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Low-rank extremal positive-partial-transpose states and unextendible product bases

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It is known how to construct, in a bipartite quantum system, a unique low-rank entangled mixed state with positive partial transpose (a PPT state) from an unextendible product basis (UPB), defined as an unextendible set of orthogonal product vectors. We point out that a state constructed in this way belongs to a continuous family of entangled PPT states of the same rank, all related by nonsingular unitary or nonunitary product transformations. The characteristic property of a state ρ in such a family is that its kernel Ker ρ has a generalized UPB, a basis of product vectors, not necessarily orthogonal, with no product vector in Im ρ, the orthogonal complement of Ker ρ. The generalized UPB in Ker ρ has the special property that it can be transformed to orthogonal form by a product transformation. In the case of a system of dimension 3×3, we give a complete parametrization of orthogonal UPBs. This is then a parametrization of families of rank 4 entangled (and extremal) PPT states, and we present strong numerical evidence that it is a complete classification of such states. We speculate that the lowest rank entangled and extremal PPT states also in higher dimensions are related to generalized, nonorthogonal UPBs in similar ways.

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I. INTRODUCTION

For a composite quantum system, with two separate parts A and B, the mixed quantum states are described by density matrices that can be classified as being either entangled or separable (nonentangled). However, there is in general no easy way to classify a given density matrix as being separable or not. This problem is referred to as the separability problem, and it has been approached in the literature in different ways over the past several years [1]. As a part of this discussion there has been a focus on a subset of the density matrices which includes, but is generally larger than, the set of separable states. This is the set of the so-called positive partial transpose (PPT) states, the density matrices that remain positive under a *partial* matrix transposition, with respect to one of the subsystems, either A or B [2].

Since it is straightforward to establish whether a density matrix is a PPT state, the separability problem is reduced to identifying the subset of *entangled* PPT states. We refer here to the set of separable states as $\mathcal{S}$ and the set of PPT states as $\mathcal{P}$, with $\mathcal{S} \subset \mathcal{P}$. These are both *convex* subsets of the full convex set of density matrices, which we denote as $\mathcal{D}$, and in principle the two sets are therefore defined by their extremal states. The extremal separable states are the pure product states, and these are also extremal states of the set $\mathcal{P}$. Since $\mathcal{P}$ is in general larger than $\mathcal{S}$, it has additional extremal states, and these states are not fully known. The problem of finding and classifying these additional extremal states is therefore an important part of the problem to identify the PPT states that are entangled.

We have in two previous publications studied, in different ways, the problem of finding extremal PPT states in systems of low dimensions. In [3] a criterion for extremality was established and a method was described to numerically search for extremal PPT states. This method was applied to different composite systems, and several types of extremal states were found. In a recent paper [4] this study has been followed up by a systematic search for PPT states of different ranks. Series of extremal PPT states have there been identified and tabulated for different bipartite systems of low dimensions.

The study in [4] seems to show that the extremal PPT states with *lowest rank* are somehow special compared to the other extremal states. In particular we have found that these density matrices have no product vectors in their image but do have a finite, complete set of product vectors in their kernel. This was found to be a common property of the lowest rank extremal PPT states studied there, for all systems with subsystems of dimensions larger than two. This property relates these states to a particular construction, where *unextendible product bases* (UPBs) are used in a method to construct entangled PPT states [5–7].

The motivation for the present paper is to follow up this apparent link between the lowest rank extremal PPT states and the UPB construction. Our focus is particularly on the rank 4 states of the 3×3 system. The rank 4 extremal PPT states that we find numerically by the method introduced in [4] are related by product transformations to states constructed directly from UPBs. We discuss this relation and use it to give a parametrization of the rank 4 extremal PPT states.

Although a direct application of the (generalized) UPB construction to the lowest rank extremal states is restricted to the 3×3 system, the similarity between these states and the lowest rank extremal states in higher dimensions indicates that there may exist a generalization of this construction that is more generally valid. We include at the end a brief discussion of the higher dimensional cases and only suggest that a construction method, and thereby a parametrization, of such states may exist.

