Extrapolated Quantum States, Void States, and a Huge Novel Class of Distillable Entangled States

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Abstract A nice and interesting property of any pure tensor-product state is that each such state has distillable entangled states at an arbitrarily small distance $\varepsilon$ in its neighbourhood. We say that such nearby states are $\varepsilon$-entangled, and we call the tensor product state in that case, a “boundary separable state”, as there is entanglement at any distance from this “boundary”. Here we find a huge class of separable states that also share that property mentioned above – they all have $\varepsilon$-entangled states at any small distance in their neighbourhood. Furthermore, the entanglement they have is proven to be distillable. We then extend this result to the discordant/classical cut and show that all classical states (correlated and uncorrelated) have discordant states at distance $\varepsilon$, and provide a constructive method for finding $\varepsilon$-discordant states.

Keywords quantum computing and quantum information, entanglement, distillability, discord.

1 Introduction

Studying the structure of the set of quantum states has been a central topic in quantum information research (Bengtsen and Zyczkowski 2006). Particular emphasis is on the tensor product structure of this space in terms of entanglement (Horodecki et al 2009) and general correlations (Modi et al 2012; Brunner et al 2014; Groisman et al 2007). The study has lead to the identification of important families of states such as Werner states (Werner 1989), bound entangled states (Horodecki 1997; Bennett et al 1999b), and the W-states (Dur et al 2000), as well as interesting sets of bases such as unextendable product bases (UPB) (Bennett et al 1999b) and locally indistinguishable bases (Bennett et al 1999a).

One method which has been particularly powerful in the study of state-space is interpolation, i.e. studying the states that lay between two known states with different properties. Interpolation has been used in the study of robustness to various types of noise (Vidal and Tarrach 1999) and learning about the ball of separable state (Braunstein et al 1999). The complementary method, extrapolation, has also been used in some cases for example in the study of non-signaling theories (Acín et al 2010) where trace one Hermitian operators with negative eigenvalues were required for larger than quantum violations of Bell inequalities.

Here we use both extrapolation and interpolation to study the boundaries between various subsets of quantum spaces with particular emphasis on boundary separable states - separable states that are arbitrarily close to an entangled state cf. Definition 1.

Any pure tensor product state has entangled states near it, at any distance (i.e. arbitrarily close), making it boundary separable (cf. corollary 19). Another simple example of a boundary separable state is a Werner-state $\lambda/3|\psi_+\rangle + \rho_{\phi_+} + \rho_{\phi_-} + (1-\lambda)|\psi_-\rangle$ (built from the four Bell states) with $\lambda = 1/2$ which has entangled states near it, at any distance.

Is the property of being separable yet having entangled states nearby at any distance common? Or is it rare? Furthermore, what can we learn about the type of entanglement that those nearby entangled states have? For two qubits, it

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A preliminary version of this work (without discordant states) appeared in TPNC-2014 (Boyer and Mor 2014).
is known (Horodecki et al. 1997) that the entanglement is always distillable. For qudits, cf proposition [18]

Our main result is a number of families of boundary separable quantum states. We show that states in these families are arbitrarily close to distillable entangled states and give a constructive method for identifying these states. We also provide similar results for discord (cf. Corollary [23] for example), showing that all classical states (classically correlated and uncorrelated) are boundary classical (in fact there is a discordant and thus non classical state arbitrarily close) and providing a constructive way to find an arbitrarily close discordant state. Our results are presented in order of complexity starting from two qubit examples and continuing to more general results involving qutrits, qudits and multi-qubit systems. In most cases the results are presented through examples. The general implications are discussed at the end of each section.

1.1 The set of quantum states

Given a Hilbert space \( \mathcal{H} \), the set of quantum states (i.e. the set of positive semidefinite trace one Hermitian operators) on \( \mathcal{H} \) is convex. If the Hilbert space has a physically meaningful tensor product structure \( \mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B \) it is useful and interesting to consider subsets of states based on this structure. These subsets are often not convex and are hard to characterize. In the work presented here we will use convex and affine mixtures of states to study the states that lay at the boundary of these subsets.

One important subset of states is the set of pure states \( |\psi\rangle \langle \psi| \) (i.e. states of rank 1). In this set we identify a smaller subset of pure product states of the form \( |\psi\rangle \langle \psi| = |\phi\rangle \langle \psi| \otimes |\psi\rangle \langle \phi| \). All pure states that are not product are called entangled pure states. Pure states are extremal points in the set of all states.

There are various ways to similarly divide the set of all states. One division is into the complementary subsets: separable states and entangled states. For any bipartite system whose Hilbert spaces are of dimension at least 2, both sets, entangled and separable, have a finite volume in the set of all states (Horodecki et al. 2009). The set of entangled states is not convex and in general it is hard to identify whether a state is entangled or separable (Gurvits 2003). At the border between separable and entangled states are the boundary separable and \( \varepsilon \)-entangled states. Some properties of this boundary were previously studied in relation to non-linear entanglement witnesses (Guhne and Lütkenhaus 2007) where it was shown that the set of all separable states is not a polytope (see also Horodecki et al. 2009). Our main results are specific families of boundary separable and \( \varepsilon \)-entangled states; some of these families such as those close to thermal states are of particular importance in quantum computing. There are a number of physically meaningful ways to divide the set of entangled states. One that we will use here is to divide the set into two disjoint subsets, distillable and bound-entangled states. A state \( \rho \) is distillable if it is possible to distill many copies of \( \rho \) into a maximally entangled state. Clearly separable states cannot be distilled, but surprisingly there are entangled states that cannot be distilled. These are known as bound entangled states. It is known that states with a non-positive partial transpose are bound entangled, similarly if the total dimension of the Hilbert space is not larger than 6, all entangled states are distillable (and have non-positive partial transpose) (Horodecki et al. 2009).

