1 W_1 |\Psi\rangle\langle \Psi|) S_2$, where $W_1 = U_1 S_1^\dagger$. Since the rank of these matrices is 1, we have (due to the fact that W_1 is unitary) that either $\langle 0|W_1^\dagger|0\rangle = 0$ (which implies that $\langle 1|W_1^\dagger|1\rangle = 0$) or $\langle 1|W_1^\dagger|0\rangle = 0$ (which implies that $\langle 0|W_1^\dagger|1\rangle = 0$). Thus, $W_1 = X^{k_1} Z(\alpha_1)$ (up to a global phase), for some $k_1 \in \{0, 1\}$ and some phase α_1 . Due to the symmetry of the state the same holds true for all $W_i = U_i S_i^\dagger$. Thus, we have that $|\Psi\rangle = U_1 U_2 U_3 |\Phi\rangle$ iff there exists k_1, k_2, k_3 and phases α_i such that $|\Psi\rangle = e^{i\alpha_0} \otimes_i Z(\alpha_i) X^{k_i} |\Psi\rangle$. Of course, it is straightforward to determine the remaining parameters,

⁴Recall that the states $|\Psi\rangle$ and $|\Phi\rangle$ do have trace decomposition.

but in order to continue with the algorithm we use Lemma 1 to show for which values of k_i the states are up to phase gates local unitary equivalent. The first condition, $|\langle \mathbf{i} | \Psi \rangle| = |\langle \mathbf{i} | \Phi \rangle| \forall \mathbf{i}$, implies that $k_1 = k_2 = k_3$. Then we have $|\Psi\rangle$ is LU equivalent to $|\Phi\rangle$ iff there exist phases α_i such that $|\Psi\rangle = e^{i\alpha_0} \otimes_i Z(\alpha_i) |\Phi\rangle$, which is true iff $\alpha_0 = 0$ and $e^{i(\alpha_1 + \alpha_2 + \alpha_3)} = 1$. Thus, using the preceding method we found $U_i = Z(\alpha_i) X^{k_i} S_i$, with $e^{i(\alpha_1 + \alpha_2 + \alpha_3)} = 1$ and $k_1 = k_2 = k_3$. The unitaries are not uniquely defined due to the symmetry of the state.

C. Four-qubit states

In this subsection we consider the LU equivalence of two four-qubit states, $|\Psi\rangle$ and $|\Phi\rangle$. Similarly to the other cases, we transform both states, $|\Psi\rangle$ and $|\Phi\rangle$, into their sorted trace decomposition. As before, the solution can, of course, be found using the method summarized in Sec. II. However, we will show here that also in this case it is possible to determine the unitaries V_i and W_i (and the bit values k_i) directly. That is, it will not be necessary to consider some of the unitaries as variables and to determine those unitaries by solving the equations which occur in Lemma 1.

According to the general method, we first distinguish the cases (1) there exists some system i with $\rho_i \neq \mathbb{1}$ and (2) $\rho_i = \mathbb{1}$ for any system i . In the first case we choose $i = 1$ and know that $U_1 = Z(\alpha_1)$ for some phase α_1 . Then we can either have that (1a) $\rho_{12} \neq \rho_1 \otimes \mathbb{1}$ or (1b) $\rho_{12} = \rho_1 \otimes \mathbb{1}$. In case (1a) W_2 , V_2 , and k_2 in Eq. (2) can easily be determined using the methods presented in Sec. IV. Then systems 1 and 2 can be measured in the computational basis leading to four two-qubit states. The remaining unitary operators can then be easily found. If $\rho_{12} = \rho_1 \otimes \mathbb{1}$ [case (1b)] we will show next that at least one of the unitaries V_i and W_i and the bit values k_i can be determined for $i \in \{3, 4\}$. First note that the eigenvalues of ρ_{34} are $p/2, p/2, (1-p)/2, (1-p)/2$, with $p \neq 1/2$, and therefore ρ_{34} is neither $\mathbb{1}$ nor LU equivalent to $\mathbb{1} - \lambda |\Psi^-\rangle \langle \Psi^-|$, for any value of λ . Thus, the unitaries W_i , V_i , and k_i for $i = 3, 4$ can be easily computed unless $\rho_{34} = \rho_3 \otimes \mathbb{1}$ (or $\rho_{34} = \mathbb{1} \otimes \rho_4$). However, in this case, since $\rho_{34} \neq \mathbb{1}$, the unitaries V_3 and W_3 and the bit value k_3 (or V_4 , W_4 , and the bit value k_4 , respectively) can be easily determined.

Let us now consider the remaining case where $\rho_i = \mathbb{1} \forall i$ (case 2). There, all two-qubit reduced states are LU equivalent to $\mathbb{1} + \sum_i \lambda_i \Sigma_i \otimes \Sigma_i$ and the reduced states are LU equivalent to each other iff the eigenvalues are the same (Corollary 1). We distinguish now the two cases (2a) $\rho_{12} \neq \mathbb{1}$ and (2b) $\rho_{12} = \mathbb{1}$. In the first case U_2 can be determined as a function of U_1 (see Sec. IV). Let us apply local unitaries to both states, $|\Psi\rangle$ and $|\Phi\rangle$, such that ρ_{12}, ρ_{34} and σ_{12}, σ_{34} are both Bell diagonal (see Lemma 4). We sort the eigenvalues in such a way that if there is threefold degeneracy; then the states are such that $\rho_{12} = \rho_{34} = \mathbb{1} - \lambda |\Psi^-\rangle \langle \Psi^-|$.⁵ The resulting states will again be denoted by $|\Psi\rangle, |\Phi\rangle$, respectively. If $\rho_{12} \neq \mathbb{1} - \lambda |\Psi^-\rangle \langle \Psi^-|$,

then the unitaries can be easily determined (see Sec. IV). In the ‘‘worst’’ case, where $\rho_{12} = \mathbb{1} - \lambda |\Psi^-\rangle \langle \Psi^-|$, we only find $U_2 = U_1$. We show next that also in this case U_2 , or more precisely V_2, W_2 , and k_2 in Eq. (2), can be directly computed. That is, we do not need to compute any of those unitaries as a function of some others.

