Convexity and the Separability Problem of Quantum Mechanical Density Matrices

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9 March 2001

Abstract

A finite dimensional quantum mechanical system is modeled by a density $\rho$, a trace one, positive semi-definite matrix on a suitable tensor product space $H^{[N]}$. For the system to demonstrate experimentally certain non-classical behavior, $\rho$ cannot be in $S$, a closed convex set of densities whose extreme points have a specified tensor product form. Two mathematical problems in the quantum computing literature arise from this context: (1) the determination whether a given $\rho$ is in $S$ and (2) a measure of the “entanglement” of such a $\rho$ in terms of its distance from $S$. In this paper we describe these two problems in detail for a linear algebra audience, discuss some recent results from the quantum computing literature, and prove some new results. We emphasize the roles of densities $\rho$ as both operators on the Hilbert space $H^{[N]}$ and also as points in a real Hilbert space $M$. We are able to compute the nearest separable densities $\tau_0$ to $\rho_0$ in particular classes of inseparable densities and we use the Euclidean distance between the two in $M$ to quantify the entanglement of $\rho_0$. We also show the role of $\tau_0$ in the construction of separating hyperplanes, so-called entanglement witnesses in the quantum computing literature.

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*Part of the research for this paper was done at the Centre for Quantum Computation at Oxford, and their hospitality is gratefully acknowledged.

†Support for this work was provided by the Office of Naval Research and ARDA-NSA
1 Introduction

The idea of using quantum mechanical systems as computing devices arose during the early 1980s, and examples of the theoretical efficacy of such devices were soon developed. However, the subject remained primarily a topic in the theoretical computer science and physics communities until 1994 when Peter Shor published a quantum algorithm for factoring a large composite integer $N$. Since his algorithm was polynomial rather than exponential in the number of digits of $N$, it showed that a prospective quantum computer could factor $N$ more efficiently than was (or is) known to be possible on a classical computer. As a result quantum versions of algorithms, information theory and computational complexity have become subjects of widespread theoretical study, and efforts to actually construct physical systems which could serve as components of a quantum computer have become a recognized and active part of experimental physics.

By its very nature, the field of quantum computation and quantum information theory is highly interdisciplinary and intersects with a variety of sub-specialities in mathematics, computer science, physics and even in philosophy. The purpose of this paper is to describe one particular problem in the field of quantum computation which should be of particular interest to the linear algebra community, and the rest of the paper is devoted to a mathematical overview of this topic and to the presentation of some new results. For the reader who would like more background in the subject of quantum computation, [18] is an early survey article while [21, 24, 28] contain descriptions of the subject and additional references. Other introductory material can be found on various web sites such as that maintained by the Centre for Quantum Computation at Oxford University [7].

In the next section we give the mathematical notation necessary to describe the separability problem, which is related to the physical problem of constructing a system that produces non-classical phenomena. Essentially, the mathematical context is one of two nested compact convex sets and the determination whether a point in the larger set is in the smaller set. In section 3 we briefly describe the issue of quantifying non-separability or “entanglement” and settle on a measure which is the Euclidean distance of a point to the smaller convex set. In section 4 we present some basic topological results related to the separability problem, and in section 5 we develop the role of orthogonality in the analysis. Section 6 deals with separating hyperplanes, called entanglement witnesses in the quantum computing literature, and relates them to the earlier analysis. The last two sections deal with very specific situations in which all of the computations can be carried out explicitly and which were motivated by basic examples in the quantum mechanics literature.

For those familiar with related work in the quantum computing community, we have emphasized convexity and the geometry of the underlying Hilbert space to provide a useful perspective of the separability problem and related topics such as entanglement witnesses. We have also shown how the resulting geometric insight facilitates the extension of results in [34] as well as the ex-
licit computation of the nearest separable density to certain given inseparable densities.

2 Notation and the separability problem

Here is the context. Let $H^{(N)}$ denote an $N = d_1 \times \cdots \times d_n$ dimensional complex Hilbert space defined as the tensor product $H^{(d_1)} \otimes \cdots \otimes H^{(d_n)}$. $M$ is the real Hilbert space of $N \times N$ Hermitian matrices over $H^{(N)}$ with a real inner product defined by

$$\langle\langle A, B \rangle\rangle = Tr(A^\dagger B) = \sum_{j,k} (a^\dagger_{jk} b_{kj}) = \sum_{j,k} (a_{jk} b_{kj})$$

which is independent of the particular orthogonal basis of $H^{(N)}$ used to define the matrix elements. $D$ denotes the compact, convex subset of densities; that is, $\rho$ in $D$ is a positive semidefinite, trace one, $N \times N$ Hermitian matrix which can be interpreted as the state of an $n$-particle system where the $k$'th particle has $d_k$ levels. The separable states (densities) comprise a compact convex subset $S$ of $D$, and $S$ is defined as the closed convex hull of the separable projections $\otimes_k |\psi_k\rangle \langle \psi_k|$. In this paper we will consistently use Dirac notation, so that a ket $|\psi_k\rangle$ denotes a column vector in the $d_k$ dimensional Hilbert space $H^{(d_k)}$ and the bra $\langle \psi_k|$ is a $d_k$-long row vector whose entries are the complex conjugates of those of $|\psi_k\rangle$. The outer product $|\psi_k\rangle \langle \psi_k|$ is a rank 1, $d_k \times d_k$ matrix, and the inner product of $|\psi\rangle$ and $\langle \varphi|$ is denoted by the bracket $\langle \varphi| \psi\rangle$. In the physics literature the term pure state is sometimes used for both the rank one density $|\psi\rangle \langle \psi|$ and the ket $|\psi\rangle$. Usually the meaning is clear from the context. (For an introduction to this notation in the context of quantum computing, see for example [24].)

It follows that the densities in $D$ and $S$ are both operators on the Hilbert space $H^{(N)}$ and also points in a real Hilbert space $M$. It is that dual role which underlies our analysis.

When the system of $n$ particles is modelled by densities not in $S$, some striking quantum effects can be observed. Thus, physical experiments need to be designed so that the resulting density is in $D - S = D \cap S^c$. The related separability problem is the mathematical question of how to determine if a given density $\rho$ is in $S$.

This is not an easy question to answer in this generality, and a simple example illustrates the difficulty. Consider a system with two 2-level particles, that is to say two “quantum bits” or qubits, so that $N = 4$ and $H^{(4)} = H^{(2)} \otimes H^{(2)}$. For this example choose $\rho_0 = |\psi_0\rangle \langle \psi_0|$ where $|\psi_0\rangle = \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle)$ and we are using the usual binary notation for two level systems. Thus, $\rho_0$ is a $4 \times 4$ matrix with 1/2 in the four corners and 0’s elsewhere.

Define $\rho(s) = (1 - s) D_0 + s \rho_0$, where here and throughout the paper we let the density $D_0$ denote the “normalized” identity of suitable dimension, $\frac{1}{N} I$. It is easy to show that $\rho(0) = D_0$ is in $S$ and, since $\rho_0$ is a projection and thus an
extreme point in $D$, that $\rho(1) = \rho_0$ is not in $S$. Thus there is an intermediate value $s_0$ such that $\rho(s_0)$ is in $S$ and $\rho(s) \notin S$ for $s_0 < s \leq 1$.

Peres (23) has observed that a necessary condition for a density to be separable is that its partial transposes are densities, where the $s$'th partial transpose of a density $\rho$ in a given basis respecting the tensor product is defined by

$$\rho^t_s (j_1 \ldots j_s \ldots j_n, k_1 \ldots k_s \ldots k_n) = \rho (j_1 \ldots k_s \ldots j_n, k_1 \ldots j_s \ldots k_n).$$

(2.2)

(Technically we probably should call this part of a generalized Peres condition, but that seems a bit fussy.) The necessity of the Peres condition is easy to confirm. If $\rho_s$ is a trace one, positive semidefinite matrix on $H^{(d_s)}$, then so is its (ordinary) transpose $\rho_s^t$. It then follows that the $s$'th partial transform of the separable density $\rho_1 \otimes \ldots \otimes \rho_n$ is separable, and thus if $\rho$ is a convex combination of separable densities, $\rho = \sum a_\rho a \rho_a$, the $s$'th partial transpose of $\rho$ is also in $S$. In fact for the $2 \times 2$ and $2 \times 3$ tensor product cases the Peres condition is also sufficient (11). Using that result it easy to see that for the two qubit example $s_0 = 1/3$, and in fact it is possible to find an explicit separable representation of $\rho(1/3)$, as noted below and in [25] for example. (Related and earlier references include [5, 6, 37, 41].) We discuss this example in more detail below, but suffice it to say here that the eigenvalues of $\rho(1/3)$ are strictly positive so that $\rho(1/3)$ is in the relative interior of $D$.

3 Measures of entanglement

A second theme of recent research has been to find a way to quantify the non-separability or entanglement of a system with density $\rho$. There has also been extensive work in this area, and some representative papers describing various approaches and basic properties which an entanglement measure should possess include [3, 4, 12, 33, 34, 35, 36] among others. The motivation for such a measure is the recognition that entanglement constitutes a resource which can be used operationally in communications. A prime example is teleportation in which two different parties who share the state $|\psi_0\rangle = \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle)$ are able to transfer an arbitrary quantum state $\alpha |0\rangle + \beta |1\rangle$ from one party to the other using classical communication and “local” operations. Figuratively this means that $H^{(d_1)}$ with $d_1 = 2$ is identified with one party, typically denoted as Alice, while $H^{(d_2)}$ with $d_2 = 2$ is identified with a second party, typically denoted as Bob. Alice and Bob can perform operations on their own components of $H^{(N)} = H^{(d_1)} \otimes H^{(d_2)}$ and can communicate classically which operations they performed and whatever information they obtained from their operations.

