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Smallest state spaces for which bipartite entangled quantum states are separable

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Abstract
According to usual definitions, entangled states cannot be given a separable decomposition in terms of products of local density operators. If we relax the requirement that the local operators be positive, then an entangled quantum state may admit a separable decomposition in terms of more general sets of single-system operators. This form of separability can be used to construct classical models and simulation methods when only a restricted set of measurements is available. With these motivations in mind, we ask what are the smallest sets of local operators such that a pure bipartite entangled quantum state becomes separable? We find that in the case of maximally entangled states there are many inequivalent solutions, including for example the sets of phase point operators that arise in the study of discrete Wigner functions. We therefore provide a new way of interpreting these operators, and more generally, provide an alternative method for constructing local hidden variable models for entangled quantum states under subsets of quantum measurements.

1. Overview

From early on in the development of quantum theory, alternative mathematical descriptions of the quantum formalism have been developed with the motivation of either simplifying calculations or elucidating the differences between quantum and classical theories. One of the most famous examples of this is the Wigner distribution [1], which was one of the earliest attempts at replacing quantum mechanical wavefunctions with objects that more closely resemble probability distributions.

An obstacle to the development of such classically motivated descriptions is the phenomenon of quantum entanglement. Entangled quantum systems exhibit powerful non-classical correlations that do not admit the most natural classical model, a local hidden variable theory [2]. With the advent of quantum information science, the correlations of entangled quantum systems have been identified as a powerful resource that can be used in quantum information processing protocols. Indeed, in some forms of quantum computation it is known that entanglement is a prerequisite for better-than-classical performance [3]. The non-classical features of entangled quantum states make it difficult to write down classical models that can mimic the outcomes of experiments, seemingly making it an impossible task. However, in many realistic situations the measurements that can be made on a quantum system are highly restricted, either because of experimental limitations or imperfections. In such cases one may ask whether the formalism of quantum theory can be replaced, and perhaps the measurement statistics could admit a classical description such as a local hidden variable model, even when the states are non-classical for unrestricted measurements. Indeed, there are many examples of this phenomenon. For instance, it has been known since the time of Bell that a two-qubit EPR pair has a local hidden variable (LHV) model for the Pauli measurements [4], even though it is the canonical maximally entangled quantum state, and for general measurements it can violate a Bell inequality. The fact that EPR pairs have a local...
hidden variable model for Pauli measurements can be reinterpreted as a statement that the EPR pair can be considered to be separable (i.e. non-entangled) with respect to a more general set of single-system operators that consists of cubes of Bloch vectors enclosing the usual Bloch sphere [5]. While the operators that correspond to these ‘cube’ Bloch vectors are not always physical, as we shall shortly describe, they can be considered as valid state descriptions if measurements are restricted to the Pauli operators.

The investigation of such non-quantum spaces resides in the study of generalized probabilistic theories [6, 7]. This field of research considers theories more general than quantum theory by describing single- and multi-particle systems in terms of tables of probabilities for measurement outcomes, under various natural constraints such as not allowing instant signaling. In principle such theories do not necessarily have an underlying structure in terms of Hilbert spaces and operators, and can exhibit correlations that are more powerful than quantum theory. In the context of the example discussed in the previous paragraph, a cube of Bloch vectors surrounding the Bloch sphere may not be valid state space in quantum theory as it contains non-positive operators, but if we are only considering Pauli measurements, then it gives a perfectly valid way to describe the probabilities of measurement outcomes.

With such motivations in mind, in this paper we will build upon these ideas to construct separable descriptions for entangled quantum states. In particular, we will set out to find the smallest local state spaces such that a given quantum entangled state can be considered separable. The reason for doing this is that, as we discuss later, such state spaces will typically be the most useful for constructing local descriptions of entangled states in various settings. Unlike the more general formalism of generalized probabilistic theories, however, the local state spaces that we consider still have some quantum structure in that they are sets of operators with the same dimensions as the density operators [8]. Indeed, the only correlations that we consider arise from quantum systems.

The structure of this paper is as follows. In the next two sections we set up notation and define more precisely the various problems that we consider. In section 5 we summarize the methods that we use. In section 6 we discuss connections between our problems and the study of cross norm measure of entanglement [10, 11]. In sections 7–9 we construct solutions to our problems for the case of maximally entangled states, and in section 10 we conclude.

2. Generalized separability

In the conventional quantum description of entanglement, a quantum state of two or more particles is said to be entangled if it cannot be written as a probabilistic mixture of products of single-particle quantum states [13]. The textbook example of an entangled quantum state for two d-level quantum particles is the maximally entangled state, denoted here by |φd⟩, which by a suitable local basis choice can be written in the form

||φd⟩ = 1/√d \sum_{j=0}^{d-1} |j⟩.

(1)

It is well known that this state cannot be written in the form of a separable state,

⟨φa|φa⟩ = ∑_j p_j \rho_j^A \otimes \rho_j^B,

(2)

where \rho_j^A and \rho_j^B are drawn from the sets \mathcal{Q}_A and \mathcal{Q}_B of quantum states on each subsystem, and p_j forms a probability distribution. However, if we relax the restriction that the local operators \rho_j^A and \rho_j^B be drawn from \mathcal{Q}_A and \mathcal{Q}_B, then we can indeed find separable decompositions for |φd⟩. If two convex sets of operators \mathcal{V}_A and \mathcal{V}_B are such that a given quantum state Ψ can be written as

Ψ = ∑_j p_j \rho_j^A \otimes \rho_j^B,

(3)

where \rho_j^A ∈ \mathcal{V}_A and \rho_j^B ∈ \mathcal{V}_B, and p_j forms a probability distribution, then we will say that Ψ is \mathcal{V}-separable, where \mathcal{V} denotes the pair of sets (\mathcal{V}_A, \mathcal{V}_B).

This generalized notion of separability [7] can adopt practical significance if the local operators in the separable decomposition exhibit some form of what can be referred to as generalized positivity. In the usual study of quantum separability, the notion of positivity amounts to matrix-positivity of the local operators so that they can correspond to density matrices. However, in other contexts, alternative notions of positivity may be useful. One example of such an alternative notion is positivity defined with respect to a subset of quantum measurements. This can be defined using the notion of a dual. Given a set \mathcal{X} of operators, its dual is defined as the set of operators satisfying \mathcal{X}^* = \{H | 0 ≤ \text{tr}(HG) \forall G ∈ \mathcal{X} \}. Due to its connection with the Born rule, this definition can be used to define operators that are ‘positive’ for subsets of quantum measurements.
Consider a positive-operator valued measurement (POVM) performed on a single quantum particle:

\[ \mathcal{M} = \{ M_i | \sum_i M_i = 1, \ M_i \geq 0 \} \]

We define the dual set of this measurement, denoted by \( \mathcal{M}^* \), as the set of operators that gives positive values under the Born rule:

\[ \mathcal{M}^* := \{ X | 0 \leq \text{tr}(X M_i), \ \forall M_i \in \mathcal{M} \} \]

(Notice that a POVM consists of Hermitian operators, so it is irrelevant whether we place the dagger \( ^\dagger \) on the \( M_i \).) In this context we say that the elements of \( \mathcal{M}^* \) are positive with respect to \( \mathcal{M} \), or more concisely \( \mathcal{M} \)-positive. Related definitions appear in the context of generalized probabilistic theories [6]. Some authors define the dual as consisting only of operators with restrictions on normalization. However, we do not do that here as in one application we will consider the construction of local hidden variable models, and in those contexts it turns out to be more natural to not impose that restriction. For an example that illustrates these ideas see figure 1.