A different classification of the set of all states is into the complimentary subsets: Discordant states and states that are classical with respect to A (Modi et al. 2012), the latter are sometimes called classical-quantum (see Sec. 2.5 for precise definitions). For simplicity we use \( C_A \) to denote the set of states that are classical with respect to A and note that the set of classical states, i.e. those that are classical with respect to A, B and both, is a subset of \( C_A \). The set of discordant states is \( \tilde{C}_A \). The classification into \( C_A \) and \( \tilde{C}_A \) shares some properties with the classification of pure states. For example, like the set of pure product states which is vanishingly small in the set of all pure states (i.e. it requires strictly fewer parameters to characterize a pure product state than to characterize a generic pure state), the set \( C_A \) is vanishingly small in the set of all states (Ferraro et al. 2010). Moreover, for pure states, discord and entanglement coincide. However, in general we can only say that entangled states are always discordant and classical states (with respect to \( A, B \) or both) are always separable. There is, an intermediate regime of discordant-separable or discordant states (Modi et al. 2010) (see fig. 1). As we will show below, all classical states (with respect to \( A, B \) or both) are also boundary classical, i.e. a state
is either discordant or there is a discordant state arbitrarily close to it.

Although discord refers to a specific quantity (Ollivier and Zurek 2001) other similar quantities exist (Modi et al 2012). Like entanglement monotonos each measure has its own domain but generally there is an unambiguous way to quantify states as uncorrelated (product), classically correlated, dissonant (discordant and separable) and entangled (Modi et al 2012). A caveat on the last statement is that in general discord-like measures are not necessarily defined to be symmetric with respect to the parties involved and the cut between discordant and classical depends on this choice. Here we mostly consider the asymmetric versions that were discussed in the early literature, in particular the sets $C_A$ and $C_A^+$; however all of our results apply to the various symmetric versions of discord in (Modi et al 2012).

A final classification is in terms of the eigenvectors of the state. A state has a product eigenbasis if it can be diagonalized in an orthonormal basis of product states. Surprisingly the decomposition of a state into eigenstates is not sufficient to tell us about entanglement or discord. In general non-degenerate separable states can have a non-separable eigenbasis (Groisman et al 2007). On the other hand a discordant state can have a product eigenbasis.

2 Notations and Terminology

2.1 General notation

In the majority of cases below we consider bipartite states as operators on a Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$ (in Sec. 5 we also consider multipartite systems). We use $T$ to denote the transpose map, similarly $(T \otimes 1)$ denotes partial transposition on $A$. Distance between two states $\rho$ and $\tau$ will be given by the trace distance $\delta(\rho, \tau) = \frac{1}{2} \text{Tr}|\rho - \tau|$.

2.2 Entanglement and separability

A convex mixture of pure states is called mixed. A quantum state $\rho$ on $\mathcal{H}_A \otimes \mathcal{H}_B$ is called a product state if it can be decomposed into $\rho = \rho_A \otimes \rho_B$, where $\rho_A$ and $\rho_B$ are states on $\mathcal{H}_A$ and $\mathcal{H}_B$ respectively; $\rho$ is called separable if it can be decomposed into a convex sum of product states, otherwise it is called entangled (cf Appendix A). Product states are also separable.

2.3 Boundary Separable States and $\epsilon$-Entangled States

Definition 1 A boundary separable state is a separable state $\rho_b$ such that for any $\epsilon > 0$, there is an entangled state $\rho_e$ for which $\delta(\rho_b, \rho_e) \leq \epsilon$, i.e. there are entangled states arbitrarily close to $\rho_b$.

Notice that for any density operator $\rho$, and $0 \leq \epsilon \leq 1$, if $\tau_\epsilon = (1 - \epsilon)\rho_b + \epsilon\rho$ (1)

then $\delta(\tau_\epsilon, \rho_b) = \frac{1}{2} \text{Tr}|\rho - \rho_b| = \epsilon \delta(\rho, \rho_b)$ and thus $\delta(\tau_\epsilon, \rho_b) \leq \epsilon$.

The trace distance between $\tau_\epsilon$ given by (1) and the (boundary) separable state $\rho_b$ is at most $\epsilon$ but it may be much smaller than $\epsilon$; it is $\epsilon$ iff $\delta(\rho, \rho_b) = 1$ i.e. if $\rho_b$ and $\rho$ are orthogonal (have orthogonal support).

Definition 2 An $\epsilon$-entangled state is an entangled state $\rho_e$ such that there is a boundary separable state $\rho_b$ for which $\delta(\rho_e, \rho_b) \leq \epsilon$; i.e. it is at trace distance at most $\epsilon$ from a boundary separable state.

As an example, the Werner state with $\lambda = 1/2$ is a boundary separable state and mixing it with $\rho_{\psi_-}$ gives $\epsilon$-entangled states.

There are separable states $\rho_b$ for which there exists a state $\rho$ such that all the states $\tau_\epsilon$ given by (1) are entangled for $\epsilon$ small enough, $\epsilon \neq 0$. There is a continuous path starting from $\rho_b$ and going straight in the direction of $\rho$ whose initial section contains only $\epsilon$-entangled states. Note that for $\epsilon = 0$ the resulting state $\tau_0$ is the boundary separable-state $\rho_b$ itself; $\tau_0 = \rho_b$. As an example, again, the Werner state with $\lambda = 1/2$ is a boundary separable state, such that mixing it with $\rho_{\psi_-}$ as in (1) gives epsilon-entangled states, and there is a continuous path from this Werner state and all the way to the fully entangled state $\rho_{\psi_-}$.

2.4 “Extrapolated States” and “Void States”

Given any two states $\rho_0$ and $\rho_1$, the operators $\rho_t = (1 - t)\rho_0 + t\rho_1$ are clearly always Hermitian with trace 1; when $0 \leq t \leq 1$, they are (mixed) states, all on a straight line segment between $\rho_0$ and $\rho_1$; those mixed states are obtained by interpolation (convex combination) of two states. Let us now introduce three additional definitions:

a) When $t < 0$, $\rho_t$ is on the same straight line but is no longer between $\rho_0$ and $\rho_1$; in general, if $\rho_0 \neq \rho_1$ and all the eigenvalues of $\rho_0$ are strictly positive, then there are values of $t < 0$ such that $\rho_t$ is a state; we call such states extrapolated states.
We consider a state \( \rho \) to the basis of \( \mathcal{H} \).