An example of teleportation is the following. An arbitrary quantum state $|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$ in a third Hilbert space is available to Alice. Without actually knowing $|\psi\rangle$ she performs operations on that state and on $H^{(d_1)}$ and, using classical communication, transmits the results of a measurement to Bob who can then recreate $|\psi\rangle$ in $H^{(d_2)}$, again without knowing $|\psi\rangle$. (For references and discussions see for example [2, 3, 21].)
Two of the measures of entanglement for bipartite states which have been motivated in part by teleportation are the measure of formation and the measure of distillation (see for example [3, 4, 40]). The respective contexts concern the creation of a state from pure states and “distilling” the maximum number of entangled states of the form \( |\psi_0\rangle = \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle) \) from copies of a given density \( \rho \). In a sense these particular measures can be considered as operational measures, since they deal with the creation of a mixed state or the extraction of maximally entangled pairs.

The definition of a measure of entanglement as an infimum of “distance” from \( S \) was introduced in [34] with an expanded discussion in [35]. Other authors, particularly [33, 36], took an axiomatic approach and also discussed basic properties that such a measure should possess, motivated in part by interpreting the operations in teleportation and distillation as mappings of densities in \( M \).

(For an alternate approach to entanglement using “robustness of entanglement” see [33].)

As a paradigm based on [34], we give the motivation (and terminology) for requiring that a measure of entanglement \( E \) satisfy the following three properties:

\[
\begin{align*}
\text{(a)} & \quad E[\rho] = 0 \text{ if and only if } \rho \in S, \\
\text{(b)} & \quad E[U \rho U^\dagger] = E[\rho] \text{ where } U \text{ is a local unitary mapping}, \\
\text{(c)} & \quad E[\Phi(\rho)] \leq E[\rho] \text{ where } \Phi \text{ is a local, completely positive, trace preserving operator on } D.
\end{align*}
\]

The motivation for the first property is obvious if one is measuring non-separability. A local unitary mapping \( U \) is a tensor product of unitary maps on the constituent product spaces and models the unitary transformations, such as a change of local basis, that could be taken independently on the individual spaces. Property (b) requires that entanglement should remain the same under such mappings. A completely positive trace preserving operator \( \Phi \) on \( D \) models the measurement process and can be represented [30] as

\[
\Phi(\rho) = \sum_k V_k \rho V_k^\dagger \quad \text{where} \quad \sum_k V_k^\dagger V_k = I.
\]

It is easy to confirm that \( \Phi \) maps \( D \) into \( D \). Locality is imposed by either assuming \( V_k \) is a tensor product of operators on the constituent spaces or else by simply assuming that \( \Phi \) also maps \( S \) into \( S \). The point of axiom (c) is that one should not be able to increase entanglement under local operations.

We mentioned above that the normalized identity \( D_0 \) is a separable state, and it is obvious that \( D_0 \) can be written as an (equally weighted) convex combination of any \( N \) orthogonal projections, each of which could be entangled. For example, in the two qubit case \( D_0 \) can be written as the average of the densities defined by the four orthogonal “Bell states” \( \frac{1}{\sqrt{2}} (|00\rangle \pm |11\rangle) \) and \( \frac{1}{\sqrt{2}} (|01\rangle \pm |10\rangle) \). Thus one could expect that a measure of entanglement would recognize the decrease
of entanglement under convex combinations and satisfy

$$(d) \quad E \left[ \sum p_a \rho_a \right] \leq \sum p_a E [\rho_a].$$

This property is not a standard requirement, although it is just the triangle inequality for distances, and it can be shown [35] that some of the proposed measures automatically satisfy (d).

Since our goal here is to gain insight into the geometry of the separable densities, we will not give a complete account of the various measures of entanglement which have been proposed but instead will use the measure of non-separability which comes naturally from the Hilbert space structure of $M$. Invoking the idea of minimal distance from $S$ [35], we use the Frobenius or Hilbert-Schmidt norm and define a measure of entanglement as the minimal distance of a density $\rho$ from the set of separable states:

$$m [\rho] = \inf_{\tau \in S} \| \rho - \tau \| = \inf_{\tau \in S} \sqrt{\text{Tr} (\rho - \tau)^2).} \quad (3.1)$$

This measure has been already been considered as a possible measure of entanglement by other authors such as [19, 35, 39], but since it does not seem to relate to operational uses of entanglement between parties, it has not been widely used. However, it is easy to show that $m$ satisfies most of the properties discussed above. For example $m [\rho] = 0$ if and only if $\rho$ is in $S$, and it is easy to check that $m [U \rho U^{-1}] = m [\rho]$ for all local unitary operations. $m$ also satisfies (d). Let $\rho = \sum_a p_a \rho_a$ and suppose $m [\rho_a] = \| \rho_a - \tau_a \|$. Then by the definition and the triangle inequality

$$m [\rho] \leq \left\| \sum p_a (\rho_a - \tau_a) \right\| \leq \sum p_a \| \rho_a - \tau_a \| = \sum p_a m [\rho_a].$$

Although it does not seem to be known whether $m$ satisfies condition (c) as stated, see [24, 35, 39] for discussions of this point, $m$ does satisfy a special case of (c) when $\Phi$ models a von Neumann measurement. Specifically, we also assume that $\{V_k\}$ is a complete set of orthogonal projections which map $S$ to $S$ and let $\hat{\rho} = \Phi (\rho)$. If $\tau_0$ is the nearest separable density to $\rho$, then

$$\| \Phi (\rho) - \Phi (\tau_0) \|^2 = \text{Tr} \left( \sum_j \sum_k V_j (\rho - \tau_0) V_j^\dagger V_k (\rho - \tau_0) V_k^\dagger \right)$$

$$= \text{Tr} \left( \sum_j (\rho - \tau_0) V_j^\dagger (\rho - \tau_0) \right) \leq \| \Phi (\rho) - \Phi (\tau_0) \| \cdot \| \rho - \tau_0 \|.$$

Thus $m [\hat{\rho}] \leq \| \Phi (\rho) - \Phi (\tau_0) \| \leq \| \rho - \tau_0 \| = m [\rho]$ as advertised. Since the inner product structure of $M$ also gives geometric insights to aspects of the separability problem, as shown for example in Witte and Truck's paper [39], we shall use $m$ as the measure of choice in this paper.
As a final remark on the issue of measures of entanglement, we note that Vedral and Plenio [35] suggested that condition (c) be replaced by

\[(c') \sum_k p_k E[\rho_k] \leq E[\rho]\]

where the \(\rho_k\)'s are particular densities derived from \(\rho\) via \(\Phi\):

\[\rho_k = \frac{1}{p_k} V_k \rho V_k^\dagger \text{ with } p_k = \text{Tr} \left( V_k \rho V_k^\dagger \right).\]

They give a reasonable motivation for this stronger condition, but it should be noted that if \(\rho = \sum_k p_k \rho_k\) to begin with and if \(\Phi\) is a von Neumann measurement leaving each \(\rho_k\) unchanged, then if \(E\) also satisfies the convexity property (d), \(E\) has to be linear in this case:

\[E[\rho] = \sum_k p_k E[\rho_k].\]

A measure based on relative entropy does satisfy this condition [35], but it is too strong a condition for the Frobenius norm.

### 4 Basic Theory

In each of the \(n\) Hilbert spaces \(H^{(d_k)}\) defining \(H^{(N)}\) we can define an orthogonal basis which arises from the physical properties of the \(d_k\)-level system we are modelling. In the quantum computation literature this is called the computational basis, and tensor products of these basis vectors define a basis for \(H^{(N)}\). If we define projection operators on each of the \(H^{(d_k)}\), then their tensor products are the separable projections \(\otimes_k |\psi_k\rangle \langle \psi_k|\) whose convex hull is \(S\). More generally, if we take a basis for the \(d_2^N\) dimensional space of linear operators on \(H^{(d_k)}\), then their tensor products define a basis for the \(N^2\) dimensional space \(M\).

Now it was shown in [26] that one can take what amounts to a discrete Fourier transform of a suitable arrangement of such product basis matrices and obtain a particular orthogonal unitary basis \(\{S_{(j,k)}\}\) for \(M\) which is indexed by pairs \((j, k)\) of \(n\)-long vectors \(j, k\). Using coordinate-wise addition, the set of indices defines an Abelian group \(G\) of order \(N\), and \(\{S_{(j,k)}\}\) turns out to be a projective representation of \(G \times G\). The \(S_{(j,k)}\) are unitary matrices and need not be in \(M\); rather they serve as a basis of \(N \times N\) matrices over the complex numbers. The reader is referred to [28] for details of the construction, and we limit ourselves here to recording the results we need. (See [14, 15]. We also note that Werner [38] shows the close connections among orthogonal unitary bases, dense coding and teleportation, all topics of great interest in quantum computing.)

Using \(e\) to denote \((0, 0)\) and \(a\) as a generic index \((j, k)\), the unitary matrices in \(\{S_a\}\) have the following properties: (1) \(S_e = I\), the \(N \times N\) identity, (2) \(\text{Tr} (S_a^\dagger S_a) = N\delta(a, b)\), and (3) \(S_a\) has the spectral representation
where the $P_{a,k}$ are separable orthogonal projections. Since $S_a$ is unitary, $\sum_k P_{a,k} = I$ and $|\lambda_{a,k}| = 1$. Since $\{S_a\}$ is a basis, a density $\rho$ in $D$ can be expressed as $\frac{1}{N} \sum_a s_a S_a$, and the last particular property is that $|s_a| \leq 1$ and $s_e = 1$.