This definition can be extended to collections of quantum measurements. If instead of a single POVM we consider a collection \( \mathcal{F} \) of POVMs on the same particle, then we define the dual \( \mathcal{F}^* \) as the intersection of sets of operators that give valid probability distributions for all of the measurements in the collection

\[ \mathcal{F}^* := \bigcap_{\mathcal{M} \in \mathcal{F}} \mathcal{M}^* \]

and we describe the elements of \( \mathcal{F}^* \) as being \( \mathcal{F} \)-positive. Note that to be positive with respect to any set of measurements, an operator must have a non-negative trace. The full dual set \( \mathcal{F}^* \) forms a convex cone, i.e. if \( X_A, X_B \in \mathcal{F}^* \), then so is \( x_A X_A + x_B X_B \) for any coefficients \( x_A, x_B \geq 0 \).

If the local operators appearing in a generalized separable decomposition are positive with respect to the measurements on each particle, then this can help to provide classical descriptions for the state of a bipartite (or for that matter multipartite) system. If, for example, the sets \( \mathcal{V}_A \) and \( \mathcal{V}_B \) are subsets of the cones of \( \mathcal{F}_A \)-positive and \( \mathcal{F}_B \)-positive operators on particles \( A \) and \( B \), respectively, and if a quantum state \( \Psi \) is \( \mathcal{V} \)-separable, then the separable decomposition supplies a local hidden variable model for measurements from \( \mathcal{F}_A \) and \( \mathcal{F}_B \) made on \( \Psi \) (for convenience the reason for this is explained in 4). Moreover, in some cases such separable decompositions can help to efficiently classically simulate quantum entangled systems under \( \mathcal{F} \); see for instance \([5, 14–16]\).

With such applications in mind, our goal in this work will be to try to identify the smallest choices for \( \mathcal{V}_A \) and \( \mathcal{V}_B \) such that the maximally entangled state \( |\phi^+_A\rangle \) is \( \mathcal{V} \)-separable. While we make our definitions of ‘small’ more precise in the rest of the paper, the motivation for this problem is that for most reasonable forms of generalized positivity, the positivity of a set of operators guarantees the positivity of any of its subsets, and this means that identifying the smallest state spaces under which a given state is separable will lead us to ‘more positive’ separable descriptions of the state. Consider, for instance, two sets \( \mathcal{V}_A \subset \mathcal{V}_A' \) for which we know that a quantum state \( \Psi \) is \( (\mathcal{V}_A, \mathcal{V}_B) \)-separable (and hence also \( (\mathcal{V}_A', \mathcal{V}_B) \)-separable), because product operators from \( (\mathcal{V}_A, \mathcal{V}_B) \) are also products from \( (\mathcal{V}_A', \mathcal{V}_B) \). Then, the set of measurements for which \( \mathcal{V}_A \) is positive cannot be smaller than the set of measurements for which \( \mathcal{V}_A' \) is positive. This in turn implies that \( (\mathcal{V}_A', \mathcal{V}_B) \)-separability supplies an LHV model for a no-smaller class of measurements than \( (\mathcal{V}_A, \mathcal{V}_B) \)-separability (we make this discussion more precise when describing problem 3 in the next section).
While there can be many definitions of ‘size’ for the sets $V_A$ and $V_B$, we will choose definitions that enable us to make analytical progress, and in the process identify choices of $V_A$ and $V_B$ that are the ‘smallest’ possible—in that no strict subsets of them can be chosen while keeping $|\phi_d|$ separable. However, we will see that there are many such inequivalent solutions. Amongst them is the set of phase point operators which is used to describe the discrete Wigner function [18] (see figure 2).

3. Variants of the problem

There are many different ways that one could define the ‘size’ of the sets $V_A$, $V_B$. We will not consider specific measurements or specific types of generalized positivity in this work, so initially we will adopt an approach where we use various norms to define the size of an operator set. Our aim is to identify state spaces that could be useful in a broad range of situations, even though they may not be the best choice for specific cases.

Ideally, the method we use to quantify the size of the sets $V_A$, $V_B$ should reflect how far from matrix-positive the operators within $V_A$, $V_B$ are. This is because if $V_A$, $V_B$ consist only of matrix-positive operators (which is of course not possible for an entangled state such as $|\phi_d\rangle$), then they will be in the dual of all quantum measurements and hence have an LHV model for all quantum measurements. If we restrict ourselves to sets $V_A$, $V_B$ of Hermitian operators, then the trace norm $\| \cdot \|_\text{tr}$ captures this distance from matrix-positivity in a satisfying way. Indeed, for Hermitian operators $X$ the quantity $(\| X \|_1 - \text{tr}(X))/2 \geq 0$ is equal to the sum of the negative eigenvalues. If we further restrict our attention to local state spaces of only unit trace operators, then because the tensor products of these operators will also be unit trace, and because the trace norm is multiplicative for the tensor products of operators (i.e. $\| A \otimes B \|_1 = \| A \|_1 \| B \|_1$), the trace norm also quantifies the non-positivity for composite systems. This suggests that if we restrict our attention to sets $V_A$, $V_B$ of the unit trace operators, then we could define the size of a single set $S$ by

$$\| S \|_1 := \sup \{ \| X \|_1 | X \in S \},$$

and then define the size of both sets $V_A$, $V_B$ together by the product of their individual sizes $\| V_A \|_1 \| V_B \|_1$.

However, finding the smallest sets using the trace norm while incorporating the requirement of Hermiticity and unit trace appears to be difficult. So initially we will begin by analyzing a different problem where we abandon the condition of unit trace, and allow ourselves to consider more general norms $\| \cdot \|$ in place of the trace norm so that now we define the size of a single set by

$$\| S \| := \sup \{ \| X \| | X \in S \},$$

although we consider the problem with or without the restriction of Hermiticity. This is the first problem that we consider.