Using Lemma 4 it is easy to see that any state $|\Psi\rangle$ with $\rho_{12} = \mathbb{1} - \lambda |\Psi^-\rangle \langle \Psi^-|$, is LU-equivalent (up to a global phase) to a state $|\Phi^+\rangle |\Phi^+\rangle + e^{i\gamma_1} |\Phi^-\rangle |\Phi^-\rangle + e^{i\gamma_2} |\Psi^+\rangle |\Psi^+\rangle + \sqrt{1 - \lambda} e^{i\gamma_3} |\Psi^-\rangle |\Psi^-\rangle$, for some phases γ_i . Since the operations $\Sigma_i \otimes \Sigma_i$ for $i \in \{1, 2, 3\}$ always change the sign of two states out of the four Bell states, we can choose $\gamma_1, \gamma_2 \leq \pi$. We are going to show next that two states of this form with the choice $\gamma_1, \gamma_2 \leq \pi$ are LU equivalent iff the complex coefficients which occur here coincide.

Let us denote by U_{mb} the 4×4 unitary matrix, which transforms the computational basis into the magic basis, that is, $U_{\text{mb}}|00\rangle = |\Phi^+\rangle, U_{\text{mb}}|01\rangle = -i|\Phi^-\rangle, U_{\text{mb}}|10\rangle = |\Psi^-\rangle, U_{\text{mb}}|11\rangle = -i|\Psi^+\rangle$. It is a well-known fact that for any U_1, U_2 unitary we have that $U_{\text{mb}}^\dagger U_1 \otimes U_2 U_{\text{mb}} = O$, where O is a real and orthogonal 4×4 matrix. Furthermore, it is easy to see that $O_i \equiv U_{\text{mb}}^\dagger U_i \otimes U_i U_{\text{mb}}$ can be written as $O_i = \tilde{O}_i \oplus |01\rangle \langle 01|$ ($U_{\text{mb}}|01\rangle = |\Psi^-\rangle$), where \tilde{O}_i is a three-dimensional rotation.

Since $\rho_{12} = \sigma_{12} = \mathbb{1} - \lambda |\Psi^-\rangle \langle \Psi^-|$ and therefore $\rho_{34} = \sigma_{34} = \mathbb{1} - \lambda |\Psi^-\rangle \langle \Psi^-|$, we know that there exist local unitaries U_i which map $|\Phi\rangle$ into $|\Psi\rangle$ iff $U_2 = U_1$ and $U_4 = U_3$. Thus, we have $|\Psi\rangle \simeq_{\text{LU}} |\Phi\rangle$ iff there exist real orthogonal matrices, $O_i = \tilde{O}_i \oplus |01\rangle \langle 01|$, with \tilde{O}_i a three-dimensional rotation such that

$$|\tilde{\Psi}\rangle \equiv U_{\text{mb}}^\dagger \otimes U_{\text{mb}}^\dagger |\Psi\rangle = O_1 \otimes O_3 |\tilde{\Phi}\rangle. \quad (10)$$

Note that $|\tilde{\Psi}\rangle = |00\rangle|00\rangle - e^{i\gamma_1}|10\rangle|10\rangle - e^{i\gamma_2}|11\rangle|11\rangle + \sqrt{1 - \lambda} e^{i\gamma_3}|01\rangle|01\rangle$ and that the phases γ_i are not local phases. Similarly, we have $|\tilde{\Phi}\rangle \equiv U_{\text{mb}}^\dagger \otimes U_{\text{mb}}^\dagger |\Phi\rangle = e^{i\tilde{\gamma}_0}(|00\rangle|00\rangle + e^{i\tilde{\gamma}_1}|10\rangle|10\rangle + e^{i\tilde{\gamma}_2}|11\rangle|11\rangle + \sqrt{1 - \lambda} e^{i\tilde{\gamma}_3}|01\rangle|01\rangle)$ for some phases $\tilde{\gamma}_i$ and coefficient $\tilde{\lambda}$. Using now that the real and orthogonal matrices O_1, O_3 are of the form $\tilde{O}_i \oplus |01\rangle \langle 01|$, it is easy to see that $|\Psi\rangle \simeq_{\text{LU}} |\Phi\rangle$; that is, Eq. (10) is satisfied iff $\{e^{i\tilde{\gamma}_i}\}_{i=1}^2 = \{e^{i\tilde{\gamma}_i}\}_{i=1}^2$ and $\sqrt{1 - \lambda} e^{i\tilde{\gamma}_3} = \sqrt{1 - \tilde{\lambda}} e^{i\tilde{\gamma}_3}$.

For the case (2b), where $\rho_{12} = \mathbb{1}$, which implies that $\rho_{34} = \mathbb{1}$ we write $|\Psi\rangle = \sum_{ij} |i, j\rangle |\psi_{i,j}\rangle$, with $\langle \psi_{ij} | \psi_{kl} \rangle = \delta_{ik} \delta_{jl}$. Since these states form an orthonormal (ON) basis, we can find a 4×4 unitary U such that $|\psi_{i,j}\rangle = U|i,j\rangle$. Recall that any two-qubit unitary operator U can be written as $U = U_1 \otimes U_2 U_d V_1 \otimes V_2$, where U_d , the nonlocal content of U , is diagonal in the magic basis, that is, $U_d = e^{i(\phi_1 X \otimes X + \phi_2 Y \otimes Y + \phi_3 Z \otimes Z)}$, for some phases ϕ_i [23]. Note that U_d can be made unique by imposing certain conditions on the phases, ϕ_i [29]. We transform the state by local unitary operations into the form $\mathbb{1}_{12} \otimes U_d \sum_{ij} |ij\rangle |ij\rangle = \mathbb{1}_{12} \otimes U_d |\Phi^+\rangle_{13} |\Phi^+\rangle_{24}$. Then the two states, $|\Psi\rangle = \mathbb{1}_{12} \otimes U_d(\Psi) \sum_{ij} |\Phi^+\rangle_{13} |\Phi^+\rangle_{24}$ and $|\Phi\rangle = \mathbb{1}_{12} \otimes U_d(\Phi) \sum_{ij} |\Phi^+\rangle_{13} |\Phi^+\rangle_{24}$ are LU equivalent iff $U_d(\Psi) = U_d(\Phi)$. Thus, these LU-equivalence classes are characterized by $E_{ij}(|\Psi\rangle) = 2$ for some systems i, j and the three parameters, ϕ_1, ϕ_2, ϕ_3 , which define the nonlocal content of U_d . In Sec. VIII we give a physical meaning to these parameters and discuss its generalization.

