

Absolutely maximally entangled state equivalence and the construction of infinite quantum solutions to the problem of 36 officers of Euler


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Ordering and classifying multipartite quantum states by their entanglement content remains an open problem. One class of highly entangled states, useful in quantum information protocols, the absolutely maximally entangled (AME) ones, are especially hard to compare as all their subsystems are maximally random. While it is well known that there is no AME state of four qubits, many analytical examples and numerically generated ensembles of four-qutrit AME states are known. However, we prove the surprising result that there is truly only *one* AME state of four qutrits up to local unitary equivalence. In contrast, for larger local dimensions, the number of local unitary classes of AME states is shown to be infinite. Of special interest is the case of local dimension 6, where it was established recently that a four-party AME state does exist, providing a quantum solution to the classically impossible Euler problem of 36 officers. Based on this, an infinity of quantum solutions are constructed, and we prove that these are not equivalent. The methods developed can be usefully generalized to multipartite states of any number of particles.

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I. INTRODUCTION

Quantum entanglement between two distant parties, with its counterintuitive nonclassical features, has been experimentally verified [1–4] via violations of Bell–Clauser–Horne–Shimony–Holt (CHSH) inequalities [5]. Multipartite entanglement, which is at the heart of quantum information, computation, and many-body physics, is still poorly understood. Studying the entanglement content in them via interconvertibility and classifying them are of fundamental importance. A putative maximally entangled class called absolutely maximally entangled (AME) states are such that there is maximum entanglement between any subset of particles and the rest [6]. They have been related to error-correcting codes [7], both classical and quantum, combinatorial designs such as orthogonal Latin squares (OLSs) [8–10], quantum parallel teleportation and secret sharing [6], and holography [11]. It is therefore of considerable interest to find structure among such highly entangled multipartite states; in particular, can some AME states have more nonlocal resources than others?

Given N particles with d levels each (the local dimension is d), there is no guarantee that an AME state, denoted $\text{AME}(N, d)$, exists. For example, $\text{AME}(4, 2)$ does not exist; four qubits cannot be absolutely maximally entangled [12]. It is known that $\text{AME}(N, 2)$ exists only for $N = 2, 3, 5$, and 6 [7,13,14]. A table of known $\text{AME}(N, d)$

constructions is maintained [15], and a recent update is presumably $\text{AME}(4, 6)$ [16]. This state long defied construction and provided a quantum solution to the classically impossible problem of “36 officers of Euler.” This state was dubbed the “golden AME” state due to the unexpected appearance of the golden ratio in it. Recent works have appeared elucidating the nature of the solution and its geometric implications [17,18].

Given that any type of entanglement cannot on average increase under local operations and classical communication (LOCC), two states $|\psi_1\rangle$ and $|\psi_2\rangle$ are said to be LOCC equivalent if they can be converted into each other under such operations [19,20]. A finer, but easily defined, equivalence is local unitary (LU) equivalence:

$$|\psi_1\rangle \stackrel{\text{LU}}{\sim} |\psi_2\rangle \quad (1)$$

if and only if there exists local unitary operators u_i , such that $|\psi_2\rangle = (u_1 \otimes \cdots \otimes u_N)|\psi_1\rangle$. A coarser classification is provided by stochastic LOCC (SLOCC), wherein conversion occurs with a nonzero probability of success [21,22]. Mathematically, this replaces the unitary u_i in the LU equivalence by invertible matrices. For pure AME states such as the ones this work addresses, SLOCC (and hence also LOCC) equivalence is identical to LU equivalence [23].

However, LU equivalence among AME states is a long-standing problem that is notoriously hard to resolve [23–25] as all the subsystem states are maximally mixed. There have been several examples of $\text{AME}(4, 3)$ in the literature, from those based on graph states and combinatorial structures [8,9,26–28] to numerically generated ensembles [29,30].

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Despite this, we prove the surprising conjecture [31] that there is exactly *one* LU-equivalence class of AME(4, 3) states. We show that they are all equivalent to each other and hence equivalent to one with minimal support or rank such as

$$|\Psi_{P_9}\rangle = (|1111\rangle + |1222\rangle + |1333\rangle + |2123\rangle + |2231\rangle + |2312\rangle + |3132\rangle + |3213\rangle + |3321\rangle)/3. \quad (2)$$

The minimal support or rank here refers to the minimum natural number r such that the corresponding state can be represented as a superposition of r orthonormal product states [32]. For an AME(N, d) state with $N, d \geq 2$, the minimal support is found to be $d^{\lfloor N/2 \rfloor}$ [33].

We provide a set of invariants such that when they coincide for two states their LU equivalence is implied. For $d > 3$, but $d \neq 6$, orthogonal Latin squares (OLSs) can be used to construct AME(4, d) states [8,9]. We show that a continuous parametrization based on multiplication of suitable components by phases gives invariants that can take an uncountable infinity of values and hence lead to an infinity of LU-equivalence classes. For the special case of $d = 6$, there are no OLS constructions [34], but we use the recently constructed ‘‘golden state’’ [16] as a basis for a similar construction which leads to an infinity of LU-equivalence classes in this case as well. The methods developed can be generalized to a larger number of particles and provide a different outlook into highly entangled multipartite states.

A unitary matrix U of order d^2 can be used to define a four-party state

$$|\Psi_U\rangle = \frac{1}{d} \sum_{i\alpha j\beta} U_{j\beta}^{i\alpha} |i\alpha j\beta\rangle, \quad (3)$$

where $U_{j\beta}^{i\alpha} := \langle i\alpha | U | j\beta \rangle$. The state $|\Psi_U\rangle$ is a vectorization of the matrix U [35,36]. If the unitary U is 2-unitary (defined in the next section), then the corresponding state is an AME(4, d). A unitary operator U is LU equivalent to U' if there exist single-qudit gates u_i and v_i such that

$$U' = (u_1 \otimes u_2)U(v_1 \otimes v_2). \quad (4)$$

The corresponding four-party states are also LU equivalent as $|\Psi_{U'}\rangle = (u_1 \otimes u_2 \otimes v_1^T \otimes v_2^T) |\Psi_U\rangle$, where T is the usual transpose. Therefore the equivalence among AME(4, d) states can be studied via equivalence of 2-unitary operators. In this paper, we construct and use LU invariants that are based on unitary operators rather than directly the coefficients of states. Based on four permutations of n copies, these are easily computed and are in principle complete, in the sense that if all of them are equal, then the operators or corresponding states are LU equivalent [37].

The fact that there is only one LU class of AME(4, 3) states implies that there is only *one* 2-unitary matrix of order 9 denoted P_9 , up to multiplication by local unitaries on either side, and no genuinely orthogonal quantum Latin square [10,38] in $d = 3$. It should also be noted that while generic states of four parties (even for qubits) have an infinity of LU-equivalence classes, the case of AME states forms an exceptional set.

II. PRELIMINARIES AND DEFINITIONS

In this section, we recall necessary background on classical and quantum orthogonal Latin squares, and 2-unitary operators.

A. Orthogonal Latin squares

A Latin square (LS) of order d is a $d \times d$ array filled by numbers $[d] = \{1, 2, \dots, d\}$, each appearing exactly once in each row and column. Two Latin squares K and L of order d , with entries K_{ij} and L_{ij} in the i th row and j th column, are called orthogonal Latin squares if the d^2 pairs (K_{ij}, L_{ij}) , $i, j \in [d]$, occur exactly once.

As mentioned earlier, a pair of orthogonal Latin squares of order d can be used to construct an AME(4, d) state. If the orthogonal Latin squares are K and L with order d , the corresponding AME(4, d) state can be constructed as follows:

$$|\psi_{(K,L)}\rangle = \frac{1}{d} \sum_{i,j} |ij\rangle |K_{ij}L_{ij}\rangle. \quad (5)$$

Such a construction exists for all d , except $d = 2$ and $d = 6$, where there are no OLSs.