**Problem 1.** For a quantum state $\Psi$ and for a suitable norm $\| \cdot \|$ what is the infimum product size $\| V_A \|_1 \| V_B \|_1$ of all pairs of convex sets ($V_A$, $V_B$) (with or without the Hermiticity constraint) such that $\Psi$ is $V$-separable?
In section 6 we will find that (at least for multiplicative norms that satisfy the cross property, defined for any two operators $A$ and $B$ as $\|A \otimes B\| = \|A\| \|B\|$) this problem is equivalent to computing the so-called projective tensor norm (also known as greatest cross norm) that has been used already in the study of entanglement theory [10, 11, 17]. This will enable us to draw on explicit formulas that have already been derived in previous works, as well as make strong connections to entanglement measures.

A drawback of problem 1, whichever norm we use, is that there could be two choices $\mathcal{V}_A$, $\mathcal{V}_B$ and $\mathcal{V}'_A$, $\mathcal{V}'_B$ with the same size as measured by a norm, while still having (say) $\mathcal{V}_A \subset \mathcal{V}'_A$, and/or $\mathcal{V}_B \subset \mathcal{V}'_B$. In such cases, the sets $\mathcal{V}_A$, $\mathcal{V}_B$ will be the preferential choice, as under most notions of positivity if a set of operators is positive, then so must be any subset. So ideally we would like to know if there are smallest choices for $(\mathcal{V}_A, \mathcal{V}_B)$, in the following sense:

**Problem 2.** Can we identify convex sets $(\mathcal{V}_A, \mathcal{V}_B)$ such that $\Psi$ is $(\mathcal{V}_A, \mathcal{V}_B)$-separable, and there exist no smaller sets $(\mathcal{R}_A, \mathcal{R}_B) \subset (\mathcal{V}_A, \mathcal{V}_B)$ with $\mathcal{R}_A \subseteq \mathcal{V}_A$ and $\mathcal{R}_B \subseteq \mathcal{V}_B$ such that $\Psi$ is $(\mathcal{R}_A, \mathcal{R}_B)$-separable?

In section 7 will see that there are many such ‘smallest’ solutions in the case of the maximally entangled state $|\phi_2\rangle\langle \phi_2|$, and we will present methods of constructing a number of them. We will do this by initially tackling problem 1 with the norm chosen to be the 2-norm, and then showing how the solutions to problem 1 also contain solutions to problem 2. In fact, in section 8 we will find that for the 2-norm and the maximally entangled state we are also able to incorporate additional requirements of strictly positive or unit trace quite straightforwardly—these conditions are useful both for meeting positivity requirements and for technical reasons. In section 9 we will use them for constructing solutions to another variant of the problem that we describe below. In the appendix we also present a solution of problem 2 in the case of non-maximally entangled bipartite pure states; however, it does not incorporate the requirement of Hermiticity, and the product operators appearing in the separable decomposition are only in the dual of commuting local measurements.

In the context of constructing local hidden variable models for quantum states, there is yet another more natural variant of the problem involving convex cone state spaces [7]. Roughly speaking the cone state spaces that we will consider are obtained by dropping the normalization constraints that are imposed when defining convex state spaces. The article [7] was the first (as far as we are aware) to consider the properties of generalized cone state spaces, partly motivated by the study of anyons. In our context we will use them simply because they are a more elegant way of constructing local hidden variable models than the use of convex state spaces. In this section and the next we discuss why this is, and at the same time lay out the third problem that we will consider in this work.

We will need some terminology that is used in the study of cones; readers not familiar with cone spaces may find more background in [9] or [7]. The **conic hull** $\text{coni}(\mathcal{Y})$ generated by a set of operators $\mathcal{Y}$ is defined to be the smallest convex cone containing $\mathcal{Y}$, and it can be generated by taking linear combinations of elements of $\mathcal{Y}$ with non-negative coefficients [9]. In this context we say that the elements of $\mathcal{Y}$ are **generators** of $\text{coni}(\mathcal{Y})$. For readers familiar with the notion of a convex hull, the only difference between a conic hull and a convex hull is that in a convex hull the coefficients are required to be both positive and sum to 1, whereas in a conic hull the coefficients are required to be only positive. It is not difficult to see from the definition of the dual that if local state spaces $\mathcal{V}_A$ and $\mathcal{V}_B$ are contained in the dual of a collection of measurements $\mathcal{F}$, then so are the sets $\text{coni}(\mathcal{V}_A)$ and $\text{coni}(\mathcal{V}_B)$. This is because if two operators $X_1, X_2 \in \mathcal{V}_A$ satisfy $\text{tr} \{X_i M\} \geq 0$ for an $M \in \mathcal{F}$, then it must be the case that for two real $x_1, x_2 \geq 0$

$$\text{tr} \left( x_1 X_1 + x_2 X_2 \right) M = x_1 \text{tr}(X_1 M) + x_2 \text{tr}(X_2 M) \geq 0,$$

so that any conic combination must also be contained in the dual.

Moreover, note that as the conic hull of a set contains the set itself, i.e. $\mathcal{V}_A \subset \text{coni}(\mathcal{V}_A)$ and $\mathcal{V}_B \subset \text{coni}(\mathcal{V}_B)$, if an operator is separable with respect to sets $\mathcal{V}_A$ and $\mathcal{V}_B$ then it is also separable with respect to the cones $\text{coni}(\mathcal{V}_A)$ and $\text{coni}(\mathcal{V}_B)$. This means that if we are interested in using generalized separable decompositions to construct a local hidden variable model for as many quantum measurements as possible, then considering conic hulls can only increase the set of states that are separable. Moreover, it turns out that separability with respect to the conic hull of a convex set gives a local hidden variable model (see the next section) for precisely the same set of measurements for which separability with respect to the generating convex set implies the existence of a local hidden variable model. So if we are concerned with local hidden variable models from separable decompositions, our goal should not be to look for the smallest convex state spaces for which the quantum state is separable, but the smallest convex cone state spaces for which the quantum state is separable.

In this context it is important to note another issue that can arise. Consider one of the two subsystems, say $A$. Suppose that we have two convex cones $\mathcal{T}, \mathcal{U}$ of operators on $A$ such that $\mathcal{T}$ is strictly contained within $\mathcal{U}$, i.e. $\mathcal{T} \subset \mathcal{U}$. In such cases, one might assume that a separable decomposition involving $\mathcal{T}$ would give stronger LHV
models than a separable decomposition involving \( \mathcal{U} \). However, in spite of the fact that \( T \subset \mathcal{U} \), it could be the case that both sets are positive for identical sets of quantum measurements, that is, the differences in their duals could be made up of operators that are not positive and hence not valid quantum measurements. In such cases the separable decompositions would give local hidden variable models for exactly the same sets of measurements, and there would be no advantage in demonstrating separability using \( T \) rather than \( \mathcal{U} \), even though \( T \) is smaller.