⁵Note that if $\rho_{12} = \mathbb{1} - \lambda |\Psi^-\rangle \langle \Psi^-|$, then $\rho_{34} = \mathbb{1} - \lambda |\Psi^-\rangle \langle \Psi^-|$ follows from the fact that all single-qubit reduced states are completely mixed and that the state describing all four systems is pure.

Using the fact that any four-qubit state with $\rho_{12} = \mathbb{1}$ is LU equivalent to the state $|\Psi\rangle = \mathbb{1}_{12} \otimes U_d \sum_{ij} |ij\rangle|ij\rangle$, where $U_d = U_{\text{mb}} \text{diag}(1, e^{i\phi_1}, e^{i\phi_2}, e^{i\phi_3}) U_{\text{mb}}^\dagger$ for some phases ϕ_i , it is also easy to rederive the result that there exists no four-qubit state with the property that all two-qubit reduced states are completely mixed, that is, $\rho_{ij} = \mathbb{1} \forall i, j$ [30]. This can be seen as follows. Since $|\Psi\rangle = \mathbb{1}_{12} \otimes U_d \sum_{ij} |ij\rangle|ij\rangle$, we find $\rho_{13} = \text{tr}_4(U_d |\Phi^+\rangle \langle \Phi^+|_{13} \otimes \mathbb{1}_4 U_d^\dagger)$. Then the conditions $\rho_{13} = \rho_{23} = \mathbb{1}$ imply that $\cos(\phi_i) = 0$ and $\cos(\phi_i - \phi_j) = 0 \forall i, j$. Since it is impossible to fulfill those equations simultaneously, we have that there exists no four-qubit state such that $\rho_{ij} = \mathbb{1} \forall i, j$. This implies that the case (2b) is actually contained in (2a). In fact, it corresponds to the case where $\lambda = 0$.

In summary, for the four-qubit case we have the following possibilities:

(1a) There exist some systems i and j with $\rho_i \neq \mathbb{1}$ and $\rho_{ij} \neq \rho_i \otimes \mathbb{1}$: Without loss of generality, we choose $i = 1$ and $j = 2$. Then $W_1 = V_1 = \mathbb{1}$ and $k_1 = 0$ in Eq. (2) and V_2, W_2 , and k_2 can be easily computed using the methods presented in Sec. IV.

(1b) There exists some system i with $\rho_i \neq \mathbb{1}$ and some system j with $\rho_{ij} = \rho_i \otimes \mathbb{1}$: Without loss of generality, we chose $i = 1$ and $j = 2$. Then the unitaries W_i, V_i , and k_i for $i = 3, 4$ can be easily computed by considering ρ_{34} , which can be neither $\mathbb{1}$ nor $\mathbb{1} - \lambda|\Psi^-\rangle \langle \Psi^-|$ for any value of λ .

In both cases at least for two systems the operators V_i and W_i and the bit values k_i can be determined. Thus, measuring those two systems in the computational basis leads to four equations for two-qubit states. The missing operators V_i and W_i and the bit values k_i can then be easily computed. The states are LU equivalent iff there exist some phases α_i such that Eq. (2) has a solution, which can easily be checked using Lemma 1.

(2a) For any system i , $\rho_i = \mathbb{1}$ and there exists a system j such that $\rho_{ij} \neq \mathbb{1}$ for some system i : Without loss of generality, we chose $i = 1$ and $j = 2$. First, we apply local unitaries to both states, $|\Psi\rangle$ and $|\Phi\rangle$, such that ρ_{12}, ρ_{34} and σ_{12}, σ_{34} are all Bell diagonal (see Sec IV A). The resulting states are again denoted by $|\Psi\rangle, |\Phi\rangle$, respectively. If $\rho_{12} \neq \mathbb{1} - \lambda|\Psi^-\rangle \langle \Psi^-|$ for any $\lambda \in \mathbf{R}$ (which implies that $\rho_{34} \neq \mathbb{1} - \lambda|\Psi^-\rangle \langle \Psi^-|$ for any $\lambda \in \mathbf{R}$), the unitaries V_i, W_i , and k_i in Eq. (2) can be directly computed using the methods of Sec. IV. If $\rho_{12} = \mathbb{1} - \lambda|\Psi^-\rangle \langle \Psi^-|$ for some $\lambda \in \mathbf{R}$ we map $|\Psi\rangle$ into the form $|\Phi^+\rangle|\Phi^+\rangle + e^{i\gamma_1}|\Phi^-\rangle|\Phi^-\rangle + e^{i\gamma_2}|\Psi^+\rangle|\Psi^+\rangle + \sqrt{\lambda}e^{i\gamma_3}|\Psi^-\rangle|\Psi^-\rangle$, for some phases γ_i with $\gamma_{1,2} < \pi$. Two states of this form are LU equivalent iff their complex coefficients which occur here coincide.

(2b) For any system i , $\rho_i = \mathbb{1}$ and there exists a system j such that $\rho_{ij} = \mathbb{1}$ for some system i : Without loss of generality we chose $i = 1$ and $j = 2$. In this case the state is LU equivalent to the state $|\Psi\rangle = \mathbb{1}_{12} \otimes U_d(\Psi) \sum_{ij} |ij\rangle|ij\rangle$, where $U_d(\Psi) = U_{\text{mb}} \text{diag}(1, e^{i\phi_1}, e^{i\phi_2}, e^{i\phi_3}) U_{\text{mb}}^\dagger$ can be chosen uniquely. Then two states are LU equivalent iff $U_d(\Psi) = U_d(\Phi)$. Note that since there exists no four-qubit state with $\rho_{ij} = \mathbb{1} \forall i, j$ case (2b) is contained in (2a).