II. AN EXTENSION OF THE UPB CONSTRUCTION OF ENTANGLED PPT STATES

We consider in the following a bipartite quantum system with a Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ of dimension $N = N_A N_B$. By definition, a separable state can be written as a density operator of the form

$$\rho = \sum_k p_k \psi_k \psi_k^\dagger, \tag{1}$$

with $p_k \geqslant 0$, $\sum_k p_k = 1$, and with $\psi_k = \phi_k \otimes \chi_k$ as normalized product vectors. The image of ρ, Im ρ, is spanned by these vectors. The fact that Im ρ must be spanned by product vectors if ρ is separable is the basis for the UPB construction, which was introduced in Ref. [5] and used there to find low-rank entangled PPT states of the 3×3 system. We review here this construction and discuss a particular generalization.

Consider $\mathcal{U}$ to be a subspace of $\mathcal{H}$ that is spanned by a set of *orthonormal* product vectors

$$\psi_k = \phi_k \otimes \chi_k, \quad k = 1,2,\ldots,p, \tag{2}$$

which cannot be extended further in $\mathcal{H}$ to a set of $p+1$ orthogonal product vectors. This defines the set as an unextendible product basis. Let $\mathcal{U}^\perp$ be the orthogonal complement to $\mathcal{U}$. The state proportional to the orthogonal projection onto $\mathcal{U}^\perp$,

$$\rho_1 = a_1 \left(\mathbb{1} - \sum_k \psi_k \psi_k^\dagger \right), \tag{3}$$

with $a_1 = 1/(N-p)$ as a normalization factor, is then an entangled PPT state. It is nonseparable because Im $\rho_1 = \mathcal{U}^\perp$ contains no product vector, and it is a PPT state because ρ_1^P, the partial transpose of ρ_1 with respect to subsystem B, is proportional to a projection of the same form,

$$\rho_1^P = a_1 \left(\mathbb{1} - \sum_k \tilde{\psi}_k \tilde{\psi}_k^\dagger \right), \tag{4}$$

with $\tilde{\psi}_k = \phi_k \otimes \chi_k^*$. The vector χ_k^* is the complex conjugate of χ_k, in the same basis in $\mathcal{H}_B$ as is used for the partial transposition.

The set of product vectors $\{\tilde{\psi}_k = \phi_k \otimes \chi_k^*\}$ is a new orthonormal UPB, which generally spans a different subspace than the original set $\{\psi_k = \phi_k \otimes \chi_k\}$. However, it may happen that there exists a basis for the Hilbert space $\mathcal{H}_B$ of the second subsystem in which all the vectors χ_k have real components. In such a basis the two UPB sets are identical and the state ρ_1 is a PPT state for the simple reason that it is invariant under partial transposition, $\rho_1^P = \rho_1$. All the states given as examples in Ref. [5] are of this special kind.

An entangled PPT state ρ_1 defined by this UPB construction is a rather special density operator. Ker ρ_1 is spanned by product vectors, while Im ρ_1 contains no product vector. Since ρ_1 is proportional to the orthogonal projection onto the subspace Im ρ_1, it is the maximally mixed state on this subspace. There is also a symmetry between ρ_1 and ρ_1^P, such that ρ_1^P shares with ρ_1 all the properties just mentioned and has the same rank $N - p$, where $N = N_A N_B$ is the dimension of the Hilbert space and p is the number of product vectors in the UPB.

Implicitly the construction implies limits to the rank of ρ_1. Thus, for a given Hilbert space of dimension $N = N_A N_B$ there is a lower limit to the number of product vectors in a UPB, which follows from the requirement that there should exist no product vector in the orthogonal space $\mathcal{U}^\perp$. The corresponding upper bound on the rank m of ρ_1, as discussed in Ref. [4], is given by $m < N - N_A - N_B + 2$. There is also a lower bound $m > \max\{N_A, N_B\}$, which is the general lower bound on the rank of entangled PPT states with full local rank [8]. In some special cases there exist more restrictive bounds than the ones given here [9].

For the 3×3 system these two bounds allow only one value $m = 4$ for the rank of a state ρ_1 constructed from a UPB, and for this rank explicit constructions of UPBs exist [5]. Also in higher dimensions a few examples of UPB constructions have been given [6].