To get around this problem we must find a way of deciding when two sets have identical quantum measurements in their dual. We now explain how to do this, and how it leads to the third variant of the problem that we consider. First note that if \( \mathcal{Q}_A \) denotes the cone of local matrix positive operators (i.e. Hermitian operators with non-negative eigenvalues), then an operator \( N \) satisfies \( \text{tr}(N \mathcal{Q}_A) \geq 0 \) iff \( N \) is also matrix-positive. This means that an operator in the dual of a given local cone of operators (say \( \text{coni}(\mathcal{V}_A) \)) is matrix-positive and hence a possible quantum measurement operator, iff it is also in the dual of \( \mathcal{Q}_A \). An operator is in the dual of both these sets \( \{ \text{coni}(\mathcal{V}_A) \text{ and } \mathcal{Q}_A \} \) if it is in the intersection of their duals \( \{ \text{coni}(\mathcal{V}_A) \}^* \text{ and } \{ \mathcal{Q}_A \}^* \), which is equal to \( \text{coni}(\mathcal{V}_A \cup \mathcal{Q}_A) \). Hence to maximize the set of measurements for which generalized separable decompositions can supply a local hidden variable model, we should not look for the smallest local cones for which the bipartite state is separable, but instead look for the smallest local cones containing the quantum states for which the bipartite state is separable. This leads to the final variant of the problem that we consider.

**Problem 3.** Can we identify local cones \( (\mathcal{V}_A, \mathcal{V}_B) \) of operators that contain the sets of local quantum operators \( (\mathcal{Q}_A, \mathcal{Q}_B) \), such that \( \Psi \) is \( (\mathcal{V}_A, \mathcal{V}_B) \)-separable, and there exist no smaller cones \( \{ \mathcal{R}_A, \mathcal{R}_B \} \equiv (\mathcal{V}_A, \mathcal{V}_B) \) with \( \mathcal{R}_A \subseteq \mathcal{V}_A \) and \( \mathcal{R}_B \subseteq \mathcal{V}_B \) with these properties?

Any two different solutions to problem 3 will be the duals of distinct sets of quantum measurements, and hence provide local hidden variable models for different scenarios. In section 9 we will see that some of our solutions to problems 1 and 2 for the maximally entangled state also enable us to construct solutions to problem 3.

### 4. Cone separability and local hidden variable models

For convenience in this section we explain why separability with respect to cone state spaces leads to a local hidden variable model for those measurements for which the cones are the dual. Suppose that

\[
\rho = \sum_i p_i A_i \otimes B_i
\]

is a separable decomposition of normalized operator \( \rho \), where \( A_i \) and \( B_i \) are \( \mathcal{F} \)-positive (for simplicity we assume that the same measurements are available to both parties). Then for local POVMs \( \mathcal{M} \) and \( \mathcal{N} \) the outcome probabilities are given by

\[
\text{tr} \left( \rho M_k \otimes N_l \right) = \sum_i p_i \text{tr} \left( A_i M_k \right) \text{tr} \left( B_i N_l \right),
\]

\[
= \sum_i p_i a(k|i)b(l|i),
\]

where \( a(k|i) := \text{tr}(A_i M_k) \) and \( b(l|i) := \text{tr}(B_i N_l) \). If \( a(k|i) \) and \( b(l|i) \) were conditional probability distributions, then this expression would be the local hidden variable model that we are seeking. However, while we know that \( a(k|i), b(l|i) \geq 0 \) from the fact that \( A_i, B_i \) are \( \mathcal{F} \)-positive, they need not be normalized. However, we do know that \( \sum_k a(k|i) = \text{tr}(A_i) \) and \( \sum_l b(l|i) = \text{tr}(B_i) \) from the completeness of the local POVMs, and we also know that \( \text{tr} \{ \rho \} = 1 \). These two facts are sufficient to allow us to turn equation (6) into a local hidden variable model, as we now demonstrate.

If \( A_i \) or \( B_i \) are traceless, then that means that the \( a(k|i) \) or \( b(l|i) \) will be all zero, and will not contribute to the sum in equation (6), so we may rewrite equation (6) as

\[5\) The simplest non-trivial example of this is the following. Consider a quantum entangled quantum state that it is separable w.r.t. the pair of sets \( (\mathcal{T}_A, \mathcal{V}_A) \), where \( \mathcal{T}_A \) is a strict subset of the cone of quantum operators but \( \mathcal{V}_A \) is larger than the cone of quantum operators (we pick \( \mathcal{V}_A \) in this way as otherwise the state would be quantum separable). Now pick another subset of quantum operators \( \mathcal{U}_A \) such that \( \mathcal{T}_A \subset \mathcal{U}_A \). The state will hence be separable w.r.t. \( (\mathcal{U}_A, \mathcal{V}_A) \) too. Then, even though \( \mathcal{T}_A \) is smaller than \( \mathcal{U}_A \), the set of quantum measurements in their duals is identical because, as they contain only quantum operators, they are both positive for all quantum measurements.\]
\[
\text{tr}\left(\rho M_b \otimes N_b\right) = \sum_{\{i|a(A_i)u(B_i) > 0\}} p_i a(k|i) b(l|i),
\]

\[
= \sum_{\{i|a(A_i)u(B_i) > 0\}} p_i \text{tr}(A_i) \text{tr}(B_i) \frac{a(k|i)}{\text{tr}(A_i)} \frac{b(l|i)}{\text{tr}(B_i)}.
\]

(7)

Defining the normalized probability distribution \(q_i\) and the normalized conditional probability distributions \(r(k|i)\) and \(s(l|i)\) by

\[
q_i := p_i \frac{\text{tr}(A_i) \text{tr}(B_i)}{r(k|i)},
\]

\[
r(k|i) := \frac{a(k|i)}{\text{tr}(A_i)},
\]

\[
s(l|i) := \frac{b(l|i)}{\text{tr}(B_i)},
\]

(the normalization of \(q_i\) is enforced by the fact that \(\rho\) has unit trace), we see that equation (7) supplies a local hidden variable model for the probability distribution. So we see that even though cones contain non-normalized operators, a cone separable decomposition still implies the existence of a local hidden variable model. Seeing as both a convex set and the set obtained from its conic hull are positive for precisely the same set of measurements, this means that separability with respect to the conic hull of a convex set provides a local hidden variable model for the same set of measurements.

5. Summary of results and method

The logical structure of the arguments that we use to solve these problems is as follows.

- We will first show that the solution to problem 1 is equivalent to computing a particular kind of norm (known as a cross norm) for the quantum state under consideration.
- We then show that for sets of local operators of exactly this size, a separable decomposition is only possible if the sets contain a minimum number of operators of a certain minimal size (as measured by the 2-norm).
- In the case of maximally entangled states we present examples of sets of operators that are the convex hull of such minimal sets, and argue that no strict subset of them can be chosen while keeping the state generalized separable, because any smaller subset contains too few operators of the minimal required size. These sets are hence solutions to problem 2. The argument is modified to give one solution for arbitrary bipartite pure states in the appendix.
- In the case of the maximally entangled state we show that such sets can be chosen to have unit trace (including subsets of phase point operators defining discrete Wigner functions as a particular case).
- We then show that the conic hulls generated by these unit trace convex sets provide solutions to problem 3.