Similarly to the three-qubit case, we will consider now the most complicated case (for the algorithm proposed in [16]) and show how the unitaries which transform two LU-equivalent states into each other can be determined. The most complicated

case for four qubits is the one where $\rho_{ij} = \mathbb{1}$, for some systems i, j which we chose to be 1, 2. Thus, we consider the example $|\Psi\rangle = \mathbb{1}_{12} \otimes U_{34} |\Phi^+\rangle_{13} |\Phi^+\rangle_{24}$, where we choose $U_{34} = U_{\text{mb}} \text{diag}(1, e^{i\phi}, e^{i\phi}, 1) U_{\text{mb}}^\dagger$ such that $\rho_{12} = \rho_{34} = \rho_{23} = \mathbb{1}$. It can be easily shown that $\rho_{13} = \rho_{24} = 1/4(\mathbb{1} + X \otimes X + \cos(\phi)(Z \otimes Z - Y \otimes Y))$. Our aim is to determine U_i such that $|\Psi\rangle = U_1, \dots, U_4 |\Phi\rangle$, where $|\Phi\rangle = S_1^\dagger, \dots, S_4^\dagger |\Psi\rangle$, for some given unitaries S_i . Since $\rho_{13} \neq \mathbb{1}$ and $\rho_{24} \neq \mathbb{1}$, we can compute $U_3 (U_4)$ as a function of $U_1 (U_2)$, respectively. Considering Eqs. (4) for all values of l and m simultaneously, we have $\rho_{13} = 1/4[\mathbb{1} + X \otimes X + \cos(\phi)(Z \otimes Z - Y \otimes Y)] = U_1 U_3 (S_1^\dagger S_1^\dagger \rho_{13} S_1 S_1) U_1^\dagger U_3^\dagger$. It is straightforward to see that the last equation can only be fulfilled if $U_1 S_1^\dagger = U_3 S_3^\dagger = \Sigma_k$ for $k \in \{0, 1, 2, 3\}$, where $\Sigma_0 = \mathbb{1}$. Similarly, we find $U_2 S_2^\dagger = U_4 S_4^\dagger = \Sigma_l$. Thus, we have $U_i = \Sigma_{k_i} S_i$, where $k_1 = k_3 = k$ and $k_2 = k_4 = l$. It is straightforward to show that $|\Psi\rangle = \Sigma_k \Sigma_l \Sigma_k \Sigma_l |\Psi\rangle$ for certain values of k, l (e.g., $k = 0, l = 3$ or $k = 1, l \in \{0, 1\}$). Again, the reason why the unitaries are not uniquely determined using this method is the symmetries of the state.

D. Five-qubit states

Instead of considering now, similarly to the other cases, all possible classes of five-qubit states, we consider here one of the hardest examples to illustrate the method presented in [16]. First, we construct a five-qubit state, $|\Psi\rangle$, which has the property that all the two-qubit reduced states are completely mixed. Then we consider the two states $|\Psi\rangle$ and $|\Phi\rangle = S_1 \otimes \dots \otimes S_5 |\Psi\rangle$ for some local unitaries S_i and compute the unitaries, U_i , which map $|\Phi\rangle$ into $|\Psi\rangle$, using the algorithm presented in [16] and summarized in Sec. III. We show that also in this case it will not be necessary to determine any of the unitaries as a function of some others but that it will be possible to determine them directly.

In order to construct the five-qubit state $|\Psi\rangle$ with $\rho_{ij} = \mathbb{1} \forall i, j$, we write $|\Psi\rangle = |0\rangle|\Psi_0\rangle + |1\rangle|\Psi_1\rangle$, where $\langle \Psi_i | \Psi_j \rangle = \delta_{ij}$. As shown earlier, any four-qubit state which has the property that $\rho_{12} = \mathbb{1}$ is LU equivalent to a state $\mathbb{1}_{12} \otimes U_d \sum_{ij} |ij\rangle|ij\rangle$, where $U_d = U_{\text{mb}} \text{diag}(1, e^{i\alpha_1}, e^{i\alpha_2}, e^{i\alpha_3}) U_{\text{mb}}^\dagger$. Imposing now also that $\rho_{23} = \rho_{14} = \mathbb{1}$ and that the phases α_i fulfill $0 \leq \alpha_i < \pi$, we find $|\Psi_0\rangle = \mathbb{1}_{12} \otimes U_{d_1} \sum_{i,j} |ij\rangle|ij\rangle$, where $U_{d_1} = U_{\text{mb}} \text{diag}(1, e^{i\alpha_1}, e^{i\alpha_1}, 1) U_{\text{mb}}^\dagger$. It is easy to see that two states, $|\Psi_0\rangle, |\Psi_1\rangle$, of this form are orthogonal to each other iff $\alpha_2 = \alpha_1 + \pi$. We consider now the five-qubit state $|\Psi\rangle = |0\rangle|\Psi_0\rangle + |1\rangle|\Psi_1\rangle$ with $|\Psi_0\rangle = \mathbb{1}_{12} \otimes U_{d_1} \sum_{i,j} |ij\rangle|ij\rangle$ and $|\Psi_1\rangle = \mathbb{1}_{12} \otimes U_{d_2} \sum_{i,j} |ij\rangle|ij\rangle$, with $U_{d_2} = U_{\text{mb}} \text{diag}(1, -e^{i\alpha_1}, -e^{i\alpha_1}, 1) U_{\text{mb}}^\dagger$. It is straightforward to show that all two-qubit states ρ_{ij} are completely mixed. Note that $|\Psi\rangle = |+\rangle(|\Phi^+, \Phi^+\rangle + |\Psi^+, \Psi^+\rangle) + e^{i\alpha} |-\rangle(|\Phi^-, \Phi^-\rangle + |\Psi^-, \Psi^-\rangle)$.

Let us now consider the state $|\Phi\rangle = S_1 \otimes \dots \otimes S_5 |\Psi\rangle$ for some local unitaries S_i and compute the unitaries, U_i , which map $|\Phi\rangle$ into $|\Psi\rangle$. Since $\rho_{ij} = \mathbb{1}$, we choose U_1, U_2 as parameters. Note that $\rho_{123} \neq \mathbb{1}$, since it can have at most rank 4. Thus, we can compute the unitary U_3 as a function of U_1 and U_2 considering ρ_{123} , which can be easily shown to be $1/8(\mathbb{1} + X \otimes X \otimes X)$.