It has been shown in a number of papers, initially in [41] and also in [5, 19, 26] for example, that there is an open neighborhood of the normalized identity $D_0$ which is composed entirely of separable densities. Using the properties of $\{S_a\}$ we give a short proof.

**Proposition 4.1** If $\rho$ is a density with $\sum_{a \neq e} |s_a| \leq 1$, then $\rho$ is separable. In particular, there exists an open neighborhood of $D_0$ composed of separable states.

**Proof**: Since $\rho$ is Hermitian, $\rho = \frac{1}{2} (\rho + \rho^\dagger)$. Using the various properties listed above we have

$$
\rho = \frac{1}{N} \left[ S_e + \frac{1}{2} \sum_{a \neq e} (s_a S_a + \bar{s}_a S_a^\dagger) \right] = \frac{1}{N} \left[ S_e + \sum_{a \neq e} \sum_k \frac{1}{2} (s_a \lambda_{a,k} + \bar{s}_a \bar{\lambda}_{a,k}) P_{a,k} \right] = \left( 1 - \sum_{a \neq e} |s_a| \right) \frac{1}{N} S_e + \sum_{a \neq e} \sum_k |s_a| \frac{1}{N} (1 + \cos (\theta_{a,k})) P_{a,k},
$$

where $\frac{1}{2} (s_a \lambda_{a,k} + \bar{s}_a \bar{\lambda}_{a,k}) = |s_a| \cos (\theta_{a,k})$. Since $1 + \cos (\theta_{a,k}) \geq 0$, we have written $\rho$ explicitly as a convex combination of separable densities, and thus $\rho$ is in $S$. For the last assertion the condition $\sum_{a \neq e} |s_a| < 1$ defines a relatively open set in $D$. □

In order to determine if an individual density is separable using this criterion, one has to compute each of the coefficients $s_a$. Two weaker but user friendly corollaries are immediate consequences, however.

**Corollary 4.2** If $\epsilon < \left( N^2 - 1 \right)^{-1}$, then $\{(1 - \epsilon) D_0 + \epsilon \sigma, \sigma \in D\}$ is a relatively open set of densities in $S$.

**Proof**: Let $\mu$ denote a density $(1 - \epsilon) D_0 + \epsilon \sigma$, so that the $a \neq e$ coefficient of $\mu$ is $\epsilon s_a$ where $s_a$ is the corresponding coefficient of $\sigma$. Since $\epsilon < \left( N^2 - 1 \right)^{-1}$, $\sum_{a \neq e} \epsilon |s_a| < 1$ and $\mu$ is separable. □

Generally speaking it does not appear that the eigenvalues and eigenvectors of a density are useful in distinguishing a separable from a non-separable state. One counterexample is the following result which is not particularly strong but which has an easy proof.

**Corollary 4.3** If the smallest eigenvalue of a density $\rho$ is at least $\frac{1}{N^2 - 2}$, then $\rho$ is separable.
Proof: We can use the spectral representation of $\rho$, obtaining

$$
\rho = \sum_k \left( \lambda_k - \frac{1}{N+t} \right) |\psi_k\rangle \langle \psi_k| + \frac{N}{N+t} \sum_k \frac{1}{N} |\psi_k\rangle \langle \psi_k| + \frac{N}{N+t} \sum_k \alpha_k |\psi_k\rangle \langle \psi_k|
$$

where $0 \leq \alpha_k = \frac{\lambda_k(N+t)-1}{t}$. Thus $\mu = \sum_k \alpha_k |\psi_k\rangle \langle \psi_k|$ is a density. In the unitary basis

$$
\rho = \frac{1}{N} \left[ S_e + \frac{t}{N+t} \sum_{a \neq e} s_a S_a \right]
$$

where the $s_a$ are the $\{S_a\}$ coefficients of $\rho$. Then

$$
\frac{t}{N+t} \sum_{b \neq e} |s_b| \leq \frac{t}{N+t} (N^2 - 1) \leq 1
$$

showing that $\rho$ is separable. □

As an example of Proposition 4.1, one can use the definition of the $S_a$’s as in [25] to show that the $s_a$ coefficients of the two qubit density $\rho(s)$ defined above satisfy $\sum_{a \neq e} |s_a| = 3s$. Thus $s \leq \frac{1}{3}$ is also a sufficient condition for separability, and one does not need the Horodecki-Peres result. Our main application of the preceding proposition, however, is to characterize densities in the relative interiors of $S$ and $D$.

**Proposition 4.4** A density $\rho$ in $S$ is in the relative interior of $S$ if and only if there exists a $t > 0$ such that $(1 + t) \rho - t D_0$ is in $S$. The same assertion holds if $S$ is replaced by $D$ throughout.

Proof: Suppose that $\mu = (1 + t) \rho - t D_0$ is in $S$. Then for any $\sigma$ in $D$

$$
\frac{1}{1+t} \mu + \frac{t}{1+t} (D_0 + \epsilon (\sigma - D_0)) = \rho + \frac{t \epsilon}{1+t} (\sigma - D_0)
$$

is also in $S$ provided $\epsilon < (N^2 - 1)^{-1}$. Conversely, if $\rho$ is in the relative interior of $S$, then for small $\delta$, $\rho + \delta (\sigma - D_0)$ is in $S$ for all $\sigma$ in $D$ so that choosing $\sigma = \rho$ gives a separable density $\mu = (1 + \delta) \rho - \delta D_0$. The same proof works if $S$ is replaced by $D$. □

The use of a line segment connecting a density with the normalized identity $D_0$ turns out to be a helpful tool in the analysis. Accordingly we shall refer to $(1 + t) \rho - t D_0$ as an entanglement probe and note that Vidal and Tarrach [33] made extensive use of entanglement probes in defining and investigating a “robustness” of entanglement for densities. Two easy applications show both the utility of entanglement probes and the contrast between $S$ and $D$. 

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Corollary 4.5 A density $\rho$ is on the boundary of $D$ if and only if $\rho$ has a zero eigenvalue. If $\rho$ is in $S$ and rank($\rho$) $< N$, then $\rho$ is on the boundary of $S$ and also of $D$.

Proof: If $\rho |\psi\rangle = 0 |\psi\rangle$, then $(1 + t) \langle \psi | \rho | \psi \rangle - t \langle \psi | D_0 | \psi \rangle < 0$ and $\mu = (1 + t) \rho - tD_0$ is not positive semidefinite. Conversely, if the eigenvalues of $\rho$ are bounded below by $s > 0$, then $\rho$ can be written as

$$\rho = (1 - sN) \sum_k \frac{\lambda_k - s}{1 - sN} |\psi_k\rangle \langle \psi_k| + sN D_0$$

and since $sN \leq 1$, $\rho$ is in the interior of $D$. If $\rho$ is in $S$ and rank($\rho$) $< N$, the same proof shows that $\rho$ is on the boundary of $D$ and thus also of $S$. □

There is a class of densities which satisfy the Peres partial transform condition but which are not separable, and there have been a number of detailed investigations of these densities using rather different techniques than those described above. For an introduction and additional references see Lewenstein et al in [15].

5 Orthogonality

In our running example we have seen that $\rho \left( \frac{1}{3} \right)$ on $H^2 \otimes H^2$ is the closest separable density to the inseparable density $\rho_0$ along the line connecting $D_0$ and $\rho_0$. As it happens, $\rho \left( \frac{1}{3} \right)$ is also closest to $\rho_0$ in the norm $\| \|$ defined in equation (3.1). To see this we need an alternate characterization of the density in $S$ closest to a density $\rho$ in $D - S$. This characterization is a standard result in convexity theory and has been used in [19, 20, 39] for example.

Proposition 5.1 Suppose $\rho$ in $D - S$. Then $\tau_0$ is the unique closest separable density to $\rho$ if and only if for all $\tau$ in $S$

$$\langle \langle \rho - \tau_0, \tau - \tau_0 \rangle \rangle \equiv Tr(\langle \rho - \tau_0 \rangle (\tau - \tau_0)) \leq 0.$$ (5.2)

By the convexity of $S$, it suffices to prove the inequality for all separable projections $\tau$.

Proof: Adding and subtracting $\tau_0$ gives

$$\langle \langle \rho - \tau, \rho - \tau \rangle \rangle = \langle \langle \rho - \tau_0, \rho - \tau_0 \rangle \rangle - 2 \langle \langle \rho - \tau_0, \tau - \tau_0 \rangle \rangle + \langle \langle \tau_0 - \tau, \tau_0 - \tau \rangle \rangle$$

which shows (5.1) is sufficient. Conversely, if $\langle \langle \rho - \sigma, \rho - \sigma \rangle \rangle$ is minimal over $S$ when $\sigma = \tau_0$, then $\langle \langle \rho - \tau_0, \sigma - \tau_0 \rangle \rangle \leq \frac{1}{2} \langle \langle \tau_0 - \sigma, \tau_0 - \sigma \rangle \rangle$. Using the convexity of the separable states, let $\sigma = (1 - t) \tau + t\tau_0$ with $0 < t < 1$, where $\tau$ is in $S$. It follows that

$$\langle \langle \rho - \tau_0, \tau - \tau_0 \rangle \rangle \leq \frac{1}{2} (1 - t) \langle \langle \tau_0 - \tau, \tau_0 - \tau \rangle \rangle,$$
and letting $t$ go to one gives the result. If $\tau_1$ also minimizes $\langle (\rho - \tau, \rho - \tau) \rangle$, then from $\langle (\rho - \tau_0, \tau_1 - \tau_0) \rangle \leq 0$ and $\langle (\rho - \tau_1, \tau_0 - \tau_0) \rangle \leq 0$, we can conclude that $\langle (\tau_1 - \tau_0, \tau_1 - \tau_0) \rangle \leq 0$, confirming uniqueness and completing the proof. □

An extremely useful geometric entity is the separable face nearest a given $\rho_0$ in $D - S$. Let $\tau_0$ denote the nearest separable density to $\rho_0$ and use the notation of the proposition above.