6. Connections to cross norms

In this section we show that problem 1 is closely related to the notion of cross norms. In particular we show that the cross norm \(\|\cdot\|_{\gamma}\) (defined below) is exactly the minimum possible value of \(\|\cdot\|_{\gamma_A} + \|\cdot\|_{\gamma_B}\) in problem 1.

Consider any norm \(\|\cdot\|\) such that on two state spaces it satisfies the cross property. For instance, the well-studied family of Schatten \(p\)-norms \(\|X\|_p = \text{tr}(|X|^p)^{1/p}\), where \(1 \leq p < \infty\), obeys the cross property [12]. For any fixed norm \(\|\cdot\|\) on a state space we consider the projective tensor norm, denoted by \(\|\cdot\|_{\gamma}\), on the tensor product of two spaces:

\[
\|X\|_{\gamma} := \inf \left\{ \sum \|A_i\|_{\gamma} \cdot \|B_i\|_{\gamma} : X = \sum_i A_i \otimes B_i \right\},
\]

(8)

where the infimum is over finite sums of arbitrary operators \(A_i, B_i\) (not necessarily in \(\mathcal{V}_A\) or \(\mathcal{V}_B\) respectively). If the norm \(\|\cdot\|\) inside the sum is equal to the \(p\)-norm \(\|\cdot\|_p\), then we denote the corresponding projective norm by \(\|\cdot\|_{\gamma,p}\). It has been shown by one of us [10] that a bipartite quantum state \(\rho\) is quantum separable if and only if \(\|\rho\|_{\gamma,1} = 1\). Moreover, the cases of \(\|\cdot\|_{\gamma,1}\) and \(\|\cdot\|_{\gamma,2}\) have been used in the definition of entanglement measures [10], while \(\|\cdot\|_{\gamma,2}\) was also used in [11] to formulate a computable separability criterion.
Theorem 1. Consider a general bipartite quantum state $\Psi$ (not necessarily $|\phi_{\alpha}\rangle$ or $|\phi_{\beta}\rangle$), and $\| \cdot \|$ to be a (fixed) norm on the local state spaces $V_A$ and $V_B$, then

$$\| \Psi \|_\gamma = \infty \| V_A \| \| V_B \|$$

(9)

where the infimum is taken over all local state spaces for which $\Psi$ is separable.

Proof. Assume first that $\Psi$ is $V_\gamma$-separable, then

$$\Psi = \sum_k p_k A_k \otimes B_k, \quad A_k \in V_A, \quad B_k \in V_B,$$

(10)

for some choices of operators $A_k, B_k$. From the definition of the cross norm in equation (8), it follows that

$$\| \Psi \|_\gamma \leq \sum_k p_k \| A_k \| \| B_k \| \leq \max_k \| A_k \| \| B_k \| \leq \| V_A \| \| V_B \|.$$

(11)

Hence, we see that the infimum product size of the local sets is lower-bounded by the corresponding cross norm. We now show that the opposite inequality holds. For simplicity we assume that the infimum of equation (8) is an achievable minimum (the argument can be modified to hold even when the infimum is not achievable). Under this assumption let

$$\Psi = \sum_i A_i \otimes B_i$$

(12)

be the finite decomposition of $\Psi$ that achieves $\| \Psi \|_\gamma$ in equation (8). We may define a probability distribution by $p_i := \| A_i \| \| B_i \| /\| \Psi \|_\gamma$. Then we have that

$$\Psi = \sum_i p_i \sqrt{\| \Psi \|_\gamma} A_i \otimes \sqrt{\| \Psi \|_\gamma} B_i.$$

(13)

Now let $V_A'$ be the convex hull of the set of all operators $\sqrt{\| \Psi \|_\gamma} A_i \otimes 1$, and similarly let $V_B'$ be the convex hull of the set of all operators $\sqrt{\| \Psi \|_\gamma} 1 \otimes B_i$. In the separable decomposition (13), all the local operators in the product terms from the sets $(V_A', V_B')$ have the same norm, equal to $\sqrt{\| \Psi \|_\gamma}$. The triangle inequality hence implies that $\| V_A' \| = \| V_B' \| = \sqrt{\| \Psi \|_\gamma}$, and hence that $\| V_A' \| \| V_B' \| = \| \Psi \|_\gamma$. Hence, there are choices of state spaces $V_A', V_B'$ such that $\| V_A' \| \| V_B' \| = \| \Psi \|_\gamma$, and the inequality (9) is tight. \qed

This connection allows us to use existing results on the calculation of the cross norm. In particular, the value of $\| \cdot \|_{1,2}$ and $\| \cdot \|_{1,\infty}$ has been calculated for (among others) all pure bipartite states [10], with or without the requirement of Hermiticity.

We will now build upon these results to provide solutions to problem 2. In the next section we will begin this analysis by rederiving some of the results of [10] for $\| \cdot \|_{1,\infty}$ in the case of interest to us (the maximally entangled state). We will use these observations to provide a variety of optimal solutions $V_A, V_B$, and then also provide solutions to problem 2.

7. Solutions to problem 2 for maximally entangled states

We begin by expanding a $d \times d$ matrix of a single-system operator $X \in S$ in an orthogonal basis of $d^2$ Hermitian operators $C_i$:

$$X = \sum_{i=1}^{d^2} x_i C_i,$$

(14)

where the expansion coefficients $x_i \in \mathbb{C}$ form a $d^2$-dimensional vector $x := (x_1, x_2, \ldots, x_{d^2})$, and the operator basis is chosen to satisfy the condition $\text{tr}(C_i C_j) = d \delta_{ij}$. An example of such a basis for qubit systems is the set of Pauli operators with the identity. In such an expansion, the square of the 2-norm of the operator $X$ is given by $\text{tr}(XX^\dagger) = \sum_{ij} x_i x_j^* \text{tr}(C_i C_j) = d \sum_{ij} x_i x_j^* \delta_{ij} = d \| x \|^2$, hence

$$\| X \|_2 = \sqrt{d} \| x \|,$$

(15)

where $\| x \|$ is the standard Euclidean norm of the vector $x$.

Theorem 2. Consider any convex sets of operators $V_A, V_B$ for which $|\phi_{\alpha}\rangle$ is $(V_A, V_B)$-separable. Then the following must hold: (a) $V_A, V_B$ must satisfy $\| V_A \|_2 \| V_B \|_2 \geq d \| \| V_A \|_2 \| V_B \|_2 = d$ then (b) the separable
decomposition must involve only product terms $A_k \otimes B_k$ with $\| A_k \|_2 \| B_k \|_2 = d$, and (c) a separable decomposition must contain at least $d^2$ operators from $\mathcal{V}_A$ and $\mathcal{V}_B$ each. Finally, let $\{ C_i \}$ be any orthogonal basis of Hermitian operators for $d \times d$ matrices such that each $C_i$ has 2-norm $\| C_i \|_2 = \sqrt{d}$, if $\mathcal{V}_A$ is chosen to be the convex hull of the $C_i$ and $\mathcal{V}_B$ is chosen to be the convex hull of their transpositions $C_i^\dagger$, then (d) $|\phi_{ij}\rangle$ is $(\mathcal{V}_A, \mathcal{V}_B)$-separable, and (e) $|\phi_{ij}\rangle$ is inseparable with respect to any strict subsets of $\mathcal{V}_A$, $\mathcal{V}_B$.