**Definition 4**

The state \( \rho \) is said to be classical with respect to the basis \( \{ |i\rangle \} \) of \( \mathcal{H} \) if it satisfies one of the above conditions.

Note that if \( \rho_0 = |0\rangle \langle 0| \) and \( \rho_1 = |1\rangle \langle 1| \), then \( (1-t)\rho_0 + t\rho_1 = (1-t)|0\rangle \langle 0| + t|1\rangle \langle 1| \) is not a state (it is not positive semi definite) as soon as \( t < 0 \) (or \( t > 1 \)).

There may be some value \( m < 0 \) such that \( \rho_0 \) is no longer positive semi-definite for \( t < m \), thus no longer a state (hence it is not a physical entity), while it is still positive semi-definite for \( t = m \).

The condition that the eigenvalues of \( \rho_0 \) be all positive is sufficient for defining extrapolated states, but not necessary. One can extrapolate carefully-chosen states that have some 0 eigenvalues. Extrapolation somewhat behaves like subtraction: if \( t < 0 \), then \( \rho_t = (1+|t|)\rho_0 - |t|\rho_1 \). We will be interested only with extrapolations with \( t < 0 \) though \( t > 1 \) could also provide extrapolations.

b) A void state is a quantum state that has exactly one zero eigenvalue. Namely, when diagonalized, it has exactly one zero on the diagonal.

c) A k-void state (of dimension \( N > k \)) is a quantum state that has exactly \( k \) zero eigenvalue\(^3\) (similarly, it has rank \( N - k \)).

2.5 Discord and classical correlation

We consider a state \( \rho \) of a bipartite system \( AB \) with marginals \( \rho_A \) and \( \rho_B \).

**Proposition 3**

Let \( \rho \) be a state of \( \mathcal{H}_A \otimes \mathcal{H}_B \) and \( \{ |i\rangle \} \) be a basis of \( \mathcal{H}_A \). Then the following three statements are equivalent (Modi et al 2012).

1. There is a set of states \( \{ \tau_i \} \) on \( \mathcal{H}_B \) such that
   \[
   \rho = \sum \lambda_i |i\rangle \langle i| \otimes \tau_i,
   \]
   where \( \lambda_i \geq 0 \) and \( \sum \lambda_i = 1 \).

2. There is a set of unitary operators \( U_i \) such that
   \[
   \rho = \sum \mu_{ij} |i\rangle \langle j| \otimes U_i |j\rangle \langle U_i^\dagger |j\rangle \langle j|,
   \]
   where \( \mu_{ij} \geq 0 \) are the eigenvalues of \( \rho \).

3. \( \rho \) is invariant under the action of the local dephasing channel \( D \).

**Definition 5**

A state \( \rho \) is said to be classical with respect to \( A \) if there is a basis of \( \mathcal{H}_A \) with respect to which it is classical; the set of classical states with respect to \( A \) is denoted \( \mathcal{C}_A \). A state \( \rho \) which is not in \( \mathcal{C}_A \) is called discordant (Modi et al 2012; Henderson and Vedral 2001; Ollivier and Zurek 2001)\(^4\).

The set of discordant states is \( \mathcal{C}_A \).

**Remark 6**

It is important to notice that all classical states (i.e. classical with respect to both \( A \) and \( B \)) are in \( \mathcal{C}_A \) and thus that a state not in \( \mathcal{C}_A \) (i.e. discordant) cannot be classical. We will use that fact to build non classical (in fact, discordant) states arbitrarily close to any classical state.

**Remark 7**

Any state which is not product is called correlated.

The set \( \mathcal{C}_A \) contains both correlated and uncorrelated states while all states in \( \mathcal{C}_A \) are correlated. These are sometimes called quantum correlated (Modi et al 2012).

When \( \rho_A = \sum \lambda_i |i\rangle \langle i| \) is not degenerate, i.e., \( \lambda_i \neq \lambda_j \) if \( i \neq j \), the conditions above provide a very simple method to check if \( \rho \) is in \( \mathcal{C}_A \) (Brodutch and Terno 2010). When \( \rho_A \) is degenerate one has to check over all its possible eigenbases.

2.5.1 Boundary classical states

In the same way as above it is possible to define boundary classical states and \( \epsilon \)-discordant states. As we will see this definition is superfluous since all classical states are also boundary classical; cf. Corollary 23.

3 Two Qubits

Our first example of 2-party boundary separable-states (and the derived \( \epsilon \)-entangled states) is obtained by starting from a completely mixed state and “fully subtracting” one of the eigenstates, to obtain a separable void state. Our second example uses a different—yet very interesting state to start with—the thermal state. As in the first example, a void-state is generated from the thermal state (via extrapolation) by subtracting one of the eigenstates. Our third example uses a 2-void state instead of a simple (1-)void state (and we also discuss here the case of 3-void state which in this case is a tensor product state). Our last two 2-qubit examples provide generalizations to less trivial cases including discordant states and separable states without a product eigenbasis. Since two qubit states that are entangled are all distillable (Horodecki et al 1997), the states obtained are thus also distillable.

\(^3\) Note that a separable \( N - 1 \)-void state is a tensor product state.

\(^4\) The term classical is used in a variety of ways in the literature, here we use it in the sense of correlations as in (Modi et al 2012).
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3.1 Example 1 – The Extrapolated Pseudo-Pure State of Two Qubits

Mixing a completely mixed state \( \rho_0 \) with an arbitrary state \( \rho_1 \) to yield the pseudo pure state (PPS) \( \rho = (1 - t)\rho_0 + t\rho_1 \) is found to be extremely useful in quantum information processing (e.g. in NMR quantum computing). To the best of our knowledge, an extrapolated state of the form \( \rho = (1 + |t|)\rho_0 - |t|\rho_1 \) was never used. This “extrapolated pseudo pure state” (EPPS), whenever it is a legal quantum state, shares with the conventional PPS the fact that applying any unitary transformation acts only on \( \rho_1 \).