**Definition 5.3** $F (\rho_0, \tau_0)$ denotes $\{ \tau \in S : \langle \rho_0 - \tau_0, \tau - \tau_0 \rangle = 0 \}$.

Thus $F (\rho_0, \tau_0)$ is the convex set of densities in $S$ such that as vectors $\tau - \tau_0$ is perpendicular to $\rho_0 - \tau_0$. We leave it to the reader to confirm that $F (\rho_0, \tau_0)$ is indeed a face of $S$ and that the extreme separable projections in a convex representation of $\tau_0$ necessarily lie in $F (\rho_0, \tau_0)$.

The alternate characterization of $\tau_0$ allows us to compute the nearest separable density in some cases, and we pursue that idea next. As an example, the following result includes Proposition 1 of [39] as a special case in which the density $\rho_1$ below is separable and equal to a density in $F = F (\rho_0, \tau_0)$.

**Corollary 5.4** Suppose $\tau_0$ and $\tau_1$, the nearest separable densities to $\rho_0$ and $\rho_1$ respectively, are both in $F = F (\rho_0, \tau_0)$. Then the nearest separable density to $tp_0 + (1 - t) \rho_1$ is $\tau (t) = t\tau_0 + (1 - t) \tau_1$, and thus $m [t\rho_0 + (1 - t) \rho_1] \leq tm [\rho_0] + (1 - t) m [\rho_1]$.

**Proof:** Since $\langle (\rho_0 - \tau_0, \tau (t) - \tau_0) \rangle = \langle (\rho - \tau_0, \tau (t) - \tau_0) \rangle = 0$, we have

$$
\langle (tp_0 + (1 - t) \rho_1 - \tau (t), \tau (t)) \rangle
= \langle (\rho_0 - \tau_0, \tau (t)) \rangle + (1 - t) \langle (\rho_1 - \tau_1, \tau (t)) \rangle
= t \langle (\rho_0 - \tau_0, \tau (t)) \rangle + (1 - t) \langle (\rho_1 - \tau_1, \tau (t)) \rangle \leq 0,
$$

completing the proof. □

As another application, we are able to give a geometric perspective to $\tau_0 (d)$, the separable density closest to the bipartite state $\rho_0 (d) = |\psi_d \rangle \langle \psi_d |$ where

$$
|\psi_d \rangle |\psi_d (2) \rangle = \frac{1}{\sqrt{d}} \sum_{j=0}^{d-1} |jj \rangle.
$$

This includes the motivating example as a special case. The state $\rho_0 (d)$ is known as a maximally entangled state and for $d = 2$ was used by Werner [37] in an analysis of “local reality” and the Einstein, Podolsky, Rosen paradox [1]. Now the convex combination $(1 - s) D_0 + s \rho_0 (d)$ can be interpreted as a mixture of the maximally entangled state $\rho_0 (d)$ and $D_0$, the “maximally mixed” state or random noise. In earlier studies, including [27] and [15] and references therein, the largest value of $s$ for which $(1 - s) D_0 + s \rho_0 (d)$ is separable was investigated, which is equivalent to the question of how much noise it takes to make the system unentangled. As it happens, the nearest separable density to
\(\rho_0(d)\) is such a convex combination. That result for \(d = 2\) seems to have been noticed first in \([33]\), and the proof below for arbitrary \(d\) follows their approach. An independent proof of the general case recently appeared as part of the analysis in \([19]\).

**Proposition 5.5** The state \(\tau_0(d) = (1 - s_d) D_0 + s_d \rho_0(d)\) with \(s_d = (1 + d)^{-1}\) is the nearest separable density to the maximally entangled state \(\rho_0(d)\). The analogous assertion is false if the number of product states \(n\) is bigger than 2.

**Proof:** The proof that \(\tau_0(d)\) is separable has been given in a number of references such as \([3, 17, 27, 8]\) among others. Dropping explicit mention of \(d\), we thus need to prove that for all separable projections \(\tau\)

\[
\frac{1}{1-s_d} \langle \langle \rho_0 - \tau_0, \tau - \tau_0 \rangle \rangle = \langle \langle \rho_0 - D_0, \tau - \tau_0 \rangle \rangle = \langle \langle \rho_0, \tau - \tau_0 \rangle \rangle \leq 0.
\]

First, \(\text{Tr} (|\psi_d\rangle \langle \psi_d| \tau_0) = (1 - s_d) \text{Tr} (1 2^d |\psi_d\rangle \langle \psi_d|) + s_d \text{Tr} (|\psi_d\rangle \langle \psi_d|) = \frac{d}{1 + d} + \frac{1}{1 - d} = \frac{1}{d}\). If \(\tau\) is a separable projection, then \(\tau = |\alpha\rangle \langle \alpha| \otimes |\beta\rangle \langle \beta|\) where in the computational basis \(|\alpha\rangle = \sum_{k=0}^{d-1} a_k |k\rangle\) with \(\sum_k |a_k|^2 = 1\) and with an analogous expression for \(|\beta\rangle\). Then

\[
\text{Tr} (|\psi_d\rangle \langle \psi_d| \tau) = \frac{1}{d} \left| \sum_{i,j,k} \langle ii|jk \rangle a_j b_k \right|^2 = \frac{1}{d} \left| \sum_k \langle a_k|^2 \right|^2 \leq \frac{1}{d}
\]

since \(\left| \sum_k a_k b_k \right|^2 \leq \sum_k |a_k|^2 \sum_k |b_k|^2\) by the Cauchy-Schwarz inequality. Hence \(\langle \langle \rho_0 - \tau_0, \tau - \tau_0 \rangle \rangle \leq 0\) for all separable densities and \(\tau_0(d)\) is the closest separable density to \(\rho_0(d)\) when \(n = 2\). When \(n > 2\) and \(|\psi_d(n)\rangle\) is defined analogously, \(\text{Tr} (|\psi_d(n)\rangle \langle \psi_d(n)| \tau_0)\) equals \(\frac{1 + d}{n(1 + d - 1)}\) and it is easy to see that there are separable projections with \(\text{Tr} (|\psi_d(n)\rangle \langle \psi_d(n)| \tau) = \frac{1}{d}\), completing the proof of the proposition. \(\square\)

**Corollary 5.6** Using \(m\) as the measure of entanglement, \(m[\rho_0(d)] = \sqrt{1 - \frac{n}{d+1}},\) so that entanglement increases with increasing \(d\). \(\square\)

As another application, we can compute explicitly the extreme points of \(F(\rho_0(d), \tau_0(d))\).

**Corollary 5.7** \(F(\rho_0(d), \tau_0(d))\) is the convex hull of \(|\alpha\rangle \langle \alpha| \otimes |\tilde{\alpha}\rangle \langle \tilde{\alpha}|\), where the bar denotes the complex conjugate of the entries of the row or column vector.

**Proof:** From an earlier observation, it suffices to consider densities of the form \(\tau = |\alpha\rangle \langle \alpha| \otimes |\beta\rangle \langle \beta|\). From the proof above, \(\tau\) is in \(F(\rho_0(d), \tau_0(d))\) if and only if \(\sum_k a_k b_k^2 = \sum_k |a_k|^2 \sum_k |b_k|^2\). This is the case of equality in the Cauchy-Schwarz inequality over the complex numbers and is equivalent to \(b_k = c\bar{a}_k\) for some constant \(c\) and all \(k\). (See for example \([29]\).) By the normalization
condition, $|e| = 1$ and thus does not appear as a factor in $\tau = |\alpha\rangle \langle \alpha| \otimes |\bar{\alpha}\rangle \langle \bar{\alpha}|$, completing the proof. □

As an example, when $d = n = 2$, the basis of orthogonal unitary matrices \{\(S_a\)\} defined earlier is essentially the set of four Pauli matrices: $\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, and $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$. (The only difference is that one uses $\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$ in lieu of $\sigma_y$.) It is easy to show that $\tau_0 = \rho \left(\begin{pmatrix} 1/3 \\ 2 \end{pmatrix}\right)$ is the average of the six separable projections $\frac{1}{4} (\sigma_0 \pm \sigma_z) \otimes (\sigma_0 \pm \sigma_z)$, $\frac{1}{4} (\sigma_0 \pm \sigma_z) \otimes (\sigma_0 \pm \sigma_z)$, and $\frac{1}{2} (\sigma_0 \pm \sigma_y) \otimes (\sigma_0 \pm \sigma_y)$ and that these projections have the requisite form $|\alpha\rangle \langle \alpha| \otimes |\bar{\alpha}\rangle \langle \bar{\alpha}|$.