**Proof.** Parts (a) and (c) are existing results, either following from the calculation of $\| \cdot \|_{\nu, 2}$ in [10], or from the Schmidt decomposition applied to the operator space. However, we will also rederive them as it will help us to prove the remaining parts. First, note that if there is a convex operator decomposition such as

$$
|\phi_{ij}\rangle \langle \phi_{ij}| = \sum_k p_k A_k \otimes B_k,
$$

where $p_k$ is a probability distribution and $A_k \in \mathcal{V}_A$ and $B_k \in \mathcal{V}_B$, then the Hilbert–Schmidt inner product of both sides with the basis of Hermitian operators $C_i \otimes C_j^\dagger$ must match. Expressing $A_k = \sum_i \alpha_{ik} C_i$ and $B_k = \sum_j (\beta_{jk})^* C_j^\dagger$, where $\alpha_k$ and $\beta_k$ (the conjugate is incorporated into the definition for later convenience) are complex expansion vectors representing $A_k$ and $B_k$ respectively, and using $\text{tr}(C_i C_j) = \text{tr}(C_i^\dagger C_j^\dagger) = d$ $\delta_{ij}$ and the identity $\langle \phi_{ij}| X \otimes Y |\phi_{ij}\rangle = \text{tr}(XY)/d$, we must have

$$
\delta_{ij} = d^2 \sum_k p_k \alpha_{ik}^* \beta_{jk}^*.
$$

(17)

All the statements of the theorem are short consequences of the above identity. In particular, summing over the $d^2$ terms involving $i = j$ gives:

$$
d^2 = d^2 \sum_k p_k \sum_i \alpha_{ik}^* \beta_i^* = 1 \sum_k p_k \langle \beta_i^k, \alpha_i^k \rangle,
$$

(18)

where $\langle \beta_i^k, \alpha_i^k \rangle$ represents the inner product. This means that the average of the inner products of $\alpha_i^k$ and $\beta_i^k$ is equal to 1. Hence, by convexity and the Cauchy–Schwarz inequality, it must be the case that $\text{max}_k \| \alpha_i^k \| \| \beta_i^k \| \geq 1$, and hence, using equation (15) and the fact that $\| S \|$ is no less than $| \langle \psi | S | \psi \rangle |$ for one of its elements, gives $\| \mathcal{V}_A \|_{\nu, 2} \| \mathcal{V}_B \|_{\nu, 2} \geq d$, proving (a). If we now restrict our attention to only sets satisfying $\| \mathcal{V}_A \|_{\nu, 2} \| \mathcal{V}_B \|_{\nu, 2} = d$, this means that we must have $\| \alpha_i^k \| \| \beta_i^k \| \leq 1$. Hence, by convexity and the Cauchy–Schwarz inequality, the only way that equation (18) can be true is if the Cauchy–Schwarz inequality is tight, so that $\| \alpha_i^k \| \| \beta_i^k \| = \langle \beta_i^k, \alpha_i^k \rangle = 1 \forall k$. This can only be true if $\beta_i^k$ and $\alpha_i^k$ are proportional, and from $\langle \beta_i^k, \alpha_i^k \rangle = 1$ we get that we must have $\| \beta_i^k \| \| \alpha_i^k \| = \beta_i^k$ for all $k$. This implies (b), and shows that there is a trade-off—the smaller the 2-norm of one state space is, the larger the 2-norm of the other must be.

To see that at least $d^2$ operators are required, let us put the fact that $\| \beta_i^k \|^2 \alpha_i^k = \beta_i^k$ back into equation (17) to get

$$
\delta_{ij} = d^2 \sum_k p_k \| \beta_i^k \|^2 \alpha_i^k \beta_{jk}^* = 1 \sum_k p_k \langle \beta_i^k, \alpha_i^k \rangle,
$$

(19)

where we have defined new unnormalized vectors $\tilde{\alpha}_i^k := \sqrt{p_k} \| \beta_i^k \| \alpha_i^k$. We may now reinterpret this equation in the following way. For fixed $i$ we consider the coefficients $\tilde{\alpha}_i^k$ for varying $k$ to be coefficients of a vector of length $N$, where $N$ (which in principle could be very large) is the number of different values of $k$ in the sum (19). Then equation (19) tells us that we have $d^2$ such vectors of norm $1/d$, and they form an orthogonal set (in the dimension $N$ vector space). For it to be possible to pick $d^2$ orthogonal vectors, $k$ must range over at least $d^2$ values, hence proving (c).

To show (d) note that setting $p_k = 1/d^2$, $\beta_i^k := \delta_{ik}$, and $\tilde{\alpha_i^k} := \delta_{ik}$, trivially satisfies equation (17), showing that (the convex hull of) any orthogonal basis $\{ C_i \}$ of operators satisfying $\text{tr}(C_i C_j) = d$ $\delta_{ij}$ provides suitable choices for $\mathcal{V}_A$ and $\mathcal{V}_B$ (by setting $\mathcal{V}_B = \mathcal{V}_A^\dagger$).

Finally, to show (e) note that for $\lambda \in (0, 1)$ the strict inequality $\| \lambda X + (1 - \lambda) Y \|_2 < \| X \|_2 + \| (1 - \lambda) Y \|_2 \leq \max \{ \| X \|_2, \| Y \|_2 \}$ holds if $X, Y$ are not proportional to each other (this follows from Cauchy–Schwarz, and it does not hold for the trace norm). Hence, no other operators within the convex hull of the $d^2$ operators $C_i$ can attain a 2-norm of $\sqrt{d}$, and hence a strict subset cannot satisfy the necessary condition (b).
These observations provide us with a method of constructing solutions to problems 1 and 2. However, in some contexts it is useful to make further restrictions, e.g. that the operators in $V_A$, $V_B$ are of strictly positive trace or of unit trace. It is straightforward (we describe this later) to include these requirements in the context of the 2-norm. We will use the resulting solutions to construct solutions to problem 3.

In the appendix we prove that parts of theorem 2 also generalize to arbitrary bipartite pure states, providing one solution of problem 2 for all bipartite pure states.