An interesting special case of this EPPS is when \( |t| \) is exactly sufficiently large to make one eigenvalue vanish (become zero). If \( \rho_1 \) is a pure tensor product state, then the resulting \( \rho \) is a void state. We assume here that the subtracted tensor product state is written in the computational basis, e.g., it is \( |11\rangle\langle 11| \) and \( m = t = -1/3 \).

**Proposition 8** If the standard basis is the eigenbasis of a state \( \rho \) on \( \mathcal{H}_2 \otimes \mathcal{H}_2 \), and if the eigenvalue of \( |11\rangle \) is 0, and the other three eigenvalues are \( 1/3 \), then there are states arbitrarily close to \( \rho \) that are entangled. [The same holds, with obvious adjustments, for any other tensor-product eigenstate that has a zero eigenvalue.]

We avoid proving this proposition as we later (in example 4) prove a more general result, containing the above (and also example 2) as special cases. The above mentioned (very basic) example is mainly given for historical reasons, as it was the first example we found.

For \( j \) fixed, let

\[
\rho = \frac{4}{3} \left[ \frac{1}{4} \sum_{i=0}^{3} |i\rangle\langle i| - \frac{1}{3} |j\rangle\langle j| \right] = \frac{4}{3} \sum_{i=0,j \neq j}^{3} |i\rangle\langle i|.
\]

This is obtained by choosing \( |j\rangle \) (viewed as a two bit integer from \( 0 = 00 \) to \( 3 = 11 \)) to be any product state \( j \equiv j_{AB} = j_A \otimes j_B \), where the two parties are \( A \) for Alice’s qubit and \( B \) for Bob's. In fact, for all values of \( t \) between 0 and \( -1/3 \), the Hermitian operators

\[
\rho_t = (1 - t) \left[ \frac{1}{4} \sum_{i=0}^{3} |i\rangle\langle i| \right] + t|j\rangle\langle j|
\]

are separable states; for \( t < -1/3 \), \( \rho_t \) is no longer a state since it is no longer positive semi definite, the eigenvalue of \( |j\rangle \) becoming negative. Finally, if \( |j\rangle = |11\rangle \), proposition 8 tells us that there are entangled states arbitrarily close to

\[
\frac{1}{3} \sum_{i=0}^{3} |i\rangle\langle i|.
\]

3.2 Example 2 – The Thermal State of Two Qubits

The thermal state on two qubits is the state

\[
\rho_\Theta = \frac{(1 + \eta)^2}{4} |00\rangle\langle 00| + \frac{1 - \eta^2}{4} (|01\rangle\langle 01| + |10\rangle\langle 10|)
\]

\[
+ \frac{(1 - \eta^2)}{4} |11\rangle\langle 11|.
\]

The state \( |11\rangle \) is a 0-eigenstate of \( \rho_\Theta = (1 + \eta)\rho_\Theta - \eta^2 |11\rangle\langle 11| \) if \( (1 - \eta^2)(p + 1) = 4\eta \) and a proposition similar to proposition 3 can be written for \( \rho_\Theta \). However, both cases of Sections 3.1 and 3.2 will be dealt with, by a generalization done in example 4.

The thermal state will get more attention later on, when we discuss \( N \) qubits.

3.3 Example 3 — 2-Void State

Example 3, using a 2-void state, is as follows:

**Proposition 9** In \( \mathcal{H}_2 \otimes \mathcal{H}_2 \) there are entangled states arbitrarily close to the state \( \rho = \frac{1}{2} (|01\rangle\langle 01| + |10\rangle\langle 10|) \).

**Proof** Here again, \( |11\rangle \) is an eigenstate of \( \rho \) of 0 eigenvalue. Let \( \rho_1 = |\psi_+\rangle\langle \psi_+| \) with \( |\psi_+\rangle = \frac{1}{\sqrt{2}} (|01\rangle + |10\rangle) \) and \( \rho_\varepsilon = (1 - \varepsilon)p + \varepsilon \rho_1 \). Then \((T \otimes I)(\rho_\varepsilon)\), where \( T \) is the transpose operator, is

\[
\begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 1/2 & \varepsilon/2 & 0 \\
0 & \varepsilon/2 & 1/2 & 0 \\
0 & 0 & 0 & 0
\end{pmatrix} \approx \begin{pmatrix}
0 & 0 & 0 & \varepsilon/2 \\
0 & 1/2 & 0 & 0 \\
0 & 0 & 1/2 & 0 \\
\varepsilon/2 & 0 & 0 & 0
\end{pmatrix}
\]

with characteristic equation \( (\lambda - 1/2)^2(\lambda^2 - \varepsilon^2/4) = 0 \) and eigenvalues \( 1/2, \varepsilon/2 \) and \( -\varepsilon/2 \); by the Peres criterion \( \delta(\rho, \rho_\varepsilon) \leq \varepsilon \).

Although the Peres Criterion is well known, it is provided for completeness of the exposition in appendix A.
In fact, there was no need to solve the characteristic equation to show that $(T \otimes I)(\rho_1)$ is not positive semi definite. That can be seen directly from the matrix of $(T \otimes I)(\rho_1)$ because there is a 0 on the main diagonal for which the corresponding row and column are not zero: This is a consequence of the following well known lemma with $|\varphi\rangle = |11\rangle$ and $|\psi\rangle = |00\rangle$; indeed, since by very definition of the partial transpose $(i_1f_1)(T \otimes I)(\rho_1)(i_2f_2) = (i_2f_2)(\rho_1)(i_1f_1)$, it follows that $\langle 11 | (T \otimes I)(\rho_1) | 11 \rangle = \langle 11 | \rho_1 | 11 \rangle = 0$ and $\langle 11 | (T \otimes I)(\rho_1) | 00 \rangle = \langle 01 | \rho_1 | 10 \rangle \neq 0$.