We have $U_3^\dagger|\Psi\rangle = U_1U_2\mathbb{1}U_4U_5|\Phi\rangle$ and therefore $U_3^\dagger\text{tr}_{-3}(|kl\rangle_{12}\langle ij||\Psi\rangle\langle\Psi|)U_3 = \text{tr}_{-3}(U_1^\dagger U_2^\dagger|kl\rangle_{12}\langle ij|U_1U_2|\Phi\rangle\langle\Phi|)$ for any i, j, k, l . It can be easily shown that $\text{tr}_{-3}(|00\rangle_{12}\langle 11||\Psi\rangle\langle\Psi|) = X/2$ and that $\text{tr}_{-3}(U_1^\dagger U_2^\dagger|00\rangle_{12}\langle 11|U_1U_2|\Phi\rangle\langle\Phi|) = xS_3X S_3^\dagger$, where x depends on U_1, U_2 . Since only x depends on U_1 and U_2 , U_3 can be directly computed (not only as a function of U_1, U_2). We find $U_3 = e^{i\alpha_3 X} S_3^\dagger$ for some phase α_3 . Thus, denoting by $|\tilde{\Psi}\rangle = H_3|\Psi\rangle$ we have $|\Psi\rangle \simeq_{\text{LU}} |\Phi\rangle$ iff there exist local unitaries U_1, U_2, U_4, U_5 and a phase α_3 such that $|\tilde{\Psi}\rangle = U_1U_2Z(\alpha_3)H_3S_3^\dagger U_4U_5|\Phi\rangle$, where S_3 is determined. Projecting now the third system onto $|0\rangle$, we find a state of system 1245 with the property that $\rho_{24} \propto \mathbb{1} + X \otimes X$. Imposing then the necessary condition $\rho_{24} = U_2U_4\sigma_{24}U_2^\dagger U_4^\dagger$ of LU equivalence leads immediately to $U_2 = e^{i\alpha_2 X} S_2^\dagger$ and $U_4 = e^{i\alpha_4 X} S_4^\dagger$. Similarly, we find the other unitaries. Thus, we have $|\Psi\rangle \simeq_{\text{LU}} |\Phi\rangle$ iff there exist phases α_i such that $\bigotimes_{i=1}^5 H_i|\Psi\rangle = e^{i\alpha_0} \bigotimes_i Z(\alpha_i)(\bigotimes_{i=1}^5 H_i S_i^\dagger)|\Phi\rangle$. The existence of the phases can be easily verify either by looking at the coefficients in the computational basis or by employing Lemma 1.

VI. LOCC INCOMPARABILITY

The results presented here lead also to conditions for the existence of more general operations transforming one state to the other, namely, LOCC. This is due to the fact that two multipartite states, having the same marginal one-party entropies, are either LU equivalent or LOCC incomparable [31,32]; that is, none of the states can be mapped to the other by LOCC.

In this section we show that for any $n > 2$ there exists a pair of n -qubit states, $\{|\Psi\rangle, |\Phi\rangle\}$ such that for any bipartition A/B , where A contains a qubits and B contains $n - a$ qubits, $\text{eig}(\rho_A) = \text{eig}(\sigma_A)$, but the states are not LU equivalent. In particular, the entropies of the reduced states of any subsystem coincide; that is, all bipartite entanglement, measured with the von Neumann entropy of the reduced states, is the same for both states. Since the eigenvalues of all single-qubit reduced states coincide, those states are not even LOCC comparable [31,32]. Surprisingly, in those examples $|\Phi\rangle$ will be the complex conjugation (in the computational basis) of $|\Psi\rangle$. That is, for any n ($n > 2$) there exist n -qubit states which are not even LOCC comparable to its complex conjugate. The consequence of the existence of these states will be discussed in Sec. VIII.

Note that for three-qubit states examples of such states have already been presented in [33]. There the fact that the states are not LU equivalent has been proven by employing a polynomial invariant of degree 12. Here we use the necessary and sufficient condition for LU equivalence presented in [16] and Sec. III to prove that the considered n -qubit states are not LU equivalent. First we present a three-qubit state $|\Psi\rangle$ which is not LU equivalent and therefore not even LOCC comparable to its complex conjugate. Then we will generalize this example to n -qubit states.

We consider the LME states $|\Psi\rangle = U_{123}(\phi)|+\rangle^{\otimes 3}$ and $|\Phi\rangle = U_{123}(\phi + \pi)|+\rangle^{\otimes 3}$, where $U_{123}(\alpha)$ is the three-qubit phase gate defined by $U_{123} = \mathbb{1} - (1 - e^{i\phi})|111\rangle\langle 111|$. As

mentioned in Sec. III an arbitrary LMES, $|\Psi\rangle$, can be easily transformed into its trace decomposition, $|\Psi_{\text{tr}}\rangle$, by applying the local unitary operations $HZ(\phi_i)$, where ϕ_i is chosen such that $\cot(\phi_i) = \frac{\langle X_i \rangle}{\langle Y_i \rangle}$. For the symmetric state $|\Psi\rangle$ we find $\langle X_i \rangle = 1/4[3 + \cos(\phi)]$ and $\langle Y_i \rangle = \sin(\phi)/4$ and therefore $\cot(\phi_i) = \cot(\phi) + 3 \csc(\phi)$ for $i = 1, 2, 3$. For $\phi = \pi/2$ the marginal entropies of $|\Psi\rangle$ and $|\Phi\rangle$, which is equivalent to the complex conjugate of $|\Psi\rangle$ in this case, coincide. However, it is easy to show that $|\Psi_{\text{tr}}\rangle/|\Psi_{\text{tr}}\rangle^*$ is not a product state and therefore the states $|\Psi\rangle$ and $|\Psi\rangle^*$ are not LU equivalent (see Lemma 1). Moreover, due to the fact that the eigenvalues of all the reduced states are the same for $|\Psi\rangle$ and $|\Psi\rangle^*$, those two states are not even LOCC comparable. Note that those two states have the same bipartite entanglement (considering any bipartite splitting) and the same value for the tangle [5], the value of which is the same for a state and its complex conjugate.