The notion of a Latin square can be generalized by replacing discrete symbols with vectors or pure quantum states [39]. A quantum Latin square of size d is a $d \times d$ arrangement of d -dimensional vectors such that each row and column forms an orthonormal basis. The mapping of discrete symbols in a classical Latin square to computational basis vectors ($\{i \mapsto |i\rangle, j \mapsto |j\rangle : \langle i|j\rangle = \delta_{ij}, i, j = 1, 2, \dots, d\}$) results in a quantum Latin square of size d . For $d = 2$ and 3 all quantum Latin squares are equivalent to classical ones for some appropriate choice of bases [40]. However, for $d \geq 4$ there exist quantum Latin squares that are not equivalent to classical Latin squares [40].

Analogous to orthogonality of classical Latin squares there is a notion of orthogonality of quantum Latin squares [10,38]. Two quantum Latin squares \mathcal{Q}_1 and \mathcal{Q}_2 are said to be orthogonal if together they form an orthonormal basis in \mathcal{H}_{d^2} . To be precise, if $|\psi_{ij}\rangle$ and $|\phi_{ij}\rangle$ denote single-qudit states in the i th row and j th column of orthogonal quantum Latin squares \mathcal{Q}_1 and \mathcal{Q}_2 , then the set $\{|\psi_{ij}\rangle \otimes |\phi_{ij}\rangle; i, j = 1, 2, \dots, d\}$ is an orthonormal basis. Thus orthogonal quantum Latin squares provide a special product basis in $\mathcal{H}_d \otimes \mathcal{H}_d$ in which both single-qudit bases form a quantum Latin square.

A more general notion of orthogonal quantum Latin squares allows for an entangled basis in $\mathcal{H}_d \otimes \mathcal{H}_d$. In this case a $d \times d$ array of bipartite pure states $|\Psi_{ij}\rangle \in \mathcal{H}_d^A \otimes \mathcal{H}_d^B$ form an orthogonal quantum Latin square, if they satisfy the following conditions [16,30]:

$$\begin{aligned} \langle \Psi_{ij} | \Psi_{kl} \rangle &= \delta_{ij} \delta_{kl}, \\ \text{Tr}_A \left(\sum_{k=1}^d |\Psi_{ik}\rangle \langle \Psi_{jk}| \right) &= \delta_{ij} \mathbb{1}_d = \text{Tr}_B \left(\sum_{k=1}^d |\Psi_{ik}\rangle \langle \Psi_{jk}| \right), \\ \text{Tr}_B \left(\sum_{k=1}^d |\Psi_{ki}\rangle \langle \Psi_{kj}| \right) &= \delta_{ij} \mathbb{1}_d = \text{Tr}_A \left(\sum_{k=1}^d |\Psi_{ki}\rangle \langle \Psi_{kj}| \right). \end{aligned}$$

Here, Tr_A and Tr_B denote the partial trace operations onto subsystems B and A , respectively. It is easily seen that in the

case of an unentangled basis these conditions are equivalent to the first definition.

The above definitions are equivalent to the bipartite unitary operator $U = \sum_{i,j=1}^d |i\rangle |j\rangle \langle \Psi_{ij}|$ remaining unitary under particular matrix rearrangements as explained below. Such unitary operators are called 2-unitary [9] and form the main focus of this work.

B. 2-unitary operators

A unitary operator U on $\mathbb{C}^d \otimes \mathbb{C}^d \in \mathcal{U}(d^2)$ can be expanded in a product basis as

$$U = \sum_{\alpha, \beta} \langle \alpha | U | \beta \rangle | \alpha \rangle \langle \beta |. \tag{6}$$

We recall the following matrix rearrangement operations familiar from state separability criteria [41,42].

(i) Realignment, R , is as follows:

$$\langle ij | U^R | \alpha \beta \rangle = \langle \alpha | U | j \beta \rangle. \tag{7}$$

(ii) Partial (or blockwise) transpose, Γ , is as follows:

$$\langle i \beta | U^\Gamma | j \alpha \rangle = \langle \alpha | U | j \beta \rangle. \tag{8}$$

Here, U^R and U^Γ denote the matrices obtained after realignment and partial transpose operations, respectively. These operations allow us to define the following classes of unitary operators.

Definition 1: Dual unitary. A matrix U is dual unitary if U and U^R are unitary.

Definition 2: T-dual unitary. A matrix U is called T-dual unitary if U and U^Γ are unitary.

Definition 3: 2-unitary. A matrix U is 2-unitary if it is dual unitary and T-dual unitary.

Quantum circuit models constructed from dual unitaries have been widely studied recently as models of nonintegrable many-body quantum systems [43–45], and the circuits constructed from 2-unitaries have been shown to possess extreme ergodic properties [28]. A generalization of 2-unitary matrices to multiunitary matrices allows the construction of AME states with a higher number of parties [9].

The 2-unitary matrix corresponding to the state in Eq. (5) constructed from OLSs gives a 2-unitary permutation defined as follows:

$$P = \sum_{i,j} |ij\rangle \langle K_{ij} L_{ij}|. \tag{9}$$

2-unitary permutations can be constructed from OLSs in all local dimensions $d > 2$, except $d = 6$. It is also noted that if we multiply a 2-unitary permutation with a diagonal unitary matrix, it remains 2-unitary. In fact, permutations that are dual or T-dual unitary remain dual or T-dual unitary under the multiplication of all nonvanishing (unit) elements by phases: We refer to this as *enphasing*. Thus all 2-unitary permutations remain 2-unitary under enphasing.

III. LU EQUIVALENCE OF AME(4, 3) STATES

The smallest local dimension in which four-party AME states exist is $d = 3$. It has been shown that AME states of

minimal support or rank 9 are all LU equivalent [23]. We now show the following.

Theorem 1. There is only one LU-equivalent class of AME(4, 3) states or, equivalently, one LU-equivalent class of 2-unitary gates of size 9.

Proof. A universal entangler on $\mathbb{C}^d \otimes \mathbb{C}^d$ entangles every product state, and it is known that they do not exist in $d = 2$ and $d = 3$ [46]. The fact that there are no two-qutrit universal entanglers implies that for any two-qutrit gate $U \in \mathcal{U}(9)$ there exists a product state in $\mathbb{C}^3 \otimes \mathbb{C}^3$ such that

$$U(|\alpha_1\rangle \otimes |\beta_1\rangle) = |\alpha_2\rangle \otimes |\beta_2\rangle. \tag{10}$$

Writing $|\alpha_1\rangle \otimes |\beta_1\rangle = (v_1 \otimes v_2) |11\rangle$ and $|\alpha_2\rangle \otimes |\beta_2\rangle = (u_1^\dagger \otimes u_2^\dagger) |11\rangle$, where u_i and v_i are single-qutrit unitary gates, it is easy to see that

$$U_1 = (u_1 \otimes u_2) U (v_1 \otimes v_2) \tag{11}$$

such that

$$U_1(|1\rangle \otimes |1\rangle) = |1\rangle \otimes |1\rangle. \tag{12}$$

Denoting nonzero entries of U_1 by $*$, the matrix form of U_1 becomes

$$U_1 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & * & * & * & * & * & * & * & * \\ 0 & * & * & * & * & * & * & * & * \\ \hline 0 & * & * & * & * & * & * & * & * \\ 0 & * & * & * & * & * & * & * & * \\ 0 & * & * & * & * & * & * & * & * \\ \hline 0 & * & * & * & * & * & * & * & * \\ 0 & * & * & * & * & * & * & * & * \\ 0 & * & * & * & * & * & * & * & * \end{pmatrix}. \tag{13}$$

If U is a 2-unitary operator, the LU transformation in Eq. (11) will lead to U_1 given in the matrix form in Eq. (16). The steps given below explain the reduction in the number of nonzero entries upon imposing dual unitary and T-dual unitary constraints.