The extension of the UPB construction that we shall consider here is based on a certain concept of equivalence between density operators previously discussed in [10]. The equivalence relation is defined by transformations between density operators of the form

$$\rho_2 = a_2 V \rho_1 V^\dagger, \tag{5}$$

where a_2 is a positive normalization factor, and $V = V_A \otimes V_B$, with V_A and V_B as nonsingular linear operators on $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively. The operators ρ_1 and ρ_2 are equivalent in the sense that they have in common several properties related to entanglement. In particular, the form of the operator V implies that separability as well as the PPT property is preserved under the transformation (5). Preservation of separability follows directly from the product form of the transformation, while preservation of PPT follows because the partially transposed matrix ρ_1^P is transformed in a similar way as ρ_1,

$$\rho_2^P = a_2 \tilde{V} \rho_1^P \tilde{V}^\dagger, \tag{6}$$

with $\tilde{V} = V_A \otimes V_B^*$. If ρ_1 and ρ_1^P are both positive then the transformation equations show explicitly that the same is true for ρ_2 and ρ_2^P. Furthermore, since the operators V and $\tilde{V}$ are nonsingular, the ranks of ρ_1 and ρ_2 are the same, and so are the ranks of ρ_1^P and ρ_2^P. The same is true for the *local* ranks of the operators, which are the ranks of the reduced density operators, defined with respect to the subsystems A and B. Finally, if ρ_1 is an extremal PPT state, so is ρ_2.

Let us again assume ρ_1 to be given by the expression (3). Since the product operator V is an invertible mapping from Im ρ_1 to Im ρ_2, and since Im ρ_1 contains no product vector, there is also no product vector in Im ρ_2, and hence ρ_2 is entangled. Similarly, the product operator $(V^\dagger)^{-1}$ is an invertible mapping from Ker ρ_1 to Ker ρ_2, and it maps the UPB in Ker ρ_1, Eq. (2), into a set of product vectors in Ker ρ_2,

$$\psi_k' = [(V_A^\dagger)^{-1}\phi_k] \otimes [(V_B^\dagger)^{-1}\chi_k], \quad k = 1,2,\ldots,p. \tag{7}$$

If the operators V_A and V_B are both unitary, then this is another UPB of orthonormal product vectors, and ρ_2 is proportional to a projection, just like ρ_1. More generally, however, we may allow V_A and V_B to be nonunitary. Then the product vectors ψ_k' in Ker ρ_2 will no longer be orthogonal, but ρ_2 is nevertheless an entangled PPT state. It has the same rank as ρ_1, but it is not proportional to a projection.

Since the normalization of the density operators ρ_1 and ρ_2 is taken care of by the normalization factors a_1 and a_2, we may impose the normalization condition det V_A = det $V_B = 1$, which defines the operators as belonging to the special linear (SL) groups on $\mathcal{H}_A$ and $\mathcal{H}_B$. We will say then that the two density operators ρ_1 and ρ_2, related by a transformation of the form (5), are SL $\otimes$ SL equivalent, or simply SL equivalent.

This construction motivates a generalization of the concept of a UPB, where we no longer require the product vectors to be orthogonal. This generalization has also previously been proposed in the literature [7]. In the following we will refer to an unextendible product basis of orthogonal vectors as an *orthogonal* UPB. A more general UPB is then a set of product vectors that need not be orthogonal (need not even be linearly independent) but still satisfies the condition that no product vector exists in the subspace *orthogonal* to the set. The UPB defined by (7) is a special type of generalized UPB, since it is SL equivalent to an orthogonal UPB. More general types of UPBs exist, and they are in fact easy to generate, since an arbitrarily chosen set of k product vectors is typically a generalized UPB, in the above sense, when k is sufficiently large. However, if it is *not* SL equivalent to an orthogonal UPB, then we have no guarantee that there will be any entangled PPT state in the subspace $\mathcal{U}^\perp$ orthogonal to the generalized UPB.