6 Entanglement witnesses

Suppose $\rho_0 \notin S$. Then a standard consequence of the Hahn-Banach theorem for convex spaces is that there exists a linear functional $F$ on $M$ such that $F(\rho_0) < 0 \leq \inf \{F(\tau) : \tau \in S\}$. In the context of our finite dimensional Hilbert space $M$, the Riesz representation theorem says that each linear functional is of the form $F(\rho) = \text{Tr}(A\rho)$ for some Hermitian matrix $A$. (See for example [1].) It is also a standard fact that the hyperplane $M(A) = \{B \in M : \text{Tr}(AB) = 0\}$ has dimension $\dim(M) - 1$, so that one can view $M(A_0)$ as a separating hyperplane with $\rho_0$ on one side and $S$ on the other. Since quantum mechanical observables are modelled as Hermitian matrices, the thrust of the theory is that the condition $\rho \notin S$ can be “witnessed” by a suitable observable $A$, and such Hermitian matrices have been dubbed “entanglement witnesses” in the quantum computation literature. This connection was first pointed out in [11], and the authors went on to link these ideas to the Banach algebra literature. In particular they showed that the Peres necessary condition for separability is also sufficient in the $2 \times 2$ and $2 \times 3$ tensor product cases.

The Peres condition can be couched in the language of positive operators on bounded functions on $H^{[N]}$, and, as mentioned in the introduction, one direction of research on separability has focused on densities which satisfy the Peres condition but which are not separable. A consequence of that work has been a study of entanglement witnesses in general. Recent relevant papers which contain further references include [14, 15, 16, 31, 32].

Since separating hyperplanes are not unique, it is customary to normalize in the entanglement context by requiring that $\text{Tr}(A\rho_0) = 1$ in addition to

$$\text{Tr}(A\rho_0) < 0 \leq \inf \{\text{Tr}(A\tau) : \tau \in S\} \quad (6.1)$$

for some inseparable density $\rho_0$. In [16] the authors introduced a partial order on such entanglement witnesses as follows. Let $D(A)$ denote $\{\rho \in D : \text{Tr}(A\rho) < 0\}$. Define a partial order by $A \preceq B$ if and only if $D(A) \subseteq D(B)$. Then an optimal entanglement witness is a maximal element in the partial order. We should note
that the analysis in [10] deals with general entanglement witnesses, and one of the sufficient conditions below for \( A_0 \) to be optimal appears there.

The connection with our analysis is that knowing the closest separable density \( \tau_0 \) to a nonseparable density \( \rho_0 \) also enables one to construct an entanglement witness \( A_0 \) for a class of densities related to \( \rho_0 \). This is not an assertion that actually finding \( \tau_0 \) is computationally easy. Rather, it illustrates the importance of \( \tau_0 \) and shows \( \text{Tr}(A_0 \sigma) \) has a familiar form which further reveals its geometric character.

We assume equation (6.1), but since we begin with a particular \( \rho_0 \) we use a slightly different normalization.

**Definition 6.2** \( A_0 \) is said to be optimal provided that any Hermitian \( A \) satisfying equation (6.1) together with \( \text{Tr}(A \rho_0) = \text{Tr}(A_0 \rho_0) \) and \( D(A_0) \subseteq D(A) \) necessarily equals \( A_0 \).

**Theorem 6.3** Suppose \( \tau_0 \) is the nearest separable density to a non-separable density \( \rho_0 \). Then the Hermitian matrix \( A_0 = c_0 I + \tau_0 - \rho_0 \) with \( c_0 = \text{Tr}(\tau_0 (\rho_0 - \tau_0)) \) is an entanglement witness for \( \rho_0 \). In particular for any density \( \sigma \)

\[
\text{Tr}(A_0 \sigma) = - \langle \langle \rho_0 - \tau_0, \sigma - \tau_0 \rangle \rangle
\]

so that the separating hyperplane defined by \( A_0 \) contains \( F(\rho_0, \tau_0) \). If some \( \tau \) in \( F(\rho_0, \tau_0) \) has full rank, then \( A_0 \) is optimal.

**Proof:** It is easy to check equation (6.2) so that \( A_0 \) has the asserted properties. Next, suppose that \( A \) satisfies equation (6.1) and that \( D(A_0) \subseteq D(A) \) with \( \text{Tr}(A \rho_0) = \text{Tr}(A_0 \rho_0) \). Using one of the techniques in [10], suppose that \( \text{Tr}(A_0 \rho) = 0 \). Then for \( 0 < s < 1 \), \( \text{Tr}(A_0 ((1 - s) \rho + s \rho_0)) < 0 \) implying \( \text{Tr}(A \rho) < \frac{s}{1-s} \text{Tr}(A \rho_0) \) and thus \( \text{Tr}(A \rho) \leq 0 \). In particular \( \text{Tr}(A \tau) \leq 0 \) for \( \tau \) in \( F(\rho_0, \tau_0) \), forcing \( \text{Tr}(A \tau) = 0 \).

Now suppose that there is a \( \tau \) in \( F(\rho_0, \tau_0) \) with full rank, so that its smallest eigenvalue is strictly positive. Then it’s straightforward to show that there exists a small positive \( t \) such that for any density \( \rho \), \( \mu(t) = (1 + t) \tau - t \rho \), a variant of the entanglement probes defined earlier, is in \( D \). In particular if \( \text{Tr}(A_0 \rho) = 0 \) we have

\[
\text{Tr}(A_0 \mu(t)) = 0 \geq \text{Tr}(A \mu(t)) = -t \text{Tr}(\rho) \geq 0
\]

forcing \( \text{Tr}(\rho) = 0 \). This gives the property that \( \text{Tr}(A_0 \rho) = 0 \) implies \( \text{Tr}(A \rho) = 0 \) which suffices for the rest of the proof. In fact, that property together with equation (6.1) and \( \text{Tr}(A \rho_0) = \text{Tr}(A_0 \rho_0) \) is equivalent to \( A = A_0 \).

Suppose \( \text{Tr}(A_0 \rho) > 0 \). Then \( \text{Tr}(A_0 ((1 - s) \rho + s \rho_0)) = 0 \) for some \( s \) in \((0, 1)\), and from the normalization it follows that \( \text{Tr}(A_0 \rho) = \text{Tr}(A \rho) \). In particular \( \text{Tr}(A_0 D_0) = \text{Tr}(A D_0) \). Finally, if \( \text{Tr}(A_0 \rho) < 0 \), then analogously \( \text{Tr}(A_0 ((1 - s) \rho + s D_0)) = 0 \) for some \( s \) in \((0, 1)\), and that gives \( \text{Tr}(A_0 \rho) = \text{Tr}(A \rho) \). Consequently \( \text{Tr}(A_0 \rho) = \text{Tr}(A \rho) \) for all \( \rho \) in \( D \), and it follows that \( A_0 = A \), completing the proof. \(\square\)
Corollary 6.5 \( A_0 \) is optimal if the separable eigenvectors of the rank one separable projections in \( F(\rho_0, \tau_0) \) span \( H^{(N)} \) or if there is a density \( \rho \) of full rank such that \( \rho = (1+t)\tau - t\rho_0 \) for some \( \tau \) in \( F(\rho_0, \tau_0) \).

Proof: In the first case, it is easy to see that one can construct a \( \tau \) in \( F(\rho_0, \tau_0) \) which has full rank. In the second case, the techniques in Corollary (4.3) show that \( \tau \) has full rank. \( \Box \)

As an example of this general theory we have the following specific result which includes example 5, up to a multiplicative constant, in [32].

Corollary 6.6 For the usual \( 2 \times 2 \) bivariate example, \( \tau_0 = \rho(1/3) \) has full rank and

\[
A_0 = \frac{1}{3} (I - 2\rho_0) = \frac{1}{3} \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}
\]

is an optimal entanglement witness. \( D(A_0) \) contains \( \rho_a = |\psi_a\rangle \langle \psi_a| \) for any density of the form \( \rho_a = |\psi_a\rangle \langle \psi_a| \) where \( |\psi_a\rangle = \sum_{k=0}^{d-1} a_k |kk\rangle \) with non-negative \( a_k \) such that \( \sum_k |a_k|^2 = 1 \). In the corresponding \( d \times d \) case, \( A_0 = \frac{1}{d^2} (I - d\rho_0) \).

\( \Box \)

If the matrix above is denoted as \( M_{01} \), the \( A_0 \) in the \( d \times d \) case turns out to be a multiple of \( \sum_{0 \leq j < k < d} M_{jk} \), where the \( M_{jk} \) have definitions analogous to \( M_{01} \). (See equation (7.4).) Another role for the \( M_{jk} \) is given below, where we find other nearest separable states using an extension of the methodology developed above.

7 Variations in the bivariate case.

It would be useful to be able to calculate \( m[\rho] \), the Frobenius measure of entanglement of states other than the maximally entangled states, and we can do this for states which are near to the maximally entangled state in a sense to be made more precise below. We will use the geometric insights obtained above in the context of two \( d \)-level systems and motivate the analysis with the usual two qubit case \( d = 2 \). That particular case was also studied by Witte and Trucks [32] who used a different approach to obtain Proposition 7.1 below.

Our approach is motivated by the geometry. We know that \( \rho_0 - \tau_0 \) is orthogonal to the face \( F(\rho_0, \tau_0) \), and from Corollary 5.3 we also know what the extreme points of \( F(\rho_0, \tau_0) \) are. Now suppose that \( \rho_a = |\psi_a\rangle \langle \psi_a| \) where \( \psi_a = \sum_{k=0}^{d-1} a_k |kk\rangle \) with \( 0 \leq a_k \), \( \sum_k a_k^2 = 1 \), and the \( a_k \)'s are close to \( 1/\sqrt{d} \). Then one would expect that \( \tau_a \) would also lie in \( F(\rho_0, \tau_0) \) and thus, considered as vectors, that \( \rho_a - \tau_a \) might be parallel to \( \rho_0 - \tau_0 \). This could take the form

\[
\tau_a = \rho_a + t (\tau_0 - \rho_0)
\]
where \( t = t(d,a) \) is a positive constant to be determined. This particular representation works when \( d = 2 \), and we obtain the same constraints on the parameters \( a_0 \) and \( a_1 \) found earlier in \[39\]. As a convention, we will assume that \( a_0 > a_1 \) throughout.