(1) If U_1^R is unitary, then the nine 3×3 blocks in U_1 are orthonormal to each other. This implies that all nonzero entries in the first block containing 1 vanish and in all the remaining blocks the element in the first row and the first column vanishes. Therefore the dual-unitary constraint implies that U_1 is of the form

$$U_1 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & * & * & * & * & * & * \\ 0 & 0 & 0 & * & * & * & * & * & * \\ \hline 0 & * & * & 0 & * & * & 0 & * & * \\ 0 & * & * & * & * & * & * & * & * \\ 0 & * & * & * & * & * & * & * & * \\ \hline 0 & * & * & 0 & * & * & 0 & * & * \\ 0 & * & * & * & * & * & * & * & * \\ 0 & * & * & * & * & * & * & * & * \end{pmatrix}. \tag{14}$$

This provides the most general form of the nonlocal part of two-qutrit dual-unitary gates.

(2) If U_1^Γ is unitary, U_1 takes the form

$$U_1 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & * & * & 0 & * & * \\ 0 & 0 & 0 & 0 & * & * & 0 & * & * \\ \hline 0 & 0 & 0 & 0 & * & * & 0 & * & * \\ 0 & * & * & * & * & * & * & * & * \\ 0 & * & * & * & * & * & * & * & * \\ \hline 0 & 0 & 0 & 0 & * & * & 0 & * & * \\ 0 & * & * & * & * & * & * & * & * \\ 0 & * & * & * & * & * & * & * & * \end{pmatrix}. \quad (15)$$

Note that the four columns 2, 3, 4, and 7 have only four potentially nonvanishing elements. Thus these form a four-dimensional orthonormal basis themselves and imply that the elements in the corresponding rows of columns 5, 6, 8, and 9 vanish. Therefore Eq. (15) further simplifies to

$$U_1 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & * & * & 0 & * & * \\ 0 & 0 & 0 & 0 & * & * & 0 & * & * \\ \hline 0 & 0 & 0 & 0 & * & * & 0 & * & * \\ 0 & * & * & * & 0 & 0 & * & 0 & 0 \\ 0 & * & * & * & 0 & 0 & * & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & * & * & 0 & * & * \\ 0 & * & * & * & 0 & 0 & * & 0 & 0 \\ 0 & * & * & * & 0 & 0 & * & 0 & 0 \end{pmatrix}. \quad (16)$$

The LU transformation in Eq. (11) reduces the maximum number of nonzero entries of the 2-unitary from 81 to 33.

From U_1 , we perform a series of local unitary transformations, involving only 2×2 unitaries such that $U_1 \stackrel{\text{LU}}{\sim} P_9$, reducing the total number of nonzero entries to only 9. Here P_9 is the 2-unitary permutation that takes (11,12,13,21,22,23,31,32,33) to (11,23,32,33,12,21,22,31,13) and results in the AME(4, 3) state $|\Psi_{P_9}\rangle$ in Eq. (2). The details of the LU transformations can be found in the Appendix.

Thus every 2-unitary matrix U in $\mathbb{C}^3 \otimes \mathbb{C}^3$ can be expressed in the form $U = (u_1^\dagger \otimes u_2^\dagger) P_9 (v_1^\dagger \otimes v_2^\dagger)$. The four 3×3 unitaries, $u_{1,2}$ and $v_{1,2}$ define a 33-dimensional manifold of 2-unitaries. Hence it is proven that there is only one LU class of 2-unitary gates of size 9 or, equivalently, there is only one AME(4, 3) state up to multiplication by local unitaries. ■

Corollary 1. For any 2-unitary two-qutrit gate $U \in \mathcal{U}(9)$, there exist orthonormal product bases $\{|\alpha_i \beta_j\rangle : i, j = 1, 2, 3\}$ and $\{|\alpha'_i \beta'_j\rangle : i, j = 1, 2, 3\}$ in $\mathbb{C}^3 \otimes \mathbb{C}^3$ such that

$$U |\alpha_i \beta_j\rangle = |\alpha'_i \beta'_j\rangle, \quad i, j = 1, 2, 3. \quad (17)$$

To see this, let the action of the 2-unitary permutation P_9 on the computational basis be given by $P_9 |ij\rangle = |k_{ij} l_{ij}\rangle$, where $i, j, k_{ij}, l_{ij} \in \{1, 2, 3\}$. The set of product states $\{|k_{ij} l_{ij}\rangle : i, j = 1, 2, 3\}$ also form a product basis in $\mathbb{C}^3 \otimes \mathbb{C}^3$. Any 2-unitary two-qutrit gate can be expressed as $U = (u_1^\dagger \otimes u_2^\dagger) P_9 (v_1^\dagger \otimes v_2^\dagger)$, where $u_{1,2}$ and $v_{1,2}$ are 3×3 unitaries. This allows us to define the product states $|\alpha_i \beta_j\rangle = (v_1 \otimes v_2) |ij\rangle$ and $|\alpha'_i \beta'_j\rangle = (u_1^\dagger \otimes u_2^\dagger) |k_{ij} l_{ij}\rangle$, which satisfy the condition in Eq. (17). If these local unitary operators $u_{1,2}$ and $v_{1,2}$ are used in the LU transformation in Eq. (11), the reduction to P_9 occurs in one step.

Illustration of the proof of Theorem 1

We illustrate the proof of Theorem 1 for generic two-qutrit ($d^2 = 9$) 2-unitary matrices. Such generic 2-unitary operators have all $d^4 = 3^4$ elements nonzero and can be obtained from the algorithms presented in Ref. [29]. The absolute values of the entries of one such realization of a generic 2-unitary of size 9, denoted simply as U below, are shown in Fig. 1(a). We use an algorithm similar to the one described in Ref. [47] that, given a bipartite unitary U , finds a pair of maximally entangled states $|\Phi_1\rangle$ and $|\Phi_2\rangle$ such that $U |\Phi_1\rangle = |\Phi_2\rangle$. We use the modified algorithm to find a product state that remains a product state under the action of U . The existence of such a product state is guaranteed due to the nonexistence of a two-qutrit universal entangler gate [46].

Using the product state obtained from the algorithm for the 2-unitary U , we illustrate the proof of Theorem 1 step by step for U showing that it is LU equivalent to the P_9 (2-unitary permutation) as follows.

Let $|\Psi_X\rangle$ and $|\Psi_Y\rangle$ be the product states found using the modified algorithm such that $U |\Psi_X\rangle = |\Psi_Y\rangle$. Define matrices X and Y with elements $X_{ij} = \langle ij | \Psi_X \rangle$ and $Y_{ij} = \langle ij | \Psi_Y \rangle$, respectively, where $i, j = 1, 2, \dots, d$. Let the singular value decompositions of the matrices X and Y be given by

$$X = a_1 D_1 b_1, \quad Y = a_2 D_2 b_2, \quad (18)$$

where a_1, a_2, b_1 , and b_2 are $d \times d$ unitary matrices and D_1 and D_2 are diagonal matrices with only one nonzero entry that is equal to 1. Rewriting the above equations in the vector form gives $|\Psi_X\rangle = (a_1 \otimes b_1^T) |11\rangle$ and $|\Psi_Y\rangle = (a_2 \otimes b_2^T) |11\rangle$. The unitary matrices obtained from these relations can be used to implement the LU transformation given in Eq. (11) by setting $u_1 = a_1, u_2 = b_1^T, v_1 = a_2^\dagger$, and $v_2 = b_2^*$. The transformation results in a 2-unitary matrix whose nonzero entries are shown in Fig. 1(b). Note that the number of nonzero entries is reduced from 81 to 33. The nonexistence of a two-qutrit universal entangler together with 2-unitarity conditions implies that any 2-unitary of size 9 is of the form shown in Fig. 1(b). The matrices U_1^R and U_1^Γ also have exactly the same structure for the nonzero entries.

We apply a sequence of local unitary transformations defined in Eqs. (A7)–(A11) to further simplify the 2-unitary matrix. The result of these local transformations is shown in Figs. 1(c)–1(e).