III. PARAMETRIZING THE UPBS OF THE 3 × 3 SYSTEM

We focus now on the orthogonal UPBs in the 3×3 system, which must have precisely five members. In fact, for any given set of four product vectors $\phi_k \otimes \chi_k$, there exists a product vector $\phi \otimes \chi$ orthogonal to all of them, for example with $\phi_1 \perp \phi \perp \phi_2$ and $\chi_3 \perp \chi \perp \chi_4$. And with six members in an orthogonal UPB, it would define a rank 3 entangled PPT state, which is known not to exist [8].

The general condition for five product vectors to form an orthogonal UPB in the 3×3 system was discussed in Ref. [5]. The condition implies that for any choice of *three* product vectors from the set, the first factors ϕ_k are linearly independent and so are the second factors χ_k. The orthogonality condition further implies that if the product vectors are suitably ordered, there is a cyclic set of orthogonality relations between the factors of the products of the form

$$\begin{aligned} &\phi_1 \perp \phi_2 \perp \phi_3 \perp \phi_4 \perp \phi_5 \perp \phi_1, \\ &\chi_1 \perp \chi_3 \perp \chi_5 \perp \chi_2 \perp \chi_4 \perp \chi_1. \end{aligned} \tag{8}$$

In Fig. 1 the situation is illustrated by a diagram composed of a pentagon and pentagram, where each corner represents a product vector. Each pair of vectors is interconnected by a line showing their orthogonality. A solid (blue) line indicates orthogonality between ϕ states (of subsystem A) and a dashed (red) line indicates orthogonality between χ states. As shown in the diagram, precisely two A lines and two B lines connect any given corner with the other corners of the diagram.

Introducing a complete set of orthonormal basis vectors α_j in $\mathcal{H}_A$, we write

$$\phi_k = \sum_{j=1}^{3} u_{jk}\alpha_j, \quad k = 1,2,3,4,5. \tag{9}$$

We may choose, for example, α_1 proportional to ϕ_1 and α_2 proportional to ϕ_2. If we multiply each basis vector α_j by a phase factor ω_j, and each vector ϕ_k by a normalization factor N_k, we change the 3×5 matrix u_{jk} into $\omega_j^{-1} N_k u_{jk}$. It is always possible to choose these factors so as to obtain a standard form

$$u = \begin{pmatrix} 1 & 0 & a & b & 0 \\ 0 & 1 & 0 & 1 & a \\ 0 & 0 & b & -a & 1 \end{pmatrix}, \tag{10}$$

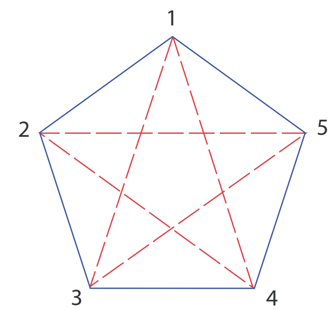

FIG. 1. (Color online) Diagrammatic representation of the orthogonality relations in a five-dimensional UPB of the 3×3 system. The corners of the diagram represent the product vectors of the UPB, and the lines represent orthogonality between pairs of states. There are two types of orthogonality, represented by the solid (blue) lines and the dashed (red) lines. The solid lines represent orthogonality between the vectors of the products that belong to subsystem A and the dashed lines represent orthogonality between the vectors belonging to subsystem B.

with a and b as real and strictly positive parameters, and with the vectors ϕ_k not normalized to length 1. A similar parametrization of the vectors of subsystem B with orthonormal basis vectors β_j gives

$$\chi_k = \sum_{j=1}^{3} v_{jk}\beta_j, \quad k = 1,2,3,4,5, \tag{11}$$

and a standard form

$$v = \begin{pmatrix} 1 & d & 0 & 0 & c \\ 0 & 1 & 1 & c & 0 \\ 0 & -c & 0 & 1 & d \end{pmatrix}, \tag{12}$$

with two more positive parameters c and d. Thus, an arbitrary orthogonal UPB is defined, up to unitary transformations in $\mathcal{H}_A$ and $\mathcal{H}_B$, by four continuous, positive parameters a,b,c,d.

Note that, for a given UPB, the parameter values are not uniquely determined, since this prescription does not specify a unique ordering of the five product vectors within the set. Any permutation that preserves the orthogonality relations pictured in Fig. 1 will generate a new set of values of the parameters that define the same UPB. These permutations form a discrete group with ten elements, generated by the cyclic shift $k \to k+1$, and the reflection $k \to 6-k$.