**Lemma 10** Let $A$ be a Hermitian operator on $\mathcal{H}$; if there are $|\varphi\rangle$ and $|\psi\rangle$ such that $\langle \varphi | A | \varphi \rangle = 0$ and $\langle \varphi | A | \psi \rangle \neq 0$ then $A$ is not positive semi definite.

**Proof** See appendix A.4

3.4 Example 4 — A Generalization

Example 4 generalizes examples 1, 2 and 3:

**Theorem 11** If the standard basis is the eigenbasis of a state $\rho$ on $\mathcal{H}_2 \otimes \mathcal{H}_2$, and if the eigenvalue of $|11\rangle$ is 0, then there are states arbitrarily close to $\rho$ that are entangled. The same holds for any eigenstate and any product eigenbasis.

**Proof** Let indeed $\rho = \lambda_{00} |00\rangle \langle 00| + \lambda_{01} |01\rangle \langle 01| + \lambda_{10} |10\rangle \langle 10|,$

i.e. $|11\rangle$ has eigenvalue $\lambda_{11} = 0.$ Let

$\rho_1 = \rho_{\varphi_0} = \frac{1}{2} \left[ |01\rangle \langle 01| + |10\rangle \langle 10| + |00\rangle \langle 01| + |10\rangle \langle 11| \right]$

and $\rho_\varepsilon = (1-\varepsilon) \rho + \varepsilon \rho_1.$

The partial transpose $(T \otimes I)(|i_1f_1\rangle \langle i_2f_2|)$ on basis states being equal to $|i_2f_2\rangle \langle i_1f_1|$, it is clear that $(T \otimes I)(\rho) = \rho.$ The partial transpose of $\rho_1$ is

$(T \otimes I)(\rho_1) = \frac{1}{2} \left[ |01\rangle \langle 01| + |11\rangle \langle 00| + |00\rangle \langle 11| + |10\rangle \langle 10| \right].$

If follows that

$\langle 11 | (T \otimes I)(\rho_1) | 11 \rangle = 0,$

and by lemma 10 $(T \otimes I)(\rho_\varepsilon)$ is not positive semi definite if $\varepsilon > 0$ and by the Peres criterion it follows that the state $\rho_\varepsilon$ is then not separable; since $\delta(\rho, \rho_\varepsilon) \leq \varepsilon$, there are states arbitrarily close to $\rho$ that are not separable. □

Notice that all that is needed is that $\lambda_{11} = 0.$ Nothing prevents $\lambda_{10} = \lambda_{01} = 0.$ That implies, after a suitable choice of basis for the two systems, that any pure product state has arbitrarily close entangled states: being two qubit states, they are also distillable (Horodecki et al. [1997]), showing that there are arbitrarily close distillable states. By symmetry, the result clearly holds if any of the other eigenvalues is known to be 0 instead of $\lambda_{11}.$ Moreover the choice of product basis is arbitrary and the same argument applies for any product basis.

3.5 Example 5. A discordant product state with a non-product eigenbasis

Take the discordant state

$\rho = \frac{1}{2} \begin{bmatrix} |00\rangle \langle 00| + |++)\langle ++| \end{bmatrix}$,

where, this time, the representation is not spectral because $|00\rangle$, $|++)\rangle$, are not part of an orthonormal basis of $\mathcal{H}_2 \otimes \mathcal{H}_2$; neither $|00\rangle$ nor $|++)\rangle$ is an eigenvector of $\rho.$ The state $\rho$ is equal to $\frac{1}{2} \begin{bmatrix} |00\rangle \langle 00| + \frac{1}{4} \sum_{ijkl} |ij\rangle \langle kl| \end{bmatrix}$ and is represented, in the standard basis, by the matrix

$$\begin{bmatrix} 5 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}$$

Since the spectral decomposition is unique, this shows that the spectral decomposition of $\rho$ has eigenvectors that are not separable even though $\rho$ is itself separable: separability of a state does not imply that its eigenbasis is made out of separable states.

As we will see in sections 3.6 and 4 the absence of a separable eigenbasis is not a necessary and sufficient condition for discord.

**Proposition 12** If $\rho = \frac{1}{2} \begin{bmatrix} |00\rangle \langle 00| + |++)\langle ++| \end{bmatrix}$ and $\rho_{\varphi_1} = |\varphi_+\rangle \langle \varphi_+|$, with $|\varphi_+\rangle = \frac{1}{\sqrt{3}} \left[ |00\rangle + |11\rangle \right]$, then for $0 < \varepsilon \leq 1$, the states $\rho_\varepsilon = (1-\varepsilon) \rho + \varepsilon \rho_{\varphi_1}$ are all entangled.

**Proof** Clearly $(T \otimes I)(\rho) = \rho.$ Also

$$(T \otimes I)(\rho_{\varphi_1}) = \frac{1}{2} \begin{bmatrix} |00\rangle \langle 00| + |10\rangle \langle 01| + |01\rangle \langle 10| + |11\rangle \langle 11| \end{bmatrix}$$

Let $|\psi_-\rangle = \frac{1}{\sqrt{2}} \left[ |01\rangle - |10\rangle \right].$ A simple calculation shows that

$$\langle \psi_- | (T \otimes I)(\rho_{\varphi_1}) | \psi_- \rangle = -\frac{1}{2}$$

and $\langle \psi_- | \rho | \psi_- \rangle = 0.$

It follows that $\langle \psi_- | (T \otimes I)(\rho_{\varphi_1}) | \psi_- \rangle = -\varepsilon/2$ which shows directly that the partial transpose of $\rho_\varepsilon$ is not positive semi definite for $\varepsilon > 0.$ The state $\rho_\varepsilon$ is consequently entangled and the discordant state $\rho$ is boundary separable. □
3.6 Example 6 - A Classical-Quantum state

As mentioned in the introduction (sec 1.1), the definition of discord is asymmetric. The following state is classical with respect to A, but it is not classical with respect to B; it becomes discordant under the interchange of the subsystems A ↔ B. Such states are often called classical-quantum (Modi et al 2012).