IV. COMPUTABLE AND COMPLETE SET OF LU INVARIANTS

In this section, we provide a complete set of LU invariants that, in principle, allow us to determine if two given operators are LU equivalent. A family of LU invariants for a general matrix $A \in \mathbb{C}^d \otimes \mathbb{C}^d$ may be constructed as follows. Take any natural number n and permutations $\sigma, \tau, \rho, \lambda \in S_n$: the symmetric group on $\{1, \dots, n\}$. From these data, compute the following number:

$$A(\sigma, \tau, \rho, \lambda) = A_{k_1 l_1}^{i_1 j_1} \cdots A_{k_n l_n}^{i_n j_n} (A^\dagger)_{i_{\sigma(1)} j_{\tau(1)}}^{k_{\rho(1)} l_{\lambda(1)}} \cdots (A^\dagger)_{i_{\sigma(n)} j_{\tau(n)}}^{k_{\rho(n)} l_{\lambda(n)}}, \quad (19)$$

where the sum over repeated indices is assumed. It is straightforward to check that this is an invariant of LU equivalence.

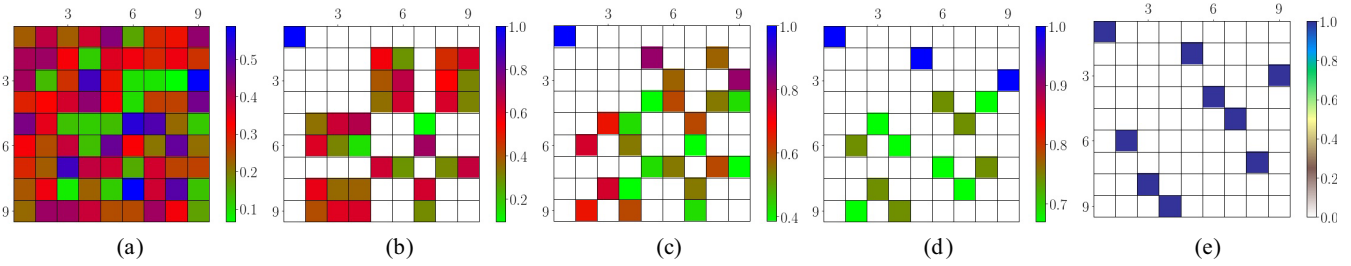


FIG. 1. (a) The absolute values of the entries of a generic 2-unitary of size 9 obtained from the M_{TR} algorithm presented in Ref. [29] are shown. All $d^4 = 81$ entries are nonzero, and the rows and columns are entangled. The numbers 1–9 on the left indicate the row number, and similarly, the numbers on the top indicate the column number. (b) The absolute values of entries of the LU-equivalent 2-unitary matrix to U , $U_1 = (u_1 \otimes u_2)U(v_1 \otimes v_2)$. The only nonzero entry in the first 3×3 block is equal to 1, and the number of nonzero entries in the 2-unitary matrix is $81 - 48 = 33$. (c) and (d) The absolute values of entries of the 2-unitary matrix are shown after performing local transformation defined in Eqs. (A7) and (A9), respectively. (e) The local transformation defined in Eq. (A12) results in 2-unitary emphasized permutation in which there is only one nonzero entry (of modulus 1) in any row and column.

The content of Propositions 8 and 20 of Ref. [37] is that the collection of all these numbers is a complete LU invariant. In other words, A and B , not necessarily unitary, are LU equivalent, if and only if $A(\sigma, \tau, \rho, \lambda) = B(\sigma, \tau, \rho, \lambda)$ for every n and choice of $\sigma, \tau, \rho, \lambda \in S_n$. In this paper, this is used to show that matrices A and B are not LU equivalent by displaying $\sigma, \tau, \rho, \lambda \in S_n$ for some n such that $A(\sigma, \tau, \rho, \lambda) \neq B(\sigma, \tau, \rho, \lambda)$.

In general, for the LU-invariant $A(\sigma, \tau, \rho, \lambda)$ to be non-trivial and not obtainable from a smaller value of n , the four permutations of length n must form a $4 \times n$ Latin rectangle; i.e., there are n different symbols in all four rows and four different symbols in all n columns. For $n < 4$, there are repetitions of symbols, and the resulting invariant reduces to a function of either trivial invariant $\text{Tr}AA^\dagger$ or known invariants based on matrix rearrangements such as realignment and partial transpose.

Our main interest is to distinguish 2-unitary operators that are not LU equivalent. The problem of LU equivalence for 2-unitaries is especially hard because all known LU invariants based on matrix rearrangements such as realignment and partial transpose are constants [48,49]. For distinguishing 2-unitaries that are not LU equivalent, we need to choose the four permutations in Eq. (19) in such a way that the resulting invariant does not reduce to a function of known invariants involving realignment and partial transpose matrix rearrangements. A possible choice of such permutations for $n = 4$ is

$$\begin{aligned} \sigma &= (1\ 2\ 3\ 4), & \tau &= (2\ 1\ 4\ 3), \\ \rho &= (3\ 4\ 1\ 2), & \lambda &= (4\ 3\ 2\ 1). \end{aligned} \tag{20}$$

Note that the above four permutations arranged in a 4×4 arrangement form a Latin square of size 4. The resulting LU invariant is equal to

$$A_{k_1 l_1}^{i_1 j_1} A_{k_2 l_2}^{i_2 j_2} A_{k_3 l_3}^{i_3 j_3} A_{k_4 l_4}^{i_4 j_4} (A^\dagger)_{i_1 j_2}^{k_3 l_4} (A^\dagger)_{i_2 j_1}^{k_4 l_3} (A^\dagger)_{i_3 j_4}^{k_1 l_2} (A^\dagger)_{i_4 j_3}^{k_2 l_1} \tag{21}$$

and is useful in distinguishing 2-unitaries that are not LU equivalent as discussed below.

V. LU-EQUIVALENCE CLASSES OF AME(4, d) STATES IN $d \geq 4$

In this section, using the LU invariants introduced above, we study the LU equivalence classes of AME states in $d \geq 4$.

Theorem 2. The number of LU-equivalence classes of 2-unitary gates of size d^2 (equivalently, the number of LU-equivalence classes of AME states of four qudits) for $d \geq 4$ is infinite.

Proof. Consider first the case of $d \geq 4$ and $d \neq 6$. We observed that 2-unitary permutations remain 2-unitary under emphasizing—multiplication of all nonvanishing (unit) elements by phases. However, such 2-unitaries are not necessarily LU equivalent.

What we actually see is that given one permutation gate, there are infinitely many LU-equivalence classes of emphasized permutation gates of the same size, the method of proof necessitating the restriction $d \neq 6$ —since permutation 2-unitary gates (which are in bijection with orthogonal Latin squares) are known to exist for all $d \geq 4$ except for $d = 6$.

Fix a permutation P of size d^2 . For every $i, j \in [d] = \{1, 2, \dots, d\}$, there exist unique $k, l \in [d]$ such that $P_{kl}^{ij} = 1$. Let $S \subseteq [d]^4$ be the set of all (i, j, k, l) as i, j vary over $[d]$ and k, l are the unique elements with $P_{kl}^{ij} = 1$. For $t = 1, 2, 3, 4$, let $\pi_t : S \rightarrow [d]$ be the t th component function, so that, for instance, $\pi_3((i, j, k, l)) = k$. Note that $|S| = d^2$ and that for each $k \in [d]$, there are exactly d elements $s \in S$ with $\pi_3(s) = k$, and similarly for each $l \in [d]$, there are exactly d elements $s \in S$ with $\pi_4(s) = l$.

We will be interested in multisubsets of S , consisting of sets that have elements of S that could be repeated. Such multisubsets construct the invariant in Eq. (19) and define functions $X(s)$ from S to $\{0, 1, 2, 3, \dots\}$ counting the number of times s occurs in X . Any such multisubset X also determines four functions from $[d]$ to $\{0, 1, 2, 3, \dots\}$. These are I_X, J_X, K_X , and L_X , where

$$I_X(p) = \sum_{s \in S, \pi_1(s)=p} X(s),$$

with analogous definitions for J_X, K_X , and L_X . These count how many times p occurs as a first, second, third, or fourth component of elements of X .