Given the orthonormal basis vectors α_j in $\mathcal{H}_A$ and β_j in $\mathcal{H}_B$, we may think of the four positive parameters a,b,c,d as defining not only one single orthogonal UPB but a continuous family of generalized UPBs that are SL equivalent to this particular orthogonal UPB. The parameter values defining one such family may be computed from any UPB in the family via SL invariant quantities, in the following way. Given the product vectors $\phi_k \otimes \chi_k$ for $k = 1,2,3,4,5$, not necessarily orthogonal, we introduce expansion coefficients as in (9) and arrange them as column vectors

$$u_k = \begin{pmatrix} u_{1k} \\ u_{2k} \\ u_{3k} \end{pmatrix}. \tag{13}$$

Then we introduce the following quantities:

$$s_1 = -\frac{\det(u_1u_2u_4)\det(u_1u_3u_5)}{\det(u_1u_2u_5)\det(u_1u_3u_4)} = a^2,$$
$$s_2 = -\frac{\det(u_1u_2u_3)\det(u_2u_4u_5)}{\det(u_1u_2u_4)\det(u_2u_3u_5)} = \frac{b^2}{a^2}, \tag{14}$$

where the values to the right are determined from the parametrization (10) of the orthogonal UPB defining the family. Similarly, we define

$$s_3 = \frac{\det(v_1v_2v_3)\det(v_1v_4v_5)}{\det(v_1v_2v_5)\det(v_1v_3v_4)} = c^2,$$
$$s_4 = \frac{\det(v_1v_3v_5)\det(v_2v_3v_4)}{\det(v_1v_2v_3)\det(v_3v_4v_5)} = \frac{d^2}{c^2}. \tag{15}$$

The quantities s_1,s_2,s_3,s_4 defined in terms of 3×3 determinants are useful because they are invariant under SL transformations as in (7), and in addition they are independent of the normalization of the column vectors u_k and v_k. Obviously, many more similar invariants may be defined from five product vectors, but these four invariants are sufficient to characterize a family of UPBs that are SL equivalent to an orthogonal UPB.

There exists a less obvious further extension of the set of invariants. In fact, there are always six vectors that can be used to define invariants, since in addition to the five linearly independent product vectors of the UPB, the space spanned by these will always contain a sixth product vector. In the case of an orthogonal UPB, given by the parameters a,b,c,d, we have found (by means of a computer algebra program) explicit polynomial expressions for the components of the one extra product vector. We have checked, both analytically and numerically, that the existence of exactly six product vectors is a generic property of a five-dimensional subspace of the 3×3 dimensional Hilbert space $\mathcal{H}$. This number of product vectors is also consistent with the formula discussed in [4], which specifies more generally, as a function of the dimensions, the number of product vectors in a subspace of $\mathcal{H}$. For an orthogonal UPB in the 3×3 system the sixth vector is singled out because it is not orthogonal to the other vectors, but for a nonorthogonal UPB there is no intrinsic difference between the six vectors of the set, which should therefore be treated on an equal footing.

For a UPB that is SL equivalent to an orthogonal UPB there are strong restrictions on the values of invariants of this kind, since they are all rational functions of the four real parameters a,b,c,d. In particular, they must all take real values. A given choice of four invariants, as in (14) and (15), is sufficient to define the parameter space for the equivalence classes of these UPBs. But since the six product vectors listed in any order define the same UPB, and the same PPT state, there is a discrete set of $6! = 720$ symmetry transformations that introduce identifications between points in the corresponding parameter space. As we shall see in the following, the requirement that all four invariants s_1,s_2,s_3,s_4 should be positive allows 60 different orderings from the total of 720.

One should note that for a generalized UPB consisting of five randomly chosen product vectors the invariants will in general be complex rather than real, and it is not a priori clear that four invariants are sufficient to parametrize the equivalence classes of random UPBs.