Proposition 13 Let

\[ \rho = \lambda_{00} |00\rangle \langle 00| + \lambda_{01} |01\rangle \langle 01| + \lambda_{1+} |1+\rangle \langle 1+| + \lambda_{1-} |1-\rangle \langle 1-| \]

(2)

If any of the eigenvalues is 0, then there are states arbitrarily close to \( \rho \) that are entangled.

Proof This time we first prove if \( \lambda_{00} = 0 \) i.e. if

\[ \rho = \lambda_{01} |01\rangle \langle 01| + \lambda_{1+} |1+\rangle \langle 1+| + \lambda_{1-} |1-\rangle \langle 1-|. \]

Let again \( \rho_1 = \frac{1}{2} \left[ |01\rangle \langle 01| + |01\rangle \langle 10| + |10\rangle \langle 01| + |10\rangle \langle 10| \right] \) and \( \rho_2 = \left( 1 - \epsilon \right) \rho + \epsilon \rho_1 \). Then \( \langle 00| (T \otimes I)(\rho_2) |00\rangle = 0 \) and \( \langle 00| (T \otimes I)(\rho_2) |11\rangle = \epsilon / 2 \) so that \( \rho_2 \) is not positive semi-definite by Lemma 10 and \( \rho_e \) is thus entangled by the Peres criterion. Had we written explicitly the matrix, we would have seen the following pattern

\[
(T \otimes I) (\rho_e) = \begin{pmatrix}
0 & 0 & 10 & 11 \\
01 & 0 & 11 & \epsilon / 2 \\
10 & 11 & 0 & \epsilon / 2 \\
11 & \epsilon / 2 & 11 & 0
\end{pmatrix}
\]

with a 0 entry on the main diagonal for which the line is not identically 0 and concluded that \( (T \otimes I)(\rho_2) \) is not positive semi definite if \( \epsilon \neq 0 \).

In this proof, it was assumed that \( \lambda_{00} = 0 \) but the same result holds if the eigenvalue of any other basis element is 0; for instance, if the eigenvalue of \( |1-\rangle \) is 0, then applying \( X \otimes X \) to the basis and [1-] onto \( |00\rangle \) for \( |1+\rangle \) we need to apply \( X \otimes H \), and for \( |01\rangle \) we apply \( I \otimes X \).

The state in equation (2) has a product eigenbasis. We can make it discordant by interchanging the subsystems A ↔ B in which case it is a discordant state with a product eigenbasis.

3.7 Two qubits - discussion

In this section we provided a number of examples of boundary separable states. More generally, we showed (Theorem 11) that any two qubit state which has a product basis and is not full rank is on the boundary. We also showed that separable states may have eigenstates which are not separable (example 5) and that discordant states can have a separable eigenstates (example 6).

4 Two qutrits

Some of the subtleties of bipartite systems cannot be seen in qubit-qubit pairs and qubit-qutrit pairs. These include UPBs and bound entangled states (Bennett et al. 1999b) and locally indistinguishable product states (Bennett et al. 1999a).

4.1 A mixture of locally indistinguishable product states

Consider the following states on a bipartite system where \( |a \pm b\rangle \) denotes the state \( \frac{1}{\sqrt{2}}(|a\rangle \pm |b\rangle) \).

\[
\begin{align*}
|\psi_1\rangle &= |1\rangle \\
|\psi_2\rangle &= |0\rangle + |1\rangle \\
|\psi_3\rangle &= |0\rangle - |1\rangle \\
|\psi_4\rangle &= |2\rangle + |1\rangle \\
|\psi_5\rangle &= |2\rangle - |1\rangle \\
|\psi_6\rangle &= |1\rangle + |2\rangle \\
|\psi_7\rangle &= |1\rangle - |2\rangle \\
|\psi_8\rangle &= |0\rangle + |1\rangle \\
|\psi_9\rangle &= |0\rangle - |1\rangle
\end{align*}
\]

Proposition 14 The state \( \rho_0 = 1/8 \sum_{i=2}^{9} |\psi_i\rangle \langle \psi_i| \) is boundary separable.

Proof Let \( |\Psi_e\rangle = \frac{1}{\sqrt{2}} [ |01\rangle \langle 01| + |10\rangle \langle 10| ] \) and \( \rho_1 = |\Psi_e\rangle \langle \Psi_e| \). Thus \( \rho_1 = \frac{1}{4} \left[ |01\rangle \langle 01| + |01\rangle \langle 10| + |10\rangle \langle 10| + |01\rangle \langle 01| \right] \). Let \( \rho_e = (1 - \epsilon) \rho_1 + \epsilon \rho_1 \). For \( 2 \leq i \leq 9 \), \( |\psi_i\rangle = 0 \) or \( \langle \psi_i| |10\rangle = 0 \) so that \( \langle 01| \rho_0 |10\rangle = 0 \) and thus \( \langle 01| \rho_e |10\rangle = \epsilon / 2 \). Also \( \langle 11| \rho_0 |11\rangle = \langle 11| \rho_1 |11\rangle = 0 \) and so \( \langle 11| \rho_e |11\rangle = 0 \). It follows that \( \langle 11| (T \otimes I)(\rho_e) |11\rangle = \langle 11| \rho_e |11\rangle = 0 \) and \( \langle 11| (T \otimes I)(\rho_e) |00\rangle = \langle 01| \rho_e |01\rangle = \epsilon / 2 \neq 0 \) and thus, for \( 0 < \epsilon < 1 \), \( \rho_e \) is entangled.

See appendix C for a matrix based argumentation.

The states in eq (3) cannot be distinguished using local operations (Bennett et al. 1999a) a property sometimes called non-locality without entanglement. In (Brody and Terno 2010) it was shown that given a set of states and a prior probability distribution, there is no relation between discord in the resulting mixed state and this property. Similarly a mixture of these 9 states is generally discordant with a product eigenbasis.