We claim that there are two distinct multisubsets X and Y of S for which all these functions are identical. To see this, note that a multisubset X of S corresponds naturally to a function $F : [d] \times [d] \rightarrow \{0, 1, 2, 3, \dots\}$. For a given such function, we could define $X : S \rightarrow \{0, 1, 2, 3, \dots\}$ by $X((i, j, k, l)) = F(i, j)$ and conversely, given X , we may define $F(i, j) = X((i, j, k, l))$, where k, l are the unique elements with $P_{kl}^{ij} = 1$.

Say that X corresponds to F and Y corresponds to G . The condition that $I_X = I_Y$ is given by $\sum_j F(i, j) = \sum_j G(i, j)$, for each $i \in [d]$. Similarly, the condition that $J_X = J_Y$ is given by $\sum_i F(i, j) = \sum_i G(i, j)$, for each $j \in [d]$. The condition that $K_X = K_Y$ is not as easily expressed since it depends on the permutation P , but it is clear that it is given by a sum of d $F(i, j)$'s on the left-hand side and the corresponding $G(i, j)$'s on the right-hand side where the (i, j) vary over those for which the corresponding k 's are equal, for each $k \in [d]$. A similar statement holds for when $L_X = L_Y$.

To summarize, two multisubsets X and Y corresponding to functions F and G have the same I, J, K , and L functions exactly (the K and L functions should not be confused with the Latin square symbols) when $4d$ homogeneous linear equations in $F(i, j) - G(i, j)$ are satisfied. However, these equations are not independent because the sum of all the $F(i, j)$ coincides with the sum of all $G(i, j)$ once $I_X = I_Y$, and so we need to consider only $d - 1$ equations for each of the J, K , and L functions. The actual number of equations is thus at most $4d - 3$. The number of variables is d^2 , namely, $F(i, j) - G(i, j)$. For $d \geq 4$, $d^2 > 4d - 3$; that is, the number of variables is greater than the number of equations. Since it is a system of homogeneous equations with more variables than equations, these equations have a nontrivial solution. The coefficients in the system of equations are rational, and hence a rational solution exists. Furthermore, by clearing all the denominators by multiplying by some number, we may assume that this solution is integral and then choose each $F(i, j)$ and $G(i, j)$ to be non-negative. The homogeneity of the equations ensures that this remains a solution.

Finally, we have two distinct multisubsets X and Y of S such that for any p , the number of elements of X with first component p equals the number of elements of Y with first component p , and similarly for the other three components too. Say that these multisubsets have N elements each. This condition implies that there exist permutations $\sigma, \tau, \rho, \lambda \in S_N$ such that if X is enumerated (arbitrarily) as $\{(i_1, j_1, k_1, l_1), \dots, (i_N, j_N, k_N, l_N)\}$, then $Y = \{(i_{\sigma(1)}, j_{\tau(1)}, k_{\rho(1)}, l_{\lambda(1)}), \dots, (i_{\sigma(N)}, j_{\tau(N)}, k_{\rho(N)}, l_{\lambda(N)})\}$. Note that $N = \sum_{i,j} F(i, j) = \sum_{i,j} G(i, j)$.

Since X and Y are distinct, there is an $s = (i, j, k, l) \in S$ for which $X(s) \neq Y(s)$. Let Q be the 2-unitary obtained from a 2-unitary permutation P by setting $Q_{kl}^{ij} = \alpha \in S^1$ with other entries untouched. The invariant $Q(\sigma, \tau, \rho, \lambda)$, by definition, is a sum of terms, each of which is a monomial in $\alpha, \bar{\alpha}$. It suffices to see that one of these terms is a nonzero power of α for this polynomial to take infinitely many values as α ranges over S^1 . However, this is true because the term corresponding to $\{(i_1, j_1, k_1, l_1), \dots, (i_N, j_N, k_N, l_N)\}$ is $\alpha^{X(s)} \bar{\alpha}^{Y(s)}$, which is a nonzero power of α . ■

To illustrate that enphasing of 2-unitary permutations leads to different LU-equivalence classes in $d = 4$, consider the permutation denoted P_{16} , and $(P_{16})_{kl}^{ij}$ elements are such that (kl) are ordered as $(11, 44, 22, 33, 43, 12, 34, 21, 24, 31, 13, 42, 32, 23, 41, 14)$ when (ij) is in the lexicographic ordering $(11, 12, \dots, 44)$. Let $P_{16}(\theta)$ denote the 2-unitary obtained from P_{16} by changing only $(P_{16})_{11}^{11}$ from 1 to $e^{i\theta}$.

The invariant given in Eq. (21) for $P_{16}(\theta)$ evaluates to the following simple continuous function of θ :

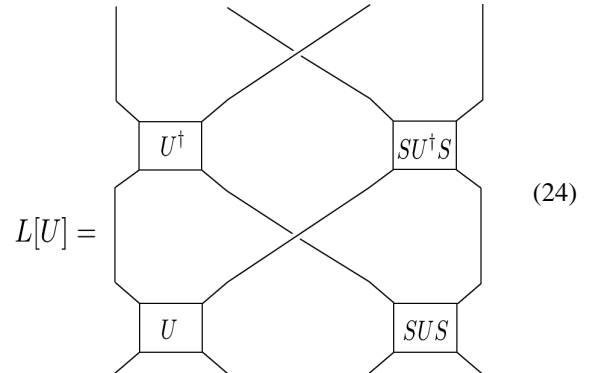
$$P_{16}(\theta; \sigma, \tau, \rho, \lambda) = 8(29 + 3 \cos \theta). \quad (22)$$

As θ ranges in $(-\pi, \pi]$, the invariant takes infinitely many distinct values, and so the corresponding 2-unitaries are not LU equivalent.

While an interpretation of this invariant is not clear, it can be related to a moment of an operator on two copies, or four parties A, B, C , and D with U acting on the pairs (A, B) and (C, D) :

$$L[U] := (S_{BD} \otimes \mathbb{1}_{AC})(U^\dagger \otimes U^\dagger)(S_{BD} \otimes \mathbb{1}_{AC})(U \otimes U), \quad (23)$$

where S_{BD} is the SWAP gate between subsystems B and D . Representing the bipartite operator with a tensor having two incoming and two outgoing indices, diagrammatic representation of $L[U]$ in terms of bipartite unitary operators U and SUS (where S is the SWAP gate) is given by



It can be easily checked that $L[U] = L[SUS]$ and all the moments, $\text{Tr} L^k[U]$; $k = 1, 2, 3, \dots$, are local unitary invariants. For example, $\text{Tr} L[U] = \text{Tr}(U^R U^{R\dagger})^2$ is related to the operator entanglement of U [29,35,36], and the invariant in Eq. (22) is equal to the second moment $\text{Tr} L^2[P_{16}(\theta)]$. Note that $\text{Tr} L[U]$ is equal to d^2 for dual unitaries and thus cannot distinguish dual unitaries in different LU-equivalence classes.

A. Proof based on orthogonal diagonal Latin squares

In this section, we give a constructive proof for Theorem 2 for the case $d \geq 4$ and $d \neq 6$ using special orthogonal Latin squares. We find explicit examples of multisets with desired properties discussed above, and construct the corresponding four permutations σ, τ, ρ , and λ .

Consider a Latin square of order d with elements from the set $[d] = \{1, 2, \dots, d\}$. A transversal of a Latin square is a set

of d distinct entries such that no two entries share the same row or column. A diagonal Latin square is one in which both the main diagonal and the main back (or “anti-”)diagonal are transversals.

Two Latin squares K and L form a pair of orthogonal diagonal Latin squares (ODLSs) if both are diagonal Latin squares and orthogonal. It is known that ODLSs exist for every order d except 2,3 and 6 [50]. An example of a pair of orthogonal diagonal Latin squares in $d = 4$ is given below:

$$\text{ODLS}(4) = \begin{array}{|c|c|c|c|} \hline 1, 2 & 3, 3 & 4, 1 & 2, 4 \\ \hline 4, 4 & 2, 1 & 1, 3 & 3, 2 \\ \hline 2, 3 & 4, 2 & 3, 4 & 1, 1 \\ \hline 3, 1 & 1, 4 & 2, 2 & 4, 3 \\ \hline \end{array}. \quad (25)$$

Given a pair of orthogonal Latin squares K and L , we can construct a 2-unitary operator P as follows:

$$P = \sum_{i,j=1}^d \alpha_{i,j} |i, j\rangle \langle K_{i,j}, L_{i,j}|, \quad (26)$$

where $\alpha_{i,j} \in S^1$. For our purpose, we set $\alpha_{i,j} = 1$, for all i, j except $\alpha_{1,1} = \alpha \neq 1$.