8. Incorporating positive or unit trace

The previous sections show that any orthogonal basis of $d^2$ Hermitian operators normalized to $\text{tr}(C_i C_i) = d$ provides a solution to both problem 1 (in the case of the 2-norm) and problem 2. However, these solutions can in principle contain operators that are not positive for some important forms of generalized positivity. For instance, if an operator has negative or complex trace, then it cannot be in the dual of any POVM. So we would like to consider adding a constraint that the trace is positive. In this section we show how this can be done straightforwardly for maximally entangled states.

To obtain such solutions we simply need to find bases of Hermitian operators with positive trace. This can be done using the Gram–Schmidt process. If we start from any Hermitian basis $C_i$ for which the first element is the identity $C_1 = 1$, and the remaining $C_i$ are traceless, then imposing the requirement that $V_A$, $V_B$ contain Hermitian operators with positive trace amounts to demanding that the expansion vectors $\alpha^k$, $\beta^k$ are real, and that their first components are positive numbers. If we consider only solutions that are constructed as the convex hull of $d^2$ orthogonal operators of 2-norm $\sqrt{d}$, then finding the appropriate vectors $\alpha^k$, $\beta^k$ is equivalent to picking a $d^2 \times d^2$ real orthogonal matrix such that the top row consists of real positive coefficients, and can be solved using the Gram–Schmidt procedure.

In the next section we will need to use solutions that are not only of positive trace, but of unit trace. We can obtain such solutions in the same way: if we consider only solutions that are constructed as the convex hull of $d^2$ orthogonal operators of 2-norm $\sqrt{d}$, then finding the appropriate vectors $\alpha^k$, $\beta^k$ is equivalent to picking a $d^2 \times d^2$ real orthogonal matrix such that the top row consists of $(1/d, 1/d, 1/d, \ldots)$, and this can also be solved using the Gram–Schmidt procedure.

Amongst these unit trace solutions there exists one type that is already widely used in the construction of classical models: the $d^2$ subsets of the phase point operators [18] that describe discrete Wigner functions. Each such subset provides a Hermitian unit trace orthogonal basis of the correct norm. In the case of $d = 2$ it can be shown that the only unit trace Hermitian operator basis satisfying $\text{tr}(C_i C_i) = 2$ are tetrahedra that are unitary rotations or transpositions of the example presented in figure 2. However, for higher dimensions $d > 2$, there are inequivalent solutions that do not share the same spectrum and hence are not unitarily equivalent to subsets of phase point operators. Our analysis shows that any quantum measurements in the dual of such sets will have local hidden variable models for the maximally entangled state, going beyond constructions available via a discrete Wigner function approach.

9. Solutions to problem 3 for the maximally entangled state

In this section we show that conic hulls generated from the unit trace operator bases in the previous section can enable us to provide solutions to problem 3. The strategy of our solutions to problems 1 and 2 was to show that if the maximally entangled state is separable with respect to given state spaces, then there must be operators in those state spaces of a big enough norm. As convex cones contain operators of arbitrary norm, we cannot apply this strategy to problem 3 without modification. We will get around this problem by restricting our attention to cones that can be generated as the conic hulls of convex sets of operators with unit trace. We will argue that these convex sets cannot be made smaller while preserving separability, and thereby also argue that the convex cones cannot be made smaller while preserving separability.

Let $W_A$, $W_B$ denote any set of unit trace orthogonal basis operators constructed in the previous section, and let $Q_A$, $Q_B$ denote the local quantum states on systems $A$, $B$ respectively. Consider $\text{coni}(W_A \cup Q_A)$ and $\text{coni}(W_B \cup Q_B)$. As the generators of these conic hulls all have strictly positive trace, all operators in the resulting cones will have strictly positive trace except for the 0 operator. This means that we can assume that any cone-separable decomposition of the maximally entangled state:

$$|\phi_d\rangle \langle \phi_d| = \sum_k p_k A_k \otimes B_k, \quad A_k \in \text{coni}(W_A \cup Q_A), \quad B_k \in \text{coni}(W_B \cup Q_B)$$

only contains local operators on the right-hand side that have strictly positive trace (any contribution from the trivial 0 operator can be discarded). Hence by dividing the operators on the right-hand side by their trace, we
may recover a separable decomposition in terms of only unit trace operators from the cones:

\[
\left| \phi_\beta \right\rangle \langle \phi_\beta \right| = \sum_k p_k \frac{\text{tr}(A_k)\text{tr}(B_k)}{\text{tr}(A_k) \otimes \text{tr}(B_k)} A_k \otimes B_k
\]

(in this equation it is easy to verify that \( p_k \text{tr}(A_k)\text{tr}(B_k) \) will be a probability distribution from the normalization of \( \left| \phi_\beta \right\rangle \langle \phi_\beta \right| \)). This means that if a state is separable with respect to the conic hulls of operators with strictly positive trace, then the state is also separable with respect to the convex subsets of the cones consisting of only unit trace operators.

To these convex subsets we may now apply theorem 2. In order for such a separable decomposition (20) to exist for the maximally entangled states, then we know that the unit trace operators on the rhs must have a minimum 2-norm of \( \sqrt{d} \). Note that any unit trace operator in the conic hulls must be a convex combination of the unit trace generators. Using the fact that for the 2-norm the strict inequality \( \|AX + (1 - \lambda)Y\|_2 < \|AX\|_2 + \|(1 - \lambda)Y\|_2 \leq \max \{\|X\|_2, \|Y\|_2\} \) holds if \( X, Y \) are not proportional to each other, we hence see that the normalized operators appearing in equation (20) must be precisely the operators from \( \mathcal{W}_A, \mathcal{W}_B \), because the quantum states have a 2-norm that is too small (their 2-norm is equal to the 2-norm of the vector of eigenvalues, and hence is \( \leq 1 \)). The only unit trace member of the conic hulls with a high enough 2-norm of \( \sqrt{d} \) are hence the \( \mathcal{W}_A, \mathcal{W}_B \)—all the extremal points of the original sets \( \mathcal{W} \) are needed for the separable decomposition because all other unit trace operators have a 2-norm that is strictly less than \( \sqrt{d} \), thereby violating the requirement of theorem 2 part (b). Hence the conic hull state spaces \( \text{coni}(\mathcal{W}_A \cup \mathcal{Q}_A) \) and \( \text{coni}(\mathcal{W}_B \cup \mathcal{Q}_B) \) cannot be made smaller, as they must contain the \( \mathcal{W}_A, \mathcal{W}_B \) as well as the local quantum states. Hence we have the following.

**Theorem 3.** Consider \( \text{coni}(\mathcal{W}_A \cup \mathcal{Q}_A) \) and \( \text{coni}(\mathcal{W}_B \cup \mathcal{Q}_B) \) where \( \mathcal{W}_A, \mathcal{W}_B \) give a unit trace solution to problem 2 for the maximally entangled state. Then \( \text{coni}(\mathcal{W}_A \cup \mathcal{Q}_A) \) and \( \text{coni}(\mathcal{W}_B \cup \mathcal{Q}_B) \) is a solution to problem 3 for the maximally entangled state.