5 Two qudits (quantum digits)

We now consider bipartite systems, with each part of dimension at least two.
5.1 The ball of separable states

**Proposition 15** All states \( \rho \) in the finite ball \( \text{Tr}\|\rho - \frac{1}{2}I\|_2 < \frac{1}{2} \) are separable and not boundary separable.

**Proof** We know from the Gurvits-Barnum bound [Gurvits and Barnum 2002] that all states \( \rho \) with \( \|\rho - \frac{1}{2}I\|_2 < \frac{1}{2} \) are separable. Using the fact that \( \|\cdot\|_2 \leq \text{Tr}\|\cdot\| \) we can see that the maximally mixed state and any state close enough to it is not boundary separable. \( \Box \)

**Corollary 16** There are separable states that are not boundary separable.

5.2 A general class of boundary separable states

We now consider states of bipartite systems \( \mathcal{H}_A \otimes \mathcal{H}_B \) for which \( \dim \mathcal{H}_A \geq 2 \) and \( \dim \mathcal{H}_B \geq 2 \).

**Lemma 17** Let \( \rho_{00} \) be a state such that \( \langle 00 | \rho_{00} | 00 \rangle = 0 \) and \( \langle 10 | \rho_{10} | 01 \rangle = 0 \). Let \( \rho_1 \) be such that \( \langle 00 | \rho_1 | 00 \rangle = 0 \) and \( \langle 10 | \rho_1 | 01 \rangle = \epsilon^r \) for \( r > 0 \). Then \( \rho_\epsilon = (1 - \epsilon) \rho_0 + \epsilon \rho_1 \) is entangled and distillable for all \( 0 < \epsilon \leq 1 \).

**Proof** The conditions on \( \rho_0 \) and \( \rho_1 \) imply that
\begin{align*}
\langle 00 | \rho_{\epsilon} | 00 \rangle &= (1 - \epsilon) \langle 00 | \rho_0 | 00 \rangle + \epsilon \langle 00 | \rho_1 | 00 \rangle = 0, \\
\langle 10 | \rho_{\epsilon} | 01 \rangle &= (1 - \epsilon) \langle 10 | \rho_0 | 01 \rangle + \epsilon \langle 10 | \rho_1 | 01 \rangle = \epsilon^r.
\end{align*}
From [3] and [5] it follows that \( \langle 00 | (T \otimes 1)(\rho_\epsilon) | 00 \rangle = 0 \) and \( \langle 00 | (T \otimes 1)(\rho_1) | 11 \rangle = \epsilon^r \neq 0 \) and consequently \( (T \otimes 1)(\rho_\epsilon) \) is not positive semi-definite and \( \rho_\epsilon \) is entangled. We can do better. Let \( \langle \Psi_b \rangle = \sin(\theta) | 11 \rangle - e^{i\phi} \cos(\theta) | 00 \rangle \). Then, since \( \langle 00 | \rho_{\epsilon} | 00 \rangle = 0 \), \( \langle 01 | \rho_{1} | 10 \rangle = \langle 10 | \rho_{1} | 01 \rangle = \epsilon^r \) and \( \langle \Psi_b \rangle = \sin(\theta) | 11 \rangle - e^{i\phi} \cos(\theta) | 00 \rangle \), it follows that
\begin{align*}
\langle \Psi_b | (T \otimes 1)(\rho_\epsilon) | \Psi_b \rangle &= \sin^2(\theta) \langle 11 | \rho_\epsilon | 11 \rangle - 2 \cos(\theta) \cos(\epsilon) \epsilon.
\end{align*}
If \( \langle 11 | \rho_{\epsilon} | 11 \rangle = 0 \), the result is negative for \( 0 < \theta < \pi/2 \). Else for all \( \epsilon \neq 0 \) there exits \( \theta \) such that \( \langle 11 | \rho_{\epsilon} | 11 \rangle < 2 \cot(\theta) \epsilon \) i.e.\ such that \( \langle \Psi_b | (T \otimes 1)(\rho_\epsilon) | \Psi_b \rangle < 0 \), which implies that \( \rho_\epsilon \) is entangled and distillable by a lemma of [Kraus et al. 2002] (cf. appendix B).

We shall now consider separable void states with a separable 0 eigenvector. They are not only boundary separable but independently of the dimensions (larger than 2), they have arbitrarily close distillable entangled states.

**Proposition 18** Let \( \rho \) be a separable state of a bipartite system \( \mathcal{H}_A \otimes \mathcal{H}_B \) (dim \( \mathcal{H}_A \geq 2 \), dim \( \mathcal{H}_B \geq 2 \)) that has a product state \( |\psi_0\rangle |\psi_0\rangle \) as eigenstate with 0 eigenvalue. Then \( \rho \) is boundary separable; moreover there are entangled states arbitrarily close to \( \rho \) that are distillable.

**Proof** We may assume that \( |\psi_0\rangle = |0\rangle_A \) and \( |\psi_0\rangle = |0\rangle_B \) (cf. Appendix A and B) so that \( \rho_{00} = |0\rangle \langle 0| \) (dropping the indices \( A \) and \( B \), as was done till now) and perform the partial transpose using the basis \( |0\rangle \), \( |1\rangle \), etc., of \( \mathcal{H}_A \). Since \( \rho \) is separable, \( (T \otimes 1)(\rho) \) is a state and, from \( \langle 00 | (T \otimes 1)(\rho) | 00 \rangle = 0 \), it follows that \( |00\rangle \) is a 0 eigenvector of \( (T \otimes 1)(\rho) \) and thus \( \langle 00 | (T \otimes 1)(\rho) | 11 \rangle = 0 \), i.e. \( (10 | \rho_{10} | 01 \rangle = 0 \). Let now \( \rho_1 \) be any state such that \( \langle 00 | \rho_1 | 00 \rangle = 0 \) and \( \langle 10 | \rho_{10} | 01 \rangle = 0 \). The conditions of Lemma 17 are satisfied and \( \rho_\epsilon = (1 - \epsilon) \rho + \epsilon \rho_1 \) is entangled and distillable for all \( 0 < \epsilon \leq 1 \).