We choose both K and L to be diagonal Latin squares such that they form a pair of orthogonal diagonal Latin squares. Let $S \subseteq [d]^{\times 4}$ be the set of all $(i, j, K_{i,j}, L_{i,j})$, $i, j \in [d]$, such that $P_{K_{i,j}, L_{i,j}}^{i,j}$ is nonzero. It is noted that the multisubsets of S construct the invariant in Eq. (19). Consider the following subsets of S constructed using the addresses and elements of main and back diagonals of K and L :

$$\begin{aligned} X &= \{(i, i, K_{i,i}, L_{i,i}), i \in [d]\}, \\ Y &= \{(i, d + 1 - i, K_{i,d+1-i}, L_{i,d+1-i}), i \in [d]\}. \end{aligned} \quad (27)$$

An element $(i, i, K_{i,i}, L_{i,i}) \in X$ is different from any element $(j, d + 1 - j, K_{j,d+1-j}, L_{j,d+1-j}) \in Y$ except the case when d is odd and $i = j = (d + 1)/2$. Therefore X and Y are distinct. However, for the multisubset X the functions I_X, J_X, K_X , and L_X are identical to the corresponding functions for the multisubset Y , both being constant functions (equal to 1). For the example in Eq. (25), $X = \{(1, 1, 1, 2), (2, 2, 2, 1), (3, 3, 3, 4), (4, 4, 4, 3)\}$ and $Y = \{(1, 4, 2, 4), (2, 3, 1, 3), (3, 2, 4, 2), (4, 1, 3, 1)\}$.

The four permutations σ, τ, ρ , and λ can be found by inspection since all the functions I, J, K , and L evaluate to 1 for the subsets X and Y . Note that the sets $\{K_{i,i}, i \in [d]\}$ and $\{L_{i,d+1-i}, i \in [d]\}$ contain elements in the main diagonal and the back diagonals of K , respectively. Since K is assumed to be a diagonal Latin square, these two sets are related by a permutation. This gives the permutation $\rho \in S_d$. A similar argument can be given in the case of sets $\{L_{i,i}, i \in [d]\}$ and $\{K_{i,d+1-i}, i \in [d]\}$, and the corresponding permutation is $\lambda \in S_d$. It is also evident that the set $[d]$ and $\{d + 1 - i, i \in [d]\}$ are related by a permutation

$$\tau = \begin{pmatrix} 1 & 2 & \dots & d \\ d & d-1 & \dots & 1 \end{pmatrix}. \quad (28)$$

Therefore, if we enumerate elements in X as $\{(i_1, j_1, k_1, l_1), \dots, (i_d, j_d, k_d, l_d)\}$, then $Y = \{(i_1, j_{\tau(1)},$

$k_{\rho(1)}, l_{\lambda(1)}), \dots, (i_d, j_{\tau(d)}, k_{\rho(d)}, l_{\lambda(d)})\}$. The permutation ρ is identity in this case. Note that the element $(1, 1, K_{1,1}, L_{1,1}) \in X$ does not belong to Y . Then, the term corresponding to $\{(i_1, j_1, k_1, l_1), \dots, (i_d, j_d, k_d, l_d)\}$ in the LU-invariant $P(1, \tau, \rho, \lambda)$ evaluates to α . Therefore $P(1, \tau, \rho, \lambda)$ can have infinitely many values as α is a continuous parameter. Hence this shows that there exist an infinite number of LU-equivalence classes of 2-unitary gates for $d \geq 4$ except $d = 6$. In $d = 3$, as proven earlier, there is only one LU-equivalence class of AME(4, 3) states. This is consistent with the fact that there are no ODLSs in $d = 3$ [50].

B. The special case of $d = 6$

Due to the nonexistence of orthogonal Latin squares of size 6 [34], 2-unitary permutations of size 36 do not exist [8], and we need to treat this case separately. However, it was shown recently in Ref. [16] that a 2-unitary matrix of size 36 denoted as \mathcal{U}_{36} , or, equivalently, an AME state of four six-level systems, AME(4, 6), $|\Psi_{\mathcal{U}_{36}}\rangle$ exists. This settled positively a long-standing open problem in quantum information theory [51].

For the sake of completeness, we show the nonzero matrix elements of the 2-unitary \mathcal{U}_{36} corresponding to the golden AME(4, 6) state [16] in Fig. 2. The pair of indices (k, l) shown in rows label the rows, and the (i, j) shown in columns label the columns in \mathcal{U}_{36} . The nonzero elements of \mathcal{U}_{36} involve the 20th root of unity, $\omega = \exp(2\pi i/20)$, and the real numbers [16]

$$a = (5 + \sqrt{5})^{-1/2}, \quad b/a = \varphi, \quad c = 1/\sqrt{2}, \quad (29)$$

where $\varphi = (1 + \sqrt{5})/2$ is the golden ratio. $\bar{\omega}$ is the complex conjugate of ω .

Here, we show that one can obtain an infinite number of 2-unitaries from \mathcal{U}_{36} by multiplying it with appropriate diagonal unitaries. Unlike 2-unitary permutations, \mathcal{U}_{36} does not remain 2-unitary under multiplication by diagonal unitaries with arbitrary phases. In order to preserve 2-unitarity, one needs to multiply particular rows or columns of the given 2-unitary with specially designed phases depending on its structure. The simplest example in the case of \mathcal{U}_{36} is the one-parameter family of 2-unitaries

$$\mathcal{U}_{36}(\theta) = \mathcal{D}(\theta)\mathcal{U}_{36}, \quad (30)$$

where $\mathcal{D}(\theta) = \text{Diag}[e^{i\theta}, 1, 1, e^{i\theta}, 1, 1, e^{i\theta}, 1, 1, e^{i\theta}, 1_{26}]$ and $\theta \in (-\pi, \pi]$. The notation 1_K is to indicate a length- K string of 1s. This yields an infinity of AME(4, 6) states parametrized by θ under the correspondence in Eq. (3). That this enphasing retains the 2-unitary property is not evident, but follows from the observation that $[\mathcal{U}_{36}(\theta)]^R = \mathcal{U}_{36}^R \mathcal{D}'(\theta)$ and $[\mathcal{U}_{36}(\theta)]^\Gamma = \mathcal{D}''(\theta)\mathcal{U}_{36}^\Gamma$, where $\mathcal{D}'(\theta) = \text{Diag}[e^{i\theta}, e^{i\theta}, 1_{16}, e^{i\theta}, e^{i\theta}, 1_{16}]$, and $\mathcal{D}''(\theta) = \text{Diag}[e^{i\theta}, e^{i\theta}, 1, 1, 1, 1, e^{i\theta}, e^{i\theta}, 1_{28}]$.