**Proposition 7.2** In the case \( d = 2 \), \( \tau_a = \rho_a + t(\tau_0 - \rho_0) \) lies in \( F(\rho_0, \tau_0) \) and is the closest separable density to \( \rho_a \) provided \( t = 2a_0a_1 \) and \( |a_0^2 - \frac{1}{3}| \leq \frac{\sqrt{3}}{6} \). The Frobenius measure of entanglement is then \( m[\rho_a] = 2a_0a_1/\sqrt{3} = 2a_0a_1m[\rho_0] \).

**Proof:** If \( \tau_a \) were in \( F(\rho_0, \tau_0) \), then \( \langle \rho_0 - \tau_0, \tau_a - \tau_0 \rangle = 0 \) and for any \( \tau \in S \)

\[
\langle \rho_0 - \tau_0, \tau - \tau_0 \rangle = t \cdot \frac{\langle \rho_0 - \tau_0, \tau - \tau_0 \rangle - \langle \rho_0 - \tau_0, \tau_a - \tau_0 \rangle}{2} \leq 0,
\]

confirming that \( \tau_a \) would be the closest separable density to \( \rho_a \). For

\[
\tau_a = \begin{pmatrix}
a_0^2 - t/6 & 0 & 0 & a_0a_1 - t/3 \\
0 & t/6 & 0 & 0 \\
a_0a_1 - t/3 & 0 & t/6 & 0 \\
a_0^2 - t/6 & 0 & 0 & a_1^2 - t/6
\end{pmatrix}
\]

to be in \( F(\rho_0, \tau_0) \) it has to be a convex combination of the extreme points of \( F(\rho_0, \tau_0) \). If the entries of \( |\beta\rangle \) are denoted by \( r_k e^{i\theta(k)} \), then the \( (j_1,j_2,k_1,k_2) \)th component of \( \tau = |\beta\rangle \langle \beta| \otimes |\bar{\beta}\rangle \langle \bar{\beta}| \) is

\[
r_{j_1,j_2}r_{k_1}r_{k_2}e^{i(\theta(j_1) - \theta(j_2) - \theta(k_1) + \theta(k_2))}.
\]

(7.3)

It follows that \( \tau_{00,11} = \tau_{11,00} = \tau_{10,10} = \tau_{01,01} = r_0^2r_1^2 \) is always real, and it is easy to see that all other entries have phase angles. Thus a necessary condition is \( a_0a_1 - t/3 = t/6 \), giving \( t = 2a_0a_1 \) as asserted.

Keeping \( r_0 \) and \( r_1 \) fixed and averaging extreme points with phase angles changed appropriately by angles of \( \pi/2 \) and \( \pi \), one can eliminate non-zero entries where phase angles appear and thus define a convex subset \( \bar{F}(\rho_0, \tau_0) \) of \( F(\rho_0, \tau_0) \) defined by densities of the form

\[
\begin{pmatrix}
0 & 0 & 0 & r_0^2r_1^2 \\
0 & r_0^2r_1^2 & 0 & 0 \\
r_0^2r_1^2 & 0 & 0 & r_1^4
\end{pmatrix}
\]

A necessary and sufficient condition for \( \tau_a \) to be in this convex subset of \( F(\rho_0, \tau_0) \) is that \( (a_0^2 - \frac{a_0a_1}{3}, a_1^2 - \frac{a_0a_1}{3}, 2a_0a_1) \) should be in the convex hull of vectors \( (r_0^4, r_1^4, 2r_0^2r_1^2) \) with \( r_0^2 + r_1^2 = 1 \). If \( x_0 \) and \( x_1 \) denote \( r_0^2 \) and \( r_1^2 \) respectively, then it is easy to check that an equivalent condition is that \( (a_0^2, a_0^2 - \frac{a_0a_1}{3}) \) should be in the convex hull of vectors \( (x_0, x_0^2) \) where \( 0 \leq x_0 \leq 1 \). But that set is precisely the set of pairs \( (x, y) \) with \( 0 \leq x \leq 1 \) and \( x^2 \leq y \leq x \). That means \( a_0^4 \leq a_0^2 - \frac{a_0a_1}{3} \) or \( 1 \leq 3a_0a_1 \), which is equivalent to the condition asserted in the statement of the proposition. (Since \( d = 2 \), the same result could be obtained by using the required positive definiteness of \( \tau_a \) and the Peres-Horodecki theorem.) The calculation of \( m[\rho_a] \) is immediate, completing the proof. □
Corollary 7.4 If \( a_0^2 = \frac{1}{2} + \frac{\sqrt{5}}{6} \), then \( r_0^2 = \left( \frac{7 + 3\sqrt{5}}{18} \right)^{1/2} \) and \( \tau_a \) is on the boundary of \( D \). □

The significance of Corollary 7.1 turns out to be that for \( a_0^2 > \frac{1}{2} + \frac{\sqrt{5}}{6} \) the vector \( \rho_a - \tau_a \) is in fact not parallel to \( \rho_0 - \tau_0 \), and the techniques above do not give \( \tau_a \). This same problem arose in [39] where it was conjectured that \( \tau_a \) could be computed using the root of a cubic polynomial. Geometrically, that cubic is based on the assumption that the nearest separable density to \( \rho_a \) is on the boundary of \( \tilde{F}(\rho_0, \tau_0) \), which is reasonable since we have already seen that \( \rho_a \) is separated from \( S \) by the hyperplane containing \( F(\rho_0, \tau_0) \). The gap in the argument is that one needs to show that \( \tau_a \) has to be in \( \tilde{F}(\rho_0, \tau_0) \).

The same approach works for \( d \geq 3 \) but with the need for additional parameters. The entries of the extreme points \( |\beta\rangle \langle \beta| \otimes |\beta\rangle \langle \beta| \) have the same sort of pattern as in the \( d = 2 \) case with real entries \( r_j^a r_k^a \) in positions \( (jk, kk) \), \( (jk, jk) \), \( (kk, jk) \), and \( (kk, jj) \) for \( 0 \leq j, k \leq d - 1 \). This means there are \( \binom{d}{2} \) sets of four entries for which the components of any density in the convex hull of the extreme points must be constant, and the single parameter \( t \) in equation (5.1) doesn’t suffice.

To obtain more parameters, we look for additional Hermitian matrices orthogonal to \( F(\rho_0, \tau_0) \). In particular, define the \( \binom{d}{2} \) matrices \( M_{jk} \), \( 0 \leq j < k < d \), whose entries are \( +1 \) at \( (jk, jk) \) and \( (kk, jk) \), \( -1 \) at entries \( (jj, kk) \) and \( (kk, jj) \) and are \( 0 \) elsewhere. Then it is easy to check that for extreme points \( \tau \) in \( F(\rho_0, \tau_0) \)

\[
\text{Tr}(M_{jk}\tau) = \tau_{jk,jk} + \tau_{kj,kj} - \tau_{kk,jj} + \tau_{kk,jj} = 0,
\]

and thus each Hermitian \( M_{jk} \) is orthogonal to densities in \( F(\rho_0, \tau_0) \). Use \( I \) to denote the \( d^2 \times d^2 \) identity and note that

\[
\sum_{j<k} M_{jk} = I - d\rho_0.
\]

As noted in the preceding section, up to a multiplicative constant \( I - d\rho_0 \) is the optimal entanglement witness \( A_0 \) based on \( \rho_0 \).

We break the analysis into two parts, first showing that the \( \tau_a \) defined below is the closest separable density to \( \rho_a \), assuming \( \tau_a \) is in \( F(\rho_0, \tau_0) \), and then obtaining sufficient conditions on the \( a_k \)'s for \( \tau_a \) to be in \( F(\rho_0, \tau_0) \). Recall that \( \rho_a \) has entries \( a_j a_k \) in positions \( (jj, kk) \) and \( (kk, jj) \) for \( 0 \leq j, k \leq d - 1 \), so that \( \sum_k a_k^2 = 1 \). As a convention we assume that \( a_0 \geq a_1 \geq \ldots \geq a_{d-1} \). Set \( a * a = \sum_{j<k} a_j a_k \) and impose the first constraint on the \( a_k \)'s:

\[
a_{d-1}^2 \geq \frac{2a * a}{d(d+1)}.
\]

Proposition 7.8 Let \( \{M_{jk}\} \) be defined as above and let \( M_a \) denote \( \sum_{j<k} u_{jk} M_{jk} \). Define

\[
\tau_a = \rho_a + t(\tau_0 - \rho_0) + M_a,
\]

\( \tau_a \) is on the boundary of \( D \). □
where \( t = \frac{2a \sqrt{a}}{d} \) and \( u_{jk} = \frac{1}{2} (a_j a_k - \frac{a_j + a_k}{d}) \). Then \( \sum_{j<k} u_{jk} = 0 \), and \( \tau_a \) is a trace one, Hermitian matrix with non-negative entries on the diagonal. Moreover, \( \rho_a - \tau_a \) is orthogonal to \( F(\rho_0, \tau_0) \). If in addition \( \tau_a \) is in \( F(\rho_0, \tau_0) \), then it is the closest separable density to \( \rho_a \) and

\[
m[\rho_a] = \sqrt{\text{Tr} \left[ (\rho_a - \tau_a)^2 \right]} = \sqrt{t^2 \left( 1 - \frac{2}{1 + d} \right) + \sum_{j<k} 4u_{jk}^2}. \tag{7.10}
\]