IV. CLASSIFYING THE RANK 4 ENTANGLED PPT STATES

We have in [4] described a method to generate PPT states ρ for given ranks (m,n) in low-dimensional systems, with $m = \text{rank}\rho$ and $n = \text{rank}\rho^P$. By repeatedly using this method with different initial data we have generated a large number of different PPT states of rank (4,4) in the 3×3 system. They are all entangled PPT states, and as a consequence they are extremal PPT states. This follows from the fact that if they were not extremal they would have to be convex combinations involving entangled PPT states of even lower ranks, and such states do not exist.

The remarkable fact is that every one of these states has a UPB in its kernel which is SL equivalent to an *orthogonal* UPB, and the state itself is SL equivalent to the state constructed from the orthogonal UPB. We regard our numerical results as strong evidence for our belief that the four real parameters which parametrize the orthogonal UPBs give a complete parametrization of the rank 4 entangled PPT states of the 3×3 system, up to the SL (or more precisely SL $\otimes$ SL) equivalence. We will describe here in more detail the numerical methods and results that lead us to this conclusion.

Assume ρ to be an entangled PPT state of rank (4,4), found by the method described in [4]. The question to examine is whether it is SL equivalent to an entangled PPT state defined by the orthogonal UPB construction. We therefore make the *ansatz* that it can be written as $\rho \equiv \rho_2 = a_2 V \rho_1 V^\dagger$, where ρ_1 is defined by a so far unknown *orthogonal* UPB, parametrized as in (10) and (12), and where the transformation V is of product form, $V = V_A \otimes V_B$. We consider how to compute the product transformation V, assuming that it exists. The fact that we are able to find such a transformation for every (4,4) state is a highly nontrivial result.

Given ρ, the first step is to find all the product vectors in Ker ρ. We solve this as a minimization problem: A normalized product vector $\psi = \phi \otimes \chi$ with $\rho\psi = 0$ is a minimum point of the expectation value $\psi^\dagger \rho \psi$. Details of the method we use are given in Ref. [4]. Empirically, we always find exactly six such product vectors $\psi_k = \phi_k \otimes \chi_k$, $k = 1,2,\ldots,6$, any five of which are linearly independent and form a UPB, typically nonorthogonal.

Although the numbering of the six product vectors is arbitrary at this stage, we compute the invariants s_1,s_2,s_3,s_4, substituting ϕ_k for u_k and χ_k for v_k, with $k = 1,2,\ldots,5$. As shown by the previous discussion all four invariants have to be real, for otherwise no solution can exist. A random UPB has complex invariants, and the empirical fact that the invariants are always real for a UPB in Ker ρ, where ρ is a rank (4,4) entangled PPT state, is a nontrivial test of the hypothesis that such a UPB can be transformed into orthogonal form.

It is not sufficient that the invariants are real. As shown by the expressions (14) and (15) there has to exist an ordering of the product vectors where all four invariants take positive values. The signs of the invariants will depend on the ordering of the product vectors, and most orderings produce both positive and negative invariants. For the rank (4,4) density matrices that we have constructed, it turns out that it is always possible to renumber the five first vectors in the set in such a way that all four invariants become positive. This is a further nontrivial test of our hypothesis.

There are in fact, in all the cases we have studied, precisely 10 of the 5! permutations of the five vectors that give positive values of the four invariants. This means that such an ordering is unique up to the symmetries noticed for the diagram in Fig. 1. However, there is a further symmetry, since the reordering which gives positive invariants works for any choice of the sixth vector of the set. The possible reorderings of all six product vectors which preserve the positivity of the invariants therefore define a discrete symmetry group with altogether $6 \times 10 = 60$ elements, which defines mappings between different, but equivalent, representations of the UPB in terms of the set of four real and positive invariants. The corresponding parameter transformations are given in the Appendix.