We show that these 2-unitaries are not LU equivalent by evaluating the invariant $\mathcal{U}_{36}(\theta; \sigma, \tau, \rho, \lambda)$ for permutation of indices given by Eq. (20). The invariant evaluates to the fol-

(1,1)	(2,2)	(1,2)	(2,1)	(6,3)	(1,3)	(2,4)	(1,4)	(2,3)	(2,5)	(1,5)	(2,6)	(1,6)	(2,5)	(4,1)
$-a$	a	$b\bar{\omega}^5$	$b\omega^5$	(1,1)	$a\omega^2$	$-a\omega^4$	$b\omega$	$b\bar{\omega}^5$	(3,3)	$a\omega$	$a\bar{\omega}$	$-b\omega^4$	$b\bar{\omega}^4$	(3,4)
		c	c	(5,6)			$c\omega^5$	$c\bar{\omega}$	(1,2)	$a\omega$	$a\omega^3$	$-b$	$b\omega^4$	(2,6)
c	c			(4,2)	$c\bar{\omega}^3$	$c\bar{\omega}$			(6,4)	$b\omega^4$	$b\bar{\omega}^2$	$a\omega^3$	$-a\bar{\omega}$	(5,5)
$-b$	b	$a\omega^5$	$a\bar{\omega}^5$		$-b\omega^4$	$-b\bar{\omega}^4$	$a\omega^3$	$-a\bar{\omega}^3$		$b\omega^2$	$-b\bar{\omega}^2$	$a\omega^5$	$a\bar{\omega}^5$	
(3,1)	(4,2)	(3,2)	(4,1)	(4,5)	(3,3)	(4,4)	(3,4)	(4,3)	(4,6)	(3,5)	(4,6)	(3,6)	(4,5)	(2,3)
$a\omega^4$	$-a$	$b\bar{\omega}^3$	$b\omega^7$	(3,2)	a	a	$b\bar{\omega}^5$	$b\bar{\omega}^5$	(6,1)	$a\omega^2$	a	$b\bar{\omega}$	$-b\omega^3$	(6,2)
		$c\omega^2$	$c\omega^2$	(2,4)			c	$-c$	(5,4)			$c\bar{\omega}^4$	c	(3,1)
$-c$	$-c\bar{\omega}^4$			(5,3)	c	$-c$			(1,5)	$-c\bar{\omega}^2$	$c\bar{\omega}^4$			(1,6)
$-b\bar{\omega}^3$	$-b\omega^3$	$-a$	a		b	b	$a\omega^5$	$a\omega^5$		$-b\omega^4$	$-b\omega^2$	$a\omega$	$a\bar{\omega}^5$	
(5,1)	(6,2)	(5,2)	(6,1)	(1,4)	(5,3)	(6,4)	(5,4)	(6,3)	(3,6)	(5,5)	(6,6)	(5,6)	(6,5)	(1,3)
$a\omega^3$	$-a\bar{\omega}^3$	b	b	(2,1)	$-a\omega^2$	$-a\omega^4$	$b\bar{\omega}^5$	$b\omega$	(5,1)	$a\bar{\omega}^2$	$a\bar{\omega}^2$	$b\omega^3$	$b\bar{\omega}^3$	(5,2)
		c	$-c$	(3,5)			$-c\omega^4$	$-c$	(2,2)			c	$-c$	(6,5)
$-c\omega^3$	$-c\bar{\omega}^3$			(6,6)	$-c\bar{\omega}^3$	$c\bar{\omega}$			(4,3)	$c\omega$	$-c\omega$			(4,4)
$-b\bar{\omega}$	$-b\omega^3$	$a\bar{\omega}^4$	$a\bar{\omega}^4$		$-b\omega^4$	$b\bar{\omega}^4$	$-a\bar{\omega}^3$	$-a\omega^3$		$-b$	$-b$	$a\omega^5$	$a\omega^5$	

FIG. 2. Nonvanishing matrix elements of the 2-unitary \mathcal{U}_{36} . The pair of indices (i, j) indicated in rows label the relevant row, $j + 6(i - 1)$, and the pair of indices (k, l) indicated in columns determine the relevant column, $l + 6(k - 1)$. $\bar{\omega}$ denotes the complex conjugate of ω .

lowing function of θ :

$$\mathcal{U}_{36}(\theta; \sigma, \tau, \rho, \lambda) = C_0 + 6 \cos \theta, \quad (31)$$

where $C_0 = 3(202 + \sqrt{5} + 2\sqrt{5 - 2\sqrt{5}})/4 \approx 154.267$ is a constant. The θ dependence proves that the invariant can take infinitely many distinct values and the corresponding $\mathcal{U}_{36}(\theta)$ are not LU equivalent. The invariant in Eq. (31) is equal to $\text{tr}L^2[\mathcal{U}_{36}(\theta)] = C_0 + 6 \cos \theta$. The realignment and partial transpose of 2-unitaries provide other 2-unitaries, and for $\mathcal{U}_{36}(\theta)$, one needs to evaluate the third moment $\text{tr}L^3[U]$ to show that these are not LU equivalent.

C. The 25-parameter family of AME(4, 6) states

Apart from the one-parameter family of enphasing discussed above, we give a more general construction consisting of 25 real parameters. Let $\mathcal{U} = \mathcal{U}_{36}$. This has 112 nonzero entries. Consider a matrix, say, \mathcal{V} , obtained from \mathcal{U} by multiplying each of these nonzero entries by a phase factor. For definiteness, suppose that each nonzero \mathcal{U}_{ij} is multiplied by $e^{i\theta_{ij}}$. We now try to understand under what conditions on the θ_{ij} the new matrix \mathcal{V} is also 2-unitary.

First \mathcal{V} must be unitary. Since its rows are still of norm 1, only the orthogonality of the rows needs to be ensured. Take any two rows, say, i_1 and i_2 of \mathcal{V} . Suppose that the columns where both these rows have nonzero entries are j_1, j_2, \dots (at most four, from the structure of \mathcal{U}). For the inner product of these rows to vanish it suffices that $\theta_{i_1 j_1} - \theta_{i_2 j_1} = \theta_{i_1 j_2} - \theta_{i_2 j_2} = \theta_{i_1 j_3} - \theta_{i_2 j_3} = \dots$. This is a set of homogeneous linear equations in the θ_{ij} . Similarly, for \mathcal{V}^R and \mathcal{V}^Γ to be unitary we get other homogeneous linear equations in the θ_{ij} .

Writing out all these homogeneous linear equations for the θ_{ij} , we get a system of 246 equations (75 for \mathcal{V} , 87 for \mathcal{V}^Γ , and 84 for \mathcal{V}^R) in 112 variables. The rank of the coefficient matrix can be computed to be 87 using, say, MATHEMATICA, thereby

yielding a 25-dimensional solution space. This is the required 25-dimensional family of 2-unitary enphasings of \mathcal{U} .

Apart from solving the difficult problem of establishing LU-equivalence classes for AME states of four parties or 2-unitary operators in any local dimension, the methods developed herein can be extended both to unequal local dimensions and to more parties. This requires as many permutations as the number of parties to construct the invariants. That the case of qutrits is special and has only one class needs further elucidation in terms of the geometry of the set of 2-unitaries in this case. We hope that these results pave the way for a deeper understanding of multipartite states and new entanglement measures.

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APPENDIX: LU TRANSFORMATIONS INVOLVED IN THE PROOF OF THEOREM 1

There exist no universal entanglers in $d = 3$. This result allows us to find a unitary operator U_1 that is LU equivalent to a given two-qutrit operator U such that the entry in the first column and first row of U_1 is equal to 1. The corresponding LU transformation, given in Eq. (11), is restated here for completeness:

$$U_1 = (u_1 \otimes u_2)U(v_1 \otimes v_2), \quad (\text{A1})$$

where $u_{1,2}$ and $v_{1,2}$ are single-qutrit unitary gates.

Requiring U to be 2-unitary and imposing 2-unitarity constraints will lead to the following matrix form of U_1 :

$$U_1 = \left(\begin{array}{ccc|ccc|ccc} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & * & * & 0 & * & * \\ 0 & 0 & 0 & 0 & * & * & 0 & * & * \\ \hline 0 & 0 & 0 & 0 & * & * & 0 & * & * \\ 0 & * & * & * & 0 & 0 & * & 0 & 0 \\ 0 & * & * & * & 0 & 0 & * & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & * & * & 0 & * & * \\ 0 & * & * & * & 0 & 0 & * & 0 & 0 \\ 0 & * & * & * & 0 & 0 & * & 0 & 0 \end{array} \right). \quad (A2)$$

From here, we apply appropriate local unitary transformations to simplify further.