Let us now generalize this example to n -qubit states (for $n > 2$). That is, the two n -qubit states, $|\Psi\rangle = U_{1,\dots,n}(\pi/2)|+\rangle^{\otimes n}$ and $|\Phi\rangle = |\Psi\rangle^*$, have the property that $\text{eig}(\rho_A) = \text{eig}(\sigma_A)$ for any subsystem A . However, the states are not even LOCC comparable. In order to prove that, we first note that the eigenvalues of ρ_A and ρ_A^* coincide for any subsystem A . Furthermore, since the state is symmetric with respect to particle exchange, all single-qubit reduced states coincide. They are of the form $\rho = |+\rangle\langle +| + 2^{-n}\{\sqrt{2}[(1+i)|1\rangle\langle +| + (1-i)|+\rangle\langle 1|] + 2|1\rangle\langle 1|\}$, with eigenvalues $1/2(1 \pm 2^{-n}\sqrt{8 - 2^{2+n} + 2^{2n}})$. Thus, none of the reduced states is proportional to the identity and therefore the states are LU equivalent iff their standard forms coincide. Since those states are LMESs, we know that their trace decompositions are of the form $[HZ(\alpha)]^{\otimes n}|\Psi\rangle$, where α is determined via the equation $\cot(\alpha) = \frac{\langle X_i \rangle}{\langle Y_i \rangle} = 1 - 2^{n-1}$. It is straightforward to show that $|\Psi_{\text{tr}}\rangle = \cos(\alpha/2)|0\rangle - i \sin(\alpha/2)|1\rangle^{\otimes n} + 2^{-n}(i-1)e^{i\alpha n/2}[|0\rangle - |1\rangle]^{\otimes n}$ and therefore none of the coefficients in the computational basis vanishes for $n > 2$. There exist now several ways to prove that $|\Psi\rangle$ is not LU equivalent to its complex conjugate. We could either compute the standard form, $|\Psi_s\rangle$, and show that it does not coincide with the one of $|\Psi\rangle^*$, that is, show that $|\Psi_s\rangle$ is not real, or we could employ Lemma 1 or Lemma 3. We use here Lemma 3 to show that the sorted trace decompositions are not related to each other by local phase gates, which proves that the states are not LU equivalent. Since the first condition [condition (i)], $|\langle i|\Psi_{\text{tr}}\rangle| = |\langle i|\Psi_{\text{tr}}^*\rangle|$ is obviously fulfilled, we have that $|\Psi\rangle \simeq_{\text{LU}} |\Psi\rangle^*$ iff $|\Psi\rangle/|\Psi\rangle^*$ is a product state. Since $|\Psi\rangle$ is symmetric, this last condition is fulfilled iff there exists a single-qubit state $|\phi\rangle$ such that $|\Psi\rangle/|\Psi\rangle^* = |\phi\rangle^{\otimes n}$. In other words, the states are LU equivalent iff there exists two phases α_0 and α_1 such that $|\Psi_{\text{tr}}\rangle = e^{i\alpha_0} Z(\alpha_1)^{\otimes n} |\Psi_{\text{tr}}^*\rangle$. This last equation is fulfilled iff there exists a phase α_1 such that $U_{1,\dots,n}(\pi/2)|+\rangle^{\otimes n} = e^{i\alpha_0} V_{\alpha_1}^{\otimes n} U_{1,\dots,n}(-\pi/2)|+\rangle^{\otimes n}$, where $V_{\alpha_1} = Z(-\alpha)HZ(\alpha_1)HZ(-\alpha) = e^{-i\alpha_1/2}[\cos(\alpha_1/2)Z(-2\alpha) - i \sin(\alpha_1/2)e^{-i\alpha} X]$. Rewriting this condition we have that the states are LU equivalent iff there exists a phase α_1 such that $|+\rangle^{\otimes n} + (i-1)|1\rangle^{\otimes n} = e^{i\alpha_0} [V_{\alpha_1}|+\rangle^{\otimes n} + (-i-1)(V_{\alpha_1}|1\rangle)^{\otimes n}]$. It can be easily shown that this condition can only be fulfilled if $V_{\alpha_1}|+\rangle \propto |e_1\rangle$ and

$V_{\alpha_1}|+\rangle \propto |e_2\rangle$, where $|e_i\rangle \in \{|1\rangle, |+\rangle\}$, for $i = 1, 2$ and $e_1 \not\propto e_2$. We consider the two possible cases, (a) $V_{\alpha_1}|+\rangle = a|1\rangle$ for some $a \in \mathcal{C}$ and (b) $V_{\alpha_1}|+\rangle = a|+\rangle$ for some $a \in \mathcal{C}$. Case (a) is possible iff $\cos(\alpha_1/2) + i \sin(\alpha_1/2)e^{-i\alpha} = 0$ and $\cos(\alpha_1)e^{-2i\alpha} + i \sin(\alpha_1)e^{-i\alpha} = a$. It is easy to see that the first condition cannot be fulfilled since α is determined as mentioned earlier. Since $V_{\alpha_1}|+\rangle = a|+\rangle$ [case (b)] implies that $\cos(\alpha_1) = 0$ it is also easy to see that in this case $V|1\rangle = \pm i e^{-i\alpha}|0\rangle$ and therefore $V|1\rangle \neq a|e_i\rangle$ with $|e_i\rangle \in \{|1\rangle, |+\rangle\}$, for $i = 1, 2$. This proves that for any $n > 2$, the two n -qubit states, $|\Psi\rangle$ and $|\Psi^*\rangle$, are not LU equivalent.

VII. LU EQUIVALENCE OF MIXED STATES AND d -LEVEL SYSTEMS

We show here that the criterion of LU equivalence presented in [16] serves also as a criterion of LU equivalence for certain mixed and also for certain multipartite states which describe a system composed of d -level systems.

For instance, if we want to find out whether two mixed states are related to each other by local unitaries and if there exists at least one eigenvalue of the mixed state which is not degenerate, then the same method can be used. This is due to the fact that the unitaries cannot change the eigenvalues; thus, if $\rho \simeq_{\text{LU}} \sigma$, then it must hold that $|\Psi\rangle \simeq_{\text{LU}} |\Phi\rangle$, where $|\Psi\rangle$ ($|\Phi\rangle$) denote the eigenstates to the nondegenerate eigenvalue of ρ (σ), respectively. In order to check then if the two mixed states are LU equivalent, one first uses the algorithm to determine the local unitaries which transform $|\Phi\rangle$ into $|\Psi\rangle$. Those unitaries must also transform σ into ρ , which can then be easily checked.