Assume now, for a given rank (4,4) state, that a "good" numbering has been chosen for the six product vectors $\psi_k = \phi_k \otimes \chi_k$ in the corresponding UPB, so that the four invariants defined by the first five vectors are all real and positive. The problem to be solved is then to find the transformation that brings the UPB into orthogonal form. This means finding 3×3 matrices C and D such that $\phi_k = N'_k C u_k$ and $\chi_k = N''_k D v_k$ for $k = 1,2,\ldots,5$, with unspecified normalization constants N'_k and N''_k. Here the vectors u_k and v_k belong to an orthogonal UPB as given by the Eqs. (10) and (12), and these vectors are all known at this stage, because the invariants s_1,s_2,s_3,s_4 determine the parameters a,b,c,d. The transformation matrices C and D correspond to $V_A^\dagger$ and $V_B^\dagger$ in (7). The condition for two vectors ϕ_k and Cu_k to be proportional is that their antisymmetric tensor product vanishes; hence we write the following homogeneous linear equations for the matrix C:

$$\phi_k \wedge (Cu_k) = \phi_k \otimes (Cu_k) - (Cu_k) \otimes \phi_k = 0, \qquad k = 1,2,\ldots,5. \tag{16}$$

Since the antisymmetric tensor product $\phi_k \wedge (Cu_k)$ has, for given k, three independent components, there are altogether fifteen linear equations for the nine unknown matrix elements C_{ij}. We may rearrange the 3×3 matrix C as a 9×1 matrix C and write a matrix equation

$$MC = 0, \tag{17}$$

where M is a 15×9 matrix. This equation implies that $(M^\dagger M)C = 0$. The other way around, the equation $(M^\dagger M)C = 0$ implies that $(MC)^\dagger(MC) = C^\dagger(M^\dagger M)C = 0$ and hence $MC = 0$. Thus we may compute the matrix C as an eigenvector with zero eigenvalue of the Hermitean 9×9 matrix $M^\dagger M$. The matrix D is computed in a similar way.

It is a final nontrivial empirical fact for the (4,4) states we have found that solutions always exist for the matrices C and D, whenever the ordering of the six product vectors $\psi_k = \phi_k \otimes \chi_k$ is such that the invariants s_1,s_2,s_3,s_4 are positive.

The result is that every rank (4,4) state of the 3×3 system which we have found in numerical searches [4] can be transformed into a projection operator with an orthogonal UPB in its kernel. We have also checked the published examples of entangled PPT states of rank (4,4), which are based on special constructions [5,6,11,12], and have obtained the same result for these states. The explicit transformations have been found numerically by the method discussed here, and in all cases the four parameters a,b,c,d have been determined, with values that are unique up to arbitrary permutations of product vectors from the 60-element symmetry group.

V. SUMMARY AND OUTLOOK

The main result of this paper is a classification of the rank 4 entangled PPT states of the 3×3 system. We find empirically that every state of this kind is equivalent, by a product transformation of the form $\mathrm{SL} \otimes \mathrm{SL}$, to a state constructed from an orthogonal unextendible product basis. We refer to this type of equivalence as SL equivalence. We have shown how to parametrize the orthogonal UPBs by four real and positive parameters, and we have described how permutations of the vectors in the UPB give rise to identifications in the four-parameter space.

The concept of SL equivalence of states and of product vectors leads to a generalization of the concept of unextendible product bases so as to include sets of nonorthogonal product vectors, and further to the concept of equivalence classes of generalized UPBs that are SL equivalent to orthogonal UPBs. Thus, the parametrization of the orthogonal UPBs by four positive parameters is at the same time a parametrization of the corresponding equivalence classes of generalized UPBs.

We have described a method for checking whether a given rank 4 entangled PPT state in the 3×3 system is equivalent, by a product transformation, to a state constructed from an orthogonal UPB. It is a highly nontrivial result that all the rank-four entangled states that we have produced numerically, and all states of this kind that we have found in the literature, are SL equivalent to states that are generated from orthogonal UPBs. This we take as a strong indication that the parametrization of the UPBs in fact gives also a parametrization of all the equivalence classes of rank 4 entangled PPT states of the 3×3 system.

Apart from the pure product states, the rank 4 entangled PPT states are the lowest rank *extremal* PPT states among the 3×3 states that we have found in numerical searches, as reported on in [4]. The property of such a state—that it has a nonorthogonal UPB in its kernel, which means that there is a complete set of product vectors in $\mathrm{Ker}\,\rho$ and no product vector in $\mathrm{Im}\,\rho$—is shared with the lowest rank extremal PPT states of the other systems that we have studied, of dimensions different from 3×3. This has led us to conjecture that this is a general feature of the lowest rank extremal PPT states, valid also in higher dimensional systems [4], and to speculate that there may exist a generalization of the construction used for the 3×3 system in terms of orthogonal UPBs and SL transformations, which can be applied in the higher dimensional systems.