In the following step, we label relevant nonzero entries and represent U_1 as

$$U_1 = \left(\begin{array}{ccc|ccc|ccc} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & p_{11} & p_{12} & 0 & q_{11} & q_{12} \\ 0 & 0 & 0 & 0 & p_{21} & p_{22} & 0 & q_{21} & q_{22} \\ \hline 0 & 0 & 0 & 0 & * & * & 0 & * & * \\ 0 & * & * & * & 0 & 0 & * & 0 & 0 \\ 0 & * & * & * & 0 & 0 & * & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & * & * & 0 & * & * \\ 0 & * & * & * & 0 & 0 & * & 0 & 0 \\ 0 & * & * & * & 0 & 0 & * & 0 & 0 \end{array} \right). \quad (A3)$$

Consider the matrices

$$P = \begin{pmatrix} p_{11} & p_{12} \\ p_{21} & p_{22} \end{pmatrix}, \quad Q = \begin{pmatrix} q_{11} & q_{12} \\ q_{21} & q_{22} \end{pmatrix}. \quad (A4)$$

The constraint that U_1 be 2-unitary gives the following conditions:

$$\left. \begin{aligned} PP^\dagger + QQ^\dagger &= \mathbb{1}_2 \quad (\text{Unitarity}), \\ P^\dagger P + Q^\dagger Q &= \mathbb{1}_2 \quad (\text{T-dual unitarity}), \\ \left. \begin{aligned} \text{tr}(P^\dagger P) &= 1 \\ \text{tr}(Q^\dagger Q) &= 1 \\ \text{tr}(P^\dagger Q) &= 0 \end{aligned} \right\} \quad (\text{Dual unitarity}). \end{aligned} \right\} \quad (A5)$$

Consider the singular value decomposition $P = V_1 D_1 W_1^\dagger$, where V_1 and W_1 are unitary matrices and $D_1 = \text{Diag}\{\sigma_1, \sigma_2\}$. The orthonormality condition $\text{tr}(P^\dagger P) = 1$ implies $\sigma_1^2 + \sigma_2^2 = 1$. From the first two relations in Eq. (A5), we get

$$\left. \begin{aligned} QQ^\dagger &= V_1 D_1^2 V_1^\dagger, \\ Q^\dagger Q &= W_1 D_1^2 W_1^\dagger, \end{aligned} \right\} \quad (A6)$$

where $D_1' = \text{Diag}\{\sigma_2, \sigma_1\}$. Therefore Q can be written as $Q = V_1 D_2 W_1^\dagger$ where D_2 is a diagonal matrix denoted by $D_2 = \text{Diag}\{\sigma_1', \sigma_2'\}$ and can in general be complex. Therefore a local unitary transformation on U_1 is given by

$$\begin{aligned} U_2 &= \left(\mathbb{1}_3 \otimes \begin{pmatrix} 1 & 0 \\ 0 & V_1^\dagger \end{pmatrix} \right) U_1 \left(\mathbb{1}_3 \otimes \begin{pmatrix} 1 & 0 \\ 0 & W_1 \end{pmatrix} \right) \\ &= \left(\begin{array}{ccc|ccc|ccc} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \sigma_1 & 0 & 0 & \sigma_1' & 0 \\ 0 & 0 & 0 & 0 & 0 & \sigma_2 & 0 & 0 & \sigma_2' \\ \hline 0 & 0 & 0 & 0 & * & * & 0 & * & * \\ 0 & * & * & * & 0 & 0 & * & 0 & 0 \\ 0 & * & * & * & 0 & 0 & * & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & * & * & 0 & * & * \\ 0 & * & * & * & 0 & 0 & * & 0 & 0 \\ 0 & * & * & * & 0 & 0 & * & 0 & 0 \end{array} \right) \\ &= \left(\begin{array}{ccc|ccc|ccc} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \sigma_1 & 0 & 0 & \sigma_1' & 0 \\ 0 & 0 & 0 & 0 & 0 & \sigma_2 & 0 & 0 & \sigma_2' \\ \hline 0 & 0 & 0 & 0 & * & * & 0 & * & * \\ 0 & 0 & * & * & 0 & 0 & * & 0 & 0 \\ 0 & * & 0 & * & 0 & 0 & * & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & * & * & 0 & * & * \\ 0 & 0 & * & * & 0 & 0 & * & 0 & 0 \\ 0 & * & 0 & * & 0 & 0 & * & 0 & 0 \end{array} \right). \quad (A7) \end{aligned}$$

The final form above has two more elements set to 0 as the 3×3 blocks have to be orthonormal.

It follows from the last two conditions in Eq. (A5) that the matrix given by

$$\sigma = \begin{pmatrix} \sigma_1 & \sigma_1' \\ \sigma_2 & \sigma_2' \end{pmatrix} \quad (A8)$$

is unitary. A local unitary transformation of the form

$$U_3 = U_2 \left(\left(\begin{pmatrix} 1 & 0 \\ 0 & \sigma^\dagger \end{pmatrix} \otimes \mathbb{1}_3 \right) \right) \quad (A9)$$

followed by considering the unitarity of U_3^Γ results in

$$U_3 = \left(\begin{array}{ccc|ccc|ccc} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ \hline 0 & 0 & 0 & 0 & 0 & c_{11} & 0 & c_{12} & 0 \\ 0 & 0 & * & 0 & 0 & 0 & * & 0 & 0 \\ 0 & * & 0 & * & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 0 & c_{21} & 0 & c_{22} & 0 \\ 0 & 0 & * & 0 & 0 & 0 & * & 0 & 0 \\ 0 & * & 0 & * & 0 & 0 & 0 & 0 & 0 \end{array} \right). \quad (A10)$$

At this stage, we notice that *all* the columns of U_3 are unentangled. Therefore we need to apply local transformations on the left to reduce further. Note that the four potentially nonzero entries labeled c_{ij} in U_3 form a 2×2 unitary matrix. Using this unitary matrix

$$C = \begin{pmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{pmatrix}, \quad (\text{A11})$$

we apply the following local unitary transformation:

$$U_4 = \left(\begin{pmatrix} 1 & 0 \\ 0 & C^\dagger \end{pmatrix} \otimes \mathbb{I}_3 \right) U_3. \quad (\text{A12})$$

The constraint of U_4 being 2-unitary gives

$$U_4 = \left(\begin{array}{ccc|ccc|ccc} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ \hline 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \alpha_2 & 0 & 0 \\ 0 & \alpha_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & \alpha_3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \alpha_4 & 0 & 0 & 0 & 0 & 0 \end{array} \right), \quad (\text{A13})$$

where $\alpha_1, \alpha_2, \alpha_3$, and α_4 are of modulus 1.

In the final step, we perform the following local unitary transformation:

$$P_9 = (\Phi_1 \otimes \Phi_2) U_4 (\Phi_3 \otimes \Phi_4) = \left(\begin{array}{ccc|ccc|ccc} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ \hline 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \end{array} \right), \quad (\text{A14})$$

where

$$\begin{aligned} \Phi_1 &= \text{Diag}\{1, (\alpha_1^* \alpha_2^*)^{\frac{1}{3}}, (\alpha_3^* \alpha_4^*)^{\frac{1}{3}}\}, \\ \Phi_2 &= \text{Diag}\{1, (\alpha_2^* \alpha_3^*)^{\frac{1}{3}}, (\alpha_1^* \alpha_4^*)^{\frac{1}{3}}\}, \\ \Phi_3 &= \text{Diag}\{1, (\alpha_1 \alpha_3 \alpha_4^*)^{\frac{1}{3}}, (\alpha_1 \alpha_3 \alpha_2^*)^{\frac{1}{3}}\}, \\ \Phi_4 &= \text{Diag}\{1, (\alpha_2 \alpha_4 \alpha_1^*)^{\frac{1}{3}}, (\alpha_2 \alpha_4 \alpha_3^*)^{\frac{1}{3}}\} \end{aligned} \quad (\text{A15})$$

are diagonal unitaries. Here, we choose the principal value of the cube root $z^{1/3}$ with argument $\arg(z) \in [0, 2\pi)$. Concerning this last step, it has already been shown that any enfusing of P_9 is LU equivalent to it [23].

Therefore we have shown that any 2-unitary two-qutrit operator is LU equivalent to P_9 . Hence there exists only one LU-equivalence class of 2-unitary gates in $d = 3$, or equivalently, there is only one AME(4, 3) state up to LU equivalence.

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