The criterion for LU equivalence for pure states can also be employed for mixed states if there does not exist a nondegenerate eigenvalue, but one which is twofold degenerate. Let us denote by $|\Psi_0\rangle, |\Psi_1\rangle$ and $|\Phi_0\rangle, |\Phi_1\rangle$, the eigenvectors corresponding to the twofold degenerate eigenvalue of ρ, σ , respectively. As before, we have that if $\rho \simeq_{\text{LU}} \sigma$, then there exist local unitaries U_i such that $|\Psi_0\rangle\langle\Psi_0| + |\Psi_1\rangle\langle\Psi_1| = \bigotimes_i U_i (|\Phi_0\rangle\langle\Phi_0| + |\Phi_1\rangle\langle\Phi_1|) \bigotimes_i U_i^\dagger$. This equation is fulfilled iff there exists a 2×2 unitary, V , with $|\Psi_k\rangle = \bigotimes_i U_i \sum_l V_{kl} |\Phi_l\rangle$, for $k = 1, 2$. Note that this is equivalent to finding the local unitaries which map the state $|\Phi\rangle = |0\rangle|\Phi_0\rangle + |1\rangle|\Phi_1\rangle$ into $|\Psi\rangle = |0\rangle|\Psi_0\rangle + |1\rangle|\Psi_1\rangle$. Thus, solving the LU-equivalence problem of mixed n -qubit states, where one eigenvalue is twofold degenerate is equivalent to solving the LU-equivalence problem of $n+1$ -qubit states, where $\rho_1 = \mathbb{1}$.

Suppose now that ρ is a n -qubit mixed state and its eigenvalue with the smallest degeneracy is l -fold degenerate. We denote by $|\Psi_k\rangle$ ($|\Phi_k\rangle$) the eigenstates of ρ (σ) corresponding to this eigenvalue. Then $\rho \simeq_{\text{LU}} \sigma$ implies that $\sum_k |k\rangle|\Psi_k\rangle = V \bigotimes_i U_i \sum_k |k\rangle|\Phi_k\rangle$, where V is a $l \times l$ unitary and all the other U_i are single-qubit unitary operations. The idea is then to first fix the unitaries U_i using the algorithm presented in [16] and at the end try to fix the unitary V .

The LU-equivalence problem for d -level systems can be investigated in a similar way. However, due to the additional degeneracy which can occur in this case, the situation gets more complicated. For instance, if a state $|\Psi\rangle$ describes a system composed out of d -level systems, then ρ_i , which

describes a single d -level system can be l -fold degenerate, where $l \leq d$. Thus, in this case the unitaries occurring in Eq. (2) can in general not be determined up to local phase gates. If there is no degeneracy, similar methods can of course be applied to solve the problem of LU equivalence.

VIII. MULTIPARTITE ENTANGLEMENT

The algorithm presented in [16] cannot only be used to solve the LU-equivalence problem, but allows us also to gain a new insight into the entanglement properties of multipartite states. Within the algorithm the classes $\rho_{n_1, \dots, n_l, k} \neq \rho_{n_1, \dots, n_l} \otimes \mathbb{1}$ and $\rho_{n_1, \dots, n_l, k} = \rho_{n_1, \dots, n_l} \otimes \mathbb{1}$ for some subset of qubits, n_1, \dots, n_l, k , are distinguished. In the first case the unitary W_k can be computed as a function of the unitaries U_{n_1}, \dots, U_{n_l} , whereas it cannot (using the proposed algorithm) be computed in the second case. Therefore, in this case a new variable, U_k is required. As explained in [16], those classes correspond also to different entanglement classes. For instance, applying any von Neumann measurement on the first subsystem described by the state $|\Psi\rangle$, with $\rho_{12} = \rho_1 \otimes \mathbb{1}$, always results in a state where the second system is maximally entangled with the remaining systems, independent of the measurement outcome. Obviously, this is not the case for a state with $\rho_{12} \neq \rho_1 \otimes \mathbb{1}$. This suggests that, in order to understand how a many-body system can be entangled, one first identifies the entanglement class (as described previously) to which the state belongs. Note that this classification is based on multipartite, not bipartite entanglement properties. However, it is easy to perform this classification since one only needs to consider the reduced state of certain subsystems. Within the identified entanglement class it is then feasible to understand how multipartite entanglement can be qualified and even quantified. For instance, as we have seen in Sec. V, the LU-equivalence classes of four-qubit states with $\rho_{ij} = \mathbb{1}$, for some systems i and j are characterized by three parameters. This is due to the fact that any state in this class (choosing, without loss of generality, $i = 1, j = 2$) can be written as $|\Psi\rangle = \mathbb{1}_{12} \otimes U_d |\Phi^+\rangle_{13} |\Phi^+\rangle_{24}$, where $U_d = e^{i(\phi_1 X \otimes X + \phi_2 Y \otimes Y + \phi_3 Z \otimes Z)}$, for some phases ϕ_i . Thus, also the entanglement contained in such a state is completely characterized by $E_{12}(|\Psi\rangle) = 2$ and the three phases, ϕ_i . Recall that any two-qubit gate, U , can be decomposed as $U = U_1 \otimes U_2 U_d V_1 \otimes V_2$, with U_d as previously denotes the nonlocal content of the gate U . Using all that allows us to give the three parameters ϕ_i the following physical meaning. Recall that the state $|\Psi\rangle = \mathbb{1}_{12} \otimes U_{34} |\Phi^+\rangle |\Phi^+\rangle$ is the Choi-Jamiolkowski state corresponding to the operation U [17]. That is, given the state $|\Psi\rangle$ the operation U can be implemented using just local operations.⁶ This shows that the nonlocal properties of a four-qubit state for which there exists a maximally entangled bipartite splitting between two versus two qubits

⁶The implementation works as follows. First, a system is prepared in the state $|\Psi\rangle$. Then local Bell measurements are performed on $|\Psi\rangle$ and the input state, ρ . In case the measurement $|\Phi^+\rangle$ is performed, the output state is $\mathcal{E}(\rho)$. In case any other measurement result is obtained, the output will be $\mathcal{E}(\sum_i \otimes \sum_j \rho \Sigma_i^\dagger \otimes \Sigma_j^\dagger)$ for properly chosen local operation $\Sigma_i \otimes \Sigma_j$.

is completely characterized by the amount of entanglement which can be generated using this state as the only nonlocal resource.