Proof: Using the definitions we first compute the non-zero entries of \( \tau_a \):

\[
\tau_a (ii, ii) = a_i^2 + \frac{td}{1 + d} \left( \frac{1}{d^2} - \frac{1}{d} \right) = a_i^2 - \frac{2a \sqrt{a}}{d(d + 1)}
\]

\[
\tau_a (jk, jk) = \frac{td}{1 + d \cdot d^2} u_{jk} = \frac{1}{2} \left( a_j a_k - \frac{2a \sqrt{a}}{d(d + 1)} \right), j \neq k,
\]

\[
\tau_a (jj, kk) = a_j a_k - \frac{td}{1 + d \cdot d^2} u_{jk} = \frac{1}{2} \left( a_j a_k - \frac{2a \sqrt{a}}{d(d + 1)} \right), j \neq k.
\]

By virtue of equation (7.5) \( \tau_a \) has non-negative entries on the diagonal and the desired pattern of values on the remaining entries. Note that these same formulas work for \( d = 2 \). One can show \( \text{Tr} (\tau_a) = 1 \) directly or by confirming that

\[
\sum_{j<k} u_{jk} = \frac{1}{2} \left( a \sqrt{a} - \left( \frac{d}{2} \right) \frac{t}{d} \right) = 0
\]

so that \( \text{Tr} (M_a) = 0 \). Since \( \text{Tr} (M_{jk}(\rho_0 - \tau_0)) = \frac{4a \sqrt{a}}{d+4} \text{Tr} (M_{jk}(\rho_0 - D_0)) = \frac{2a}{d} \),

\[
\text{Tr} (M_a(\rho_0 - \tau_0)) = \frac{-2}{d} \sum_{j<k} u_{jk} = 0.
\]

Thus, as a vector \( \rho_a - \tau_a \) can be viewed as the sum of two orthogonal vectors in \( (F(\rho_0, \tau_0))^\perp \), the linear subspace of Hermitian matrices perpendicular to \( F(\rho_0, \tau_0) \), and (7.7) follows from that observation.

So far we have only shown that \( \tau_a \) could be in \( F(\rho_0, \tau_0) \), with equation (7.5) the only constraint imposed so far on the \( a_k \)'s. To complete the proof of the proposition, we show that if \( \tau_a \) is in \( F(\rho_0, \tau_0) \) then it is the nearest separable density to \( \rho_a \). Since \( \langle \rho_a - \tau_0, \tau_a - \tau_0 \rangle = \langle M_{jk}, \tau_a \rangle = 0 \) under that hypothesis,

\[
\langle \rho_a - \tau_a, \tau - \tau_a \rangle = t \left[ \langle \rho_0 - \tau_0, \tau - \tau_a \rangle \right] - \sum_{j<k} u_{jk} \langle M_{jk}, \tau - \tau_a \rangle
\]

\[
= t \left[ \langle \rho_0 - \tau_0, \tau - \tau_0 \rangle \right] - \sum_{j<k} u_{jk} \langle M_{jk}, \tau \rangle
\]

\[
= \frac{td}{d+1} \langle \rho_0 - D_0, \tau - \tau_0 \rangle - \sum_{j<k} u_{jk} \langle M_{jk}, \tau \rangle.
\]
Hence (7.4) and we have already shown that notation and equation (7.3) separable extreme point of the form |β⟩⊗|γ⟩. We examine that problem next. What we do instead is demonstrate a methodology which shows that there exists a neighborhood of the equal entry case when \( a_k = 1/\sqrt{d} \) in which \( \tau_a \) is the related density to a choice of \( k \) in \( \hat{d} \). As we saw in the case when \( d = 2 \), further restrictions on the \( a_k \)’s are required to show that \( \tau_a \) actually is a separable density. We examine that problem next.

Now it is easy to check that

\[
\langle \rho_0 - D_0, \tau - \tau_0 \rangle = \langle \rho_0, \tau \rangle - \langle \rho_0, \tau_0 \rangle = \langle \rho_0, \tau \rangle - \frac{1}{d} \langle \rho_0 - I, \tau \rangle,
\]

where \( I \) denotes the \( d^2 \times d^2 \) identity matrix. Using \( d\rho_0 - I = -\sum_{j<k} M_{jk} \) from equation (7.4) and

\[
\sum_{j<k} u_{jk} \langle M_{jk}, \tau \rangle = \frac{1}{2} \sum_{j<k} a_j a_k \langle M_{jk}, \tau \rangle - \frac{t}{2d} \sum_{j<k} \langle M_{jk}, \tau \rangle,
\]

we have

\[
\langle \rho_a - \tau_a, \tau - \tau_a \rangle = -\frac{1}{2} \sum_{j<k} \langle M_{jk}, \tau \rangle \left( \frac{t(d-1)}{d(d+1)} + a_j a_k \right).
\]

We have already shown that \( \langle \rho_{jk}, \tau \rangle = 0 \) when \( \tau \) is in \( F(\rho_0, \tau_0) \). If \( \tau \) is a separable extreme point of the form \( |\beta⟩⟨\beta| \otimes |\gamma⟩⟨\gamma| \), then using the obvious notation and equation (7.3)

\[
\langle M_{jk}, \tau \rangle = \tau_{jk} + \tau_{kj} + \tau_{jj} - \tau_{kk} = b_j^2 c_k^2 + b_k^2 c_j^2 - 2 b_j b_k c_j c_k \cos(\theta_{jk}) \geq 0.
\]

Hence \( \langle \rho_a - \tau_a, \tau - \tau_a \rangle \) \leq 0 for all separable densities, and that completes the proof. □

As we saw in the case when \( d = 2 \), further restrictions on the \( a_k \)’s are required to show that \( \tau_a \) actually is a separable density. We examine that problem next and obtain sufficient conditions on the \( a_k \)’s for \( \tau_a \) to be in \( F(\rho_0, \tau_0) \). It then follows from the foregoing analysis that \( \tau_a \) is the separable density closest to the related density \( \rho_a \), confirming the intuition that motivated this analysis in the first place. Unfortunately the algebra appears to be too involved to get as precise a result as in the case when \( d = 2 \).

What we do instead is to demonstrate a methodology which shows that there exists a neighborhood of the equal entry case when \( a_k = 1/\sqrt{d} \) in which \( \tau_a \) is in \( F(\rho_0, \tau_0) \). We have already shown that \( \tau_a \) could be in the smaller convex set \( \hat{F}(\rho_0, \tau_0) \), and we follow the approach used in the \( d = 2 \) case. \( \tau_a \) will be in \( \hat{F}(\rho_0, \tau_0) \) if the \( (d+1)/2 \) vectors \( T(a) \) whose first \( d \) entries are \( a_i^2 - \frac{2a_{ij}a_i}{d(d+1)} \) and whose next \( \binom{d}{2} \) entries are \( a_j a_k - \frac{2a_{jk}a_i}{d(d+1)} \), \( j \neq k \); is in the convex hull of \( X(x) \) vectors with respective entries \( x_1^2 \) and \( 2x_i, x_{i+1} \), where \( \sum_i x_i = 1 \) and \( 0 \leq x_i \). Note that the components of all of the vectors in question sum to \( 1 \). In this notation \( \tau_0 \) corresponds to a \( T \)-vector \( T(0) \) with entries \( \frac{2}{d(d+1)} \).

The idea is to select a specific set of extreme \( X \) vectors and show that \( T(0) \) is in the interior of the convex hull of these particular vectors. Specifically, for each of \( 1 \leq k \leq d \) we choose \( \binom{d}{2} \) vectors \( X(k;j) \), \( 1 \leq j \leq \binom{d}{2} \), corresponding to a choice of \( k \) of the \( x_i \)’s equal to \( 1/k \) and the remainder equal to 0. Thus, \( X(k;j) \) will have \( k \) of its entries corresponding to \( x_i^2 \) equal to \( 1/k^2 \) and \( \binom{d}{2} \)
entries corresponding to $2x_1, x_2$ equal to $2/k^2$. For example, if $d = 3$ the resulting 7 vectors can be written as column vectors in a $6 \times 7$ array $V$, and the assertion that $T(0)$ is in the convex hull of these vectors is equivalent to $V\vec{p} = T(0)$ or

$$
\begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 \\
\end{pmatrix}
\begin{pmatrix}
p_0 \\
p_1 \\
p_2 \\
p_3 \\
p_4 \\
p_5 \\
\end{pmatrix}
= 
\begin{pmatrix}
\frac{1}{6} \\
\frac{1}{6} \\
\frac{1}{6} \\
\frac{1}{6} \\
\frac{1}{6} \\
\frac{1}{6} \\
\end{pmatrix}
$$

(7.11)

with non-negative $p_j$'s summing to 1. Using this approach some easy linear algebra shows that a sufficient condition for $\tau_a$ to be in $F(\rho_0, \tau_0)$ when $a_0 \geq a_1 \geq a_2$ is that

$$
\frac{1}{2}a_0a_2 \leq a_2^2 - \frac{1}{12}a_1^2,
$$

(7.12)

implying (7.5) when $d = 3$. As two examples, the $a$ corresponding to $a_0 = \sqrt{5/12}, a_1 = \sqrt{4/12}$, and $a_2 = \sqrt{3/12}$ satisfies this constraint, and the inequality (7.9) when $a_k = \frac{1}{\sqrt{3}}$ is $\frac{1}{3} \leq \frac{1}{4}$.