This implies that if we consider any two unitarily inequivalent \( \mathcal{W} = (\mathcal{W}_A, \mathcal{W}_B) \) and \( \mathcal{W}' = (\mathcal{W}'_A, \mathcal{W}'_B) \) that have been constructed for problem 2, as is possible for \( d > 2 \), then the separable decomposition resulting from the conic hulls of these states with the quantum states will supply LHV models for distinct and unitarily inequivalent sets of measurements. In this sense our constructions generalize the local hidden variable models that one can construct from discrete Wigner functions.

Figure 3 depicts (a) the convex hull of \( \mathcal{W}_A \cup \mathcal{Q}_A \), and (b) its dual, when \( d = 2 \). Operationally this means that the qubit Bell state \( |\phi^+\rangle \) has a local hidden variable model set of POVMs \( M_A \) on A and \( M_B = M_B^0 \) on B, where the elements of \( M_A \) are proportional to \( 1 + r \cdot \sigma \) and \( r \) is a vector from the convex set in figure 3(b).

**10. Conclusions**

We have determined local state spaces that admit a separable decomposition of an entangled pure state \( |\psi\rangle \) and cannot be made strictly smaller while maintaining separability. In the context of maximally entangled states, in particular where the local state spaces can be chosen to have unit trace, this has applications in constructing local hidden variable models.
Our measure of ‘smallest’ state space is given by the operator 2-norm not only because it renders the optimization of problem 1 analytically tractable, but also because it enables solutions of problem 2 and problem 3. We do note, however, that using the trace norm would be more natural when searching for states spaces of operators that are not very negative; further work is required to explore this option.

We have made a connection between cross norms and generalized separability, and it is likely that these connections can be generalized when considering other notions of positivity for the local state spaces.

It will also be interesting to know whether it is possible to extend the method from the bipartite to the multipartite case, where very little is known about classical models for quantum states.

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Appendix. A solution to problem 2 for bipartite pure states

We may obtain a solution to problem 2 for general bipartite pure states by applying similar considerations to the maximally entangled case. Consider a bipartite pure state written in Schmidt form:

$$|\psi\rangle = \sum_{i} \lambda_{i} |i\rangle,$$

with $\lambda_{i} \geq 0$. We assume that the Schmidt rank is maximal, else we truncate the local quantum state spaces to dimension $d$, where $d$ is the Schmidt rank. Using the Schmidt basis $\{|i\rangle\}$, we may construct an orthogonal basis for the local operator space consisting of the $d^2$ operators:

$$C_{ij} = |i\rangle \langle j|,$$

note that $\text{tr}(C_{ij}C_{kl}^{T}) = \delta_{ij}\delta_{kl}$. Suppose that we have a separable decomposition of $|\psi\rangle$ as follows:

$$|\psi\rangle \langle \psi| = \sum_{k=1}^{N} p_{k} A_{k} \otimes B_{k}.$$

Let us decompose the local operators as $A_{k} = \sum_{g} \alpha_{g}^{k} C_{g}$ and $B_{k} = \sum_{g} \langle \beta_{g}^{k} \rangle^{*} C_{g}^{T}$. Using these definitions we may compute

$$\langle \psi| C_{gh} \otimes C_{ij} |\psi\rangle = \lambda_{k} \lambda_{l} \delta_{gh,ij},$$

$$= \sum_{k=1}^{N} p_{k} \alpha_{g}^{k} \langle \beta_{l}^{k} \rangle^{*}. \quad (A.1)$$

Summing the equation over $g = i$, $h = j$ gives

$$\left(\sum_{g} \lambda_{g}\right)^{2} = \sum_{k} p_{k} \langle \beta_{k}^{\dagger} , \alpha_{k}^{\dagger} \rangle, \quad (A.2)$$

where $\alpha_{k}$ and $\beta_{k}$ are $d^2 \times 1$ vectors of coefficients $\alpha_{g}^{k}$ and $\beta_{g}^{k}$ respectively, and $\langle \beta_{k}^{\dagger} , \alpha_{k}^{\dagger} \rangle$ symbolizes their inner product. If we now make the restriction that the $\alpha_{k}$, $\beta_{k}$ corresponding to the local operators satisfy $\|\alpha_{k}\|_{2}, \|\beta_{k}\|_{2} \leq \sum_{g} \lambda_{g}$, then by Cauchy–Schwarz the only way that equation (A.2) can be true is if each $\alpha_{k}$ and $\beta_{k}$ are equal, and they all have 2-norm equal to $\sum_{g} \lambda_{g}$. Note that in terms of the operators we have that $\| A_{k} \|_{2} = \sqrt{\text{tr} |A_{k}^{\dagger} A_{k}|} = \| \alpha_{k} \|_{2},$ and similarly $\| B_{k} \|_{2} = \sqrt{d} \| \beta_{k} \|_{2},$ and so this condition can also be expressed as $\| A_{k} \|_{2}, \| B_{k} \|_{2} = \sum_{g} \lambda_{g}$. We may place the restriction back into equation (A.1) to get

$$\langle \psi| C_{gh} \otimes C_{ij} |\psi\rangle = \lambda_{k} \lambda_{l} \delta_{gh,ij},$$

$$= d^2 \sum_{k=1}^{N} p_{k} \alpha_{g}^{k} \langle \beta_{l}^{k} \rangle^{*}. \quad (A.3)$$

We are looking for solutions of this equation under the constraint that $\| \alpha_{k} \|_{2} = \sum_{g} \lambda_{g}$. This equation may be reinterpreted as an orthogonality relation between $d^2$ vectors labeled by $i$, $j$, with $N$ components in each vector (the size of the range of $k$). Hence we need at least $N \geq d^2$ orthogonal vectors of dimension $d^2$.

We are now in the following position: if we can find a solution to equation (A.3) involving $d^2$ operators such that each $\| \alpha_{k} \|_{2} = \sum_{g} \lambda_{g}$ then in analogy to the maximally entangled case, such a separable decomposition
will be a solution to problem 2, as no other set of operators in the convex hull will have enough operators of high enough norm.

We now exhibit such a separable decomposition. Define the operator $A^g$ as:

$$A^g := |i\rangle \langle j| \left( \sum_x \lambda_x \right).$$

It is easy to check that the 2-norm of these operators is $\sum \lambda_x$. If we define a probability distribution over $i, j$ by

$$p_{ij} := \frac{\lambda_i \lambda_j}{\left( \sum_x \lambda_x \right)^2},$$

then it is not difficult to check that

$$\sum_{i,j} p_{ij} A^g \otimes A^g = |\psi\rangle \langle \psi|.$$

Although this is a solution to problem 2 for general bipartite pure states, it has the disadvantage that the operators $A^g$ are only in the dual of measurements in the computational basis. In future work it will be interesting to explore whether alternative solutions are possible.

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