In higher dimensions the orthogonality condition is harder to satisfy, and therefore another condition may take its place as the defining characteristic of a special subset of extremal states from each SL equivalence class. This hypothetical new condition may involve the full set of product vectors in the subspace, rather than an arbitrarily selected subset as in the definition of the orthogonal UPBs. We consider examining this possibility, with the aim of parametrizing the lowest rank extremal PPT states more generally, an interesting task for further research, and we are currently looking into the problem.

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APPENDIX: EQUIVALENT ORDERINGS OF THE SIX PRODUCT VECTORS

Assume that the sequence of product vectors $\psi_k = \phi_k \otimes \chi_k$, $k = 1,2,3,4,5$, in this order, is characterized by parameter values a,b,c,d, as computed from the invariants s_1,s_2,s_3,s_4. It is convenient here to replace the parameters a,b,c,d by $\alpha = a^2$, $\beta = b^2$, $\gamma = c^2$, $\delta = d^2$.

Then the cyclic permutation $\psi_k \mapsto \tilde{\psi}_k$ with $\tilde{\psi}_1 = \psi_5$ and $\tilde{\psi}_k = \psi_{k-1}$ for $k = 2,3,4,5$ corresponds to the following parameter transformation, which is periodic with period 5:

$$\begin{aligned}\tilde{\alpha} &= \frac{\beta}{1+\alpha},\\ \tilde{\beta} &= \frac{\beta}{\alpha(1+\alpha)},\\ \tilde{\gamma} &= \frac{1}{\gamma+\delta},\\ \tilde{\delta} &= \frac{\gamma(1+\gamma+\delta)}{\delta(\gamma+\delta)}.\end{aligned} \tag{A1}$$

The inversion $\psi_1 \mapsto \tilde{\psi}_1 = \psi_1$, $\psi_k \mapsto \tilde{\psi}_k = \psi_{7-k}$ for $k = 2,3,4,5$ corresponds to the parameter transformation $\tilde{\alpha} = \alpha$, $\tilde{\gamma} = \gamma$,

$$\begin{aligned}\tilde{\beta} &= \frac{\alpha(1+\alpha)}{\beta},\\ \tilde{\delta} &= \frac{\gamma(1+\gamma)}{\delta}.\end{aligned} \tag{A2}$$

Let $\psi_6 = \phi_6 \otimes \chi_6$ be the sixth product vector in the five-dimensional subspace spanned by these five product vectors. Then the sequence $\tilde{\psi}_1 = \psi_6$, $\tilde{\psi}_2 = \psi_5$, $\tilde{\psi}_3 = \psi_3$, $\tilde{\psi}_4 = \psi_4$, $\tilde{\psi}_5 = \psi_2$ corresponds to the parameter transformation $\tilde{\alpha} = \gamma$, $\tilde{\gamma} = \alpha$,

$$\begin{aligned}\tilde{\beta} &= \frac{\beta(1+\gamma)[(\alpha+\beta)(\gamma+\delta)+\delta]}{\alpha(1+\alpha+\beta)\delta+(1+\alpha)(\alpha+\beta)(1+\gamma)},\\ \tilde{\delta} &= \frac{(1+\alpha)[\beta\delta+(\alpha+\beta)\gamma(1+\gamma+\delta)]}{[1+\alpha+(1+\alpha+\beta)(\gamma+\delta)]\delta}.\end{aligned} \tag{A3}$$

It is not easy to see by looking at the formulas that this parameter transformation is its own inverse.

Altogether, these transformations generate a transformation group of order 60 (with 60 elements), isomorphic to the symmetry group of a regular icosahedron with opposite corners identified. Equivalently, it is the group of proper rotations of the icosahedron, excluding reflections. The icosahedron has twelve corners, and we may associate the six product vectors with the six pairs of opposite corners.

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