In the general case $V$ is a $(d + \binom{d}{2}) \times \left(\sum_{k=1}^{d} \binom{d}{k}\right)$ matrix with regular structure in each of the $d$ blocks of $\binom{d}{k}$ columns. Each of the first $d$ rows will have $\binom{d-1}{k-1}$ non-zero entries equal to $1/k^2$ in the corresponding block of $\binom{d}{k}$ columns. Similarly, each of the last $\binom{d}{d}$ rows will have no positive entries in the first block of columns and $\binom{d-2}{k-2}$ non-zero entries equal to $2/k^2$ in the remaining blocks of column vectors. If we further require that each of the $\binom{d}{k}$ column vectors have equal weight $q_k/\binom{d}{k}$, then solving for $\vec{p}$ in $V\vec{p} = T(0)$ is equivalent to finding non-negative $q_k$ satisfying $\sum_k q_k = 1$ and

$$
\sum_{k=1}^{d} \frac{1}{k} q_k \binom{d-1}{k-1} = \sum_{k=2}^{d} \frac{2}{k} q_k \binom{d-2}{k-2} = \frac{2}{d(d+1)}.
$$

It is then easy to show that those three equations are equivalent to

$$
\sum_{k=1}^{d} q_k = 1, \quad \sum_{k=2}^{d} \frac{q_k}{k} = \frac{2}{d+1}.
$$

(7.13)

Note that if $2k < d$, then $q_k = k/(d+1)$, $q_{d+1-k} = (d+1-k)/(d+1)$ and $q_j$ equals zero otherwise is a particular solution. From that observation it is easy to see that one can find solutions of (7.10) which are strictly positive.

We have defined $2^d - 1$ particular vectors $X$ which span their $(d+1)$ dimensional space. Given the components $a_k$ of $a$, we want to find $\vec{p}_a$, a $(2^d - 1)$-long vector with non-negative components which sum to one and such that
\( V\vec{p}_a = T(a) \), the vector corresponding to \( \tau_a \). Equivalently, we want to solve 
\[ V\vec{p}_a = V\vec{p}_0 + V(\vec{p}_a - \vec{p}_0) = T(0) + (T(a) - T(0)). \]
By the earlier analysis we know that we can choose a \( \vec{p}_0 \) whose entries are all strictly positive, and thus the problem reduces to finding solutions of \( V\vec{x} = T(a) - T(0) \) where the components of \( \vec{x} \) sum to 0 and are sufficiently small so that the components of \( \vec{p}_a = \vec{p}_0 + \vec{x} \) are non-negative. Since \( 2^d - 1 > \left( \frac{d+1}{2} \right) \), this is always possible, provided the components of \( T(a) - T(0) \) are also sufficiently small. This proves the final assertion of this section.

**Proposition 7.14** If the components \( a_k \) of \( a \) are sufficiently close to \( \frac{1}{\sqrt{d}} \), then \( \tau_a \) is in \( F(\rho_0, \tau_0) \).

8 Orthogonality in the n qubit case

In the absence of an efficient algorithm to compute the nearest separable density to a given \( \rho_0 \) we have used the special structure of states near maximally entangled states to find \( \tau_0 \). In particular we found in Section 4 that in the bivariate case the nearest separable state to \( \rho_0(d) \) lay along the line in \( M \) connecting \( \rho_0 \) to \( D_0 \), and we also saw that was not true if there were more than two systems.

In this section we work with \( n \) qubits and show that the special structure of \( \rho_0 = \rho_0(n) = |\psi_0\rangle \langle \psi_0| \) where \( |\psi_0\rangle = \frac{1}{\sqrt{2}} (|00\ldots0\rangle + |11\ldots1\rangle) \) facilitates the analysis. In particular we will obtain some perspective on the geometry in this higher dimensional context.

The approach is straight-forward. We use the structure of \( \rho_0 \) as a matrix in the computational basis and consider the local unitary mappings which leave \( \rho_0 \) invariant. Since such operations should also leave \( \tau_0 \) invariant, we assume \( \tau_0 \) will have non-zero entries only on the diagonal and in the \((0,i),(\bar{0},\bar{i}) = (00\ldots0,11\ldots1)\) and \((\bar{1},\bar{0}) = (11\ldots1,00\ldots0)\) positions. Additional considerations of symmetry and positive definiteness reduce the calculation to a one variable problem which can be solved by minimizing \( \|\rho_0 - \tau_0\| \) over the remaining free parameter. The result of that calculation provides a judicious guess for the form of \( \tau_0 \), and the work is in the verification. These results include the two qubit case which has \( r_2 = 2 \) in the notation below.

**Theorem 8.1** For fixed \( n \geq 2 \) let \( r_n = 2^{n-1} \) and let \( \tau_0 \) denote the \( 2^n \times 2^n \) matrix with entries equal to 0 except for

\[
\tau_0(\bar{0},\bar{0}) = \tau_0(\bar{i},\bar{i}) = a_n = \frac{r_n^2 - 2 r_n + 2}{2 r_n^2 - 2 r_n + 2},
\]
\[
\tau_0(\bar{0},\bar{i}) = \tau_0(\bar{i},\bar{0}) = b_n = \frac{1}{2 r_n^2 - 2 r_n + 2},
\]
and with all other entries on the diagonal also equal to \( b_n \). Then

\[
m[\rho_0] = \|\rho_0 - \tau_0\| = \frac{1}{\sqrt{2}} \left( 1 - \frac{1}{r_n^2 - r_n + 1} \right)^{\frac{1}{2}}
\]
The extreme points of $F(\rho_0, \tau_0)$ consist of $|\hat{0}\rangle \langle \hat{0}|$, $|\hat{1}\rangle \langle \hat{1}|$, and projections of the form $\tau = \bigotimes_{k=1}^{n} |\psi_k\rangle \langle \psi_k|$ where $|\psi_k\rangle = \frac{1}{\sqrt{2}} \left( e^{i\varphi_k/2} |0\rangle + e^{-i\varphi_k/2} |1\rangle \right)$ with $\Phi = \sum_k \varphi_k \equiv 0$ modulo $2\pi$.

Proof: The calculation of $\|\rho_0 - \tau_0\|$ is routine, once we know that $\tau_0$ is the closest separable density. Thus we want to show that $Tr(A_0\tau) \geq 0$ for separable $\tau$ when $A_0 = c_0 I + \tau_0 - \rho_0$, and as usual it suffices to check the inequality for separable projections. A routine calculation of $c_0 = Tr(\tau_0 (\rho_0 - \tau_0))$ gives $c_0 = \frac{r_{0,\tau}^2}{r_{0,\tau}^2 - 2r_{0,\tau} + 2}$. A separable projection can be written as the tensor product of $n$ matrices of the form

$$
\left( \begin{array}{cc} r_k^2 (0) & r_k (0) r_k (1) e^{-i\varphi_k/2} \\ r_k (0) r_k (1) e^{i\varphi_k/2} & r_k^2 (1) \end{array} \right),
$$

and when we carry out the details we find that

$$
Tr(A_0\tau) = \frac{r_n}{2r_{0,\tau}^2 - 2r_{0,\tau} + 2} F(\tau)
$$

with

$$
F(\tau) = 1 - \prod_k r_k^2 (0) - \prod_k r_k^2 (1) - (2^n - 2) \prod_k r_k (0) r_k (1) \cos (\Phi)
$$

(8.2)

where $\Phi = \sum_k \varphi_k$. Since $r_k^2 (0) + r_k^2 (1) = 1$, we can write the 1 in $F(\tau)$ as the product of all $n$ terms $r_k^2 (0) + r_k^2 (1)$. Subtracting $\prod_k r_k^2 (0) + \prod_k r_k^2 (1)$ from that product leaves $2^n - 2$ terms of the form $\prod_k r_k^2 (j_k)$ where the binary indices $j_k$ are not all the same. These terms can be grouped in pairs so that each factor of $r_k^2 (0)$ and $r_k^2 (1)$ appears in exactly one of the two paired terms. Then $F(\tau)$ can be written as the sum of $2^{n-1} - 1$ expressions of the form

$$
\left[ \prod_k r_k^2 (j_k) + \prod_k r_k^2 (\bar{j}_k) - 2 \prod_k r_k (0) r_k (1) \cos (\Phi) \right],
$$

(8.3)

where $\bar{j}_k$ denotes the binary complement of $j_k$. Since each of these expressions is non-negative, $Tr(A_0\tau) \geq 0$ for separable $S$.

Suppose $F(\tau) = 0$ for $\tau$ a separable projection. Then it’s easy to check from equation (8.1) that if any one of the factors $r_k (0) = 1$, all of the factors $r_j (0) = 1$ and $|\hat{0}\rangle \langle \hat{0}|$ is in $F(\rho_0, \tau_0)$. Similar reasoning shows that $|\hat{1}\rangle \langle \hat{1}|$ is also in $F(\rho_0, \tau_0)$, and the only remaining case is when none of the factors equals zero. Since each expression in equation (8.2) must be zero, $\cos (\Phi) = 1$ and

$$
\prod_k r_k (j_k) = \prod_k r_k (\bar{j}_k) \neq 0
$$

for all $n$-tuples $(j_1, \ldots, j_n)$. But then it is easy to show that $r_j (0) = r_j (1) = 1/\sqrt{2}$ for all $j$, completing the characterization of the extreme points of $F(\rho_0, \tau_0)$ and the proof of the theorem. □
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