Of course, this new insight in characterizing multipartite entanglement by the amount of entanglement which can be generated using this state as the only nonlocal resource can be generalized to an arbitrary state, independent of the dimension and even for mixed states. Note that the quantum operation corresponding to a state describing n subsystems is acting only on $\lceil n/2 \rceil$ systems. As in the example of four-qubit states, the corresponding operation is acting on two qubits. This fact simplifies the characterization of multipartite entanglement, since, for example, the nonlocal properties of two-qubit operations are very well understood. It should be further noted here that the operation corresponding to the state $|\Psi\rangle$ via the Choi-Jamiolkowski isomorphism is unitary iff the state has the property that it is maximally entangled in the considered bipartite splitting.

Let us point out here that the algorithm gets more and more complicated the larger is the number of systems l for which $\rho_{n_1, \dots, n_l} = \mathbb{1}$ for any choice of n_1, \dots, n_l , since then l unitaries have to be considered as variables. In the worst case, where any bipartition of $\lceil n/2 \rceil$ qubits is maximally entangled with the rest, $\lceil n/2 \rceil$ unitaries have to be considered as variables. It is known, however, that only for very few values of n do such states exist [34]. On the other hand, the more systems are maximally entangled with the rest, the fewer parameters remain to characterize the LU-equivalence class. For instance, in the example of four qubits, the class with $\rho_{ij} = \mathbb{1}$, for some systems i, j can be characterized with only three parameters. For the other extreme case of generic states, all the parameters occurring in the standard form determine, such as in the bipartite case, the entanglement contained in the state.

Another insight into multipartite entanglement which we gained here is the fact that for any $n > 2$ there exists a n -qubit state, $|\Psi\rangle$, which is not LOCC comparable to its complex conjugate (Sec. VI). Thus, the nonlocal properties of $|\Psi\rangle$ and $|\Psi^*\rangle$ seem to be really different. Since the mapping $|\Psi\rangle \rightarrow |\Psi^*\rangle$ corresponds to the redefinition of the complex unit i by $-i$, one might expect that this change does not lead to any new physics. In fact, for any observable O , we have $\langle \Psi | O | \Psi \rangle = \langle \Psi^* | O^* | \Psi^* \rangle$. Thus, whatever measurement outcome we can get by measuring a system described by the state $|\Psi\rangle$, the same outcome can be obtained by measuring O^* on $|\Psi^*\rangle$. Due to that, there will not exist a physical measure which is capable of distinguishing those two states. This shows that it will not be possible to characterize all LU-equivalence classes by operational entanglement measures.⁷

This suggests the introduction of a function, I_1 , with $I_1(|\Psi\rangle) = 0$ if $|\Psi\rangle \simeq_{\text{LU}} |\Psi^*\rangle$ and $I_1(|\Psi\rangle) = 1$ otherwise. If $I_1(|\Psi\rangle) = 1$, the Hilbert space should be divided into two subsets, one containing $|\Psi\rangle$ and the other containing $|\Psi^*\rangle$. After making this distinction, one proceeds investigating the nonlocal properties of the state $|\Psi\rangle$ within the subset associated to it.

In [28] we will follow the approach to investigate the multipartite entanglement properties in the way outlined here. In particular, we will consider multipartite state, describing several qubits, and introduce the function which determines if a state is LU equivalent to its complex conjugate or not. Moreover, we will analyze the entanglement contained in the state by investigating the amount of entanglement which can be generated using this state as the only nonlocal resource to implement quantum operations on a smaller system.

IX. CONCLUSION

We used the criterion of LU equivalence of multipartite pure states to derive the different LU-equivalence classes of up to four qubits. For five-qubit states, which can be treated analogously, it is shown that the most complicated class of states, where all two-qubit reduced states are completely mixed, can be easily considered using the algorithm developed in [16]. Even though it is, in principle, necessary to determine some of the local unitary operations as a function of some others, it is shown that for those cases this is, in fact, not required. That is, the unitaries can always be directly computed. The algorithm suggests to distinguish different classes of entangled states, such as the one where $\rho_{12} \neq \rho_1 \otimes \mathbb{1}$ and where $\rho_{12} = \rho_1 \otimes \mathbb{1}$. We considered here all the possible classes and showed that, within certain classes, new operational entanglement parameters can be identified which completely characterize the nonlocal properties of the states. For instance, it has been shown that any four-qubit state for which one two-qubit reduced state is completely mixed is LU equivalent to a state $|\Psi\rangle = \mathbb{1} \otimes U_d |\Phi^+\rangle |\Phi^+\rangle$, where $U_d = e^{i(\alpha_1 X \otimes X + \alpha_2 Y \otimes Y + \alpha_3 Z \otimes Z)}$ with $\alpha_i \in \mathbf{R}$, is the nonlocal content of a two-qubit gate [23]. The state $|\Psi\rangle$ is the Choi-Jamiolkowski state corresponding to the operation U_d [17]. Thus, U_d can be implemented by local operations if the state $|\Psi\rangle$ is used as a resource. This new approach of characterizing the entanglement of a multipartite state by the entangling capability of the operation which can be implemented using the state as the only nonlocal resource can be generalized to arbitrary states. Moreover, we derived examples of n -qubit states (for $n > 2$) which are not LOCC comparable to their complex conjugate. This observation suggests the introduction of a new measure, which distinguishes the cases $|\Psi\rangle \simeq_{\text{LU}} |\Psi^*\rangle$ and $|\Psi\rangle \not\simeq_{\text{LU}} |\Psi^*\rangle$. If the states are not LU equivalent, two different subsets of the Hilbert space should be considered, one for $|\Psi\rangle$ and one for $|\Psi^*\rangle$, in order to further investigate the properties of multipartite entangled states. In [28] we will prove that the examples of n -qubit states, $|\Psi\rangle$, which are presented here, cannot even be mapped into their complex conjugate by allowing stochastic LOCC. That is, it is not possible to transform $|\Psi\rangle$ into $|\Psi^*\rangle$ by local operations even with an arbitrary small probability of success.

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⁷Note that in [35] it has been shown that the orbit of a state is uniquely defined by the set of all entanglement monotones.

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