**Corollary 19** All pure product states are boundary separable.

5.3 Discordant states

**Proposition 20** If \( \rho \) and \( \tau \) are classical with respect to the basis \( \{ |i\rangle \} \) then so is the state \( (1 - t)\rho + t\tau \) for any valid \( t \).

**Proof** That follows directly from Proposition 5.

**Theorem 21** The state \( (1 - t)\frac{1}{2}I + \rho \) is discordant if and only if \( \rho \) is discordant, where \( I \) is the identity of \( \mathcal{H}_A \otimes \mathcal{H}_B \) and \( d = \dim (\mathcal{H}_A \otimes \mathcal{H}_B) \).

**Proof** This follows directly from statement 4 in Proposition 3 and the fact that \( I \) is invariant under any dephasing channel.

**Proposition 22** Consider the state
\[ \rho = \sum_{i,j} \mu_{ij} |i\rangle \langle i| \otimes |U_i| |j\rangle \langle j| U_j^\dagger, \]
with the standard basis chosen such that the smallest eigenvalue is \( \mu_{00} \) and \( U_0 = I \). Let \( \rho_{00} \) be any state of the bipartite system s.t. \( \langle 00 | \rho_{00} | 00 \rangle = 0 \) and \( \langle 10 | \rho_{10} | 01 \rangle \neq 0 \); then the state \( \rho_\epsilon = (1 - \epsilon) \rho + \epsilon \rho_{10} \) is a discordant state for all \( 0 < \epsilon \leq 1 \).

**Proof** Let \( \rho_{00} = \sum_{i,j} \mu_{ij} |i\rangle \langle i| \otimes |U_i| |j\rangle \langle j| U_j^\dagger \) if \( \rho \neq \frac{1}{2} \) (the \( \mu_{ij} \) are not all equal), else let \( \rho_{00} = |00\rangle \langle 00| \); then \( \rho_{00} + (1 - z)\frac{1}{2} \) for \( z = 1 - d \mu_{00}, 0 \leq z \leq 1 \). Since \( \langle 00 | \rho_{00} | 00 \rangle = 0 \) and \( \langle 10 | \rho_{10} | 01 \rangle = 0 \). From Proposition 21 we know that \( \rho_\epsilon \) is discordant if and only if the state \( \rho_\epsilon = \rho_{00} + \epsilon \rho_{10} \) obtained by normalizing \( \rho_\epsilon = (1 - \epsilon) \rho_{00} + \epsilon \rho_{10} \) is discordant. It holds that \( \rho_\epsilon = (1 - \epsilon') \rho_{00} + \epsilon' \rho_{10} \) with \( \epsilon' = k \epsilon \) for \( 0 < \epsilon' \leq 1 \). By Lemma 17, \( \rho_\epsilon \) is entangled (and distillable), so that \( \rho_\epsilon \) is discordant and \( \rho \) is boundary classical.

**Corollary 23** All classical states are boundary classical.

We note that one could arrive at corollary 23 by using the fact that the set of classical states is nowhere dense [Ferraro et al. 2010].
Proposition 22 provides a method to construct $\varepsilon$-discordant states. If a classical state $\rho$ (or any state $\rho \in C_A$) is not boundary separable the $\varepsilon$-discordant state is also dissonant (i.e., it is separable). In general there is no direct relation between discord and boundary separable states.

**Proposition 24** There are classical states (and states in $C_A$) that are boundary separable and discordant states that are not boundary separable.

**Proof** Most of the examples of boundary separable states above are classical with respect to $A$. Moreover all pure product states are also uncorrelated and boundary separable. From proposition 21 and we know there are discordant states arbitrarily close to the maximally mixed states. From proposition 15 we know that these states are not boundary separable. □

5.4 Two qudits - discussion

In this section we showed that there are separable states that are not boundary separable (corollary 16). We then presented a general class of boundary separable states and showed that in general all pure product states are boundary separable (Corollary 19). Finally we discussed depolarized discordant states (Theorem 21), showed that all classical states are boundary classical (Corollary 23) and that there is no direct relation between discord and boundary separable states.

6 Multiple qudits

6.1 Extrapolated Pseudo-Pure States of $N$ Qubits

Let us consider states of the form

$$\rho_t = (1-t) \frac{1}{2^N} + t|11\ldots1\rangle\langle11\ldots1|$$

where $I$ is the identity matrix, but this time of size $2^N \times 2^N$, and $t < 0$. With $(1-t) + 2^N t = 0$, i.e. $t = -\frac{1}{2^N-1}$, $\rho_b = \rho_t$ becomes a 1-void state, with $|11\ldots1\rangle$ as 0-eigenvector. The states $\rho_t$ for $t \leq 0$ are all clearly separable; their matrix is diagonal in the standard basis, with non-negative eigenvalues. Only the eigenvalue of $|11\ldots1\rangle$ decreases.

6.1.1 $\rho_b$ Is a Boundary Separable State.

We choose arbitrarily the first bit and show that there are $\varepsilon$ close entangled states for which the first qubit is entangled with the others. Let $|1\rangle = |1^{N-1}\rangle$, i.e. $N-1$ bits equal to one. The eigenstate of $\rho_b$ with 0 eigenvalue can be written as $|0\rangle = |1\rangle|1\rangle$ and Proposition 18 applies.

6.1.2 Trace Distance Between $\varepsilon$-Entangled States and the Completely Mixed State.

The trace distance between $\rho_b$ and $1/2^N$ is

$$\frac{1}{2} \text{tr} \left| (1-t) \frac{1}{2^N} + t|1\rangle\langle1| \right| = \frac{|t|}{2} \text{tr} \left| \frac{1}{2^N} - |1\rangle\langle1| \right|.$$  

The trace of $|1/2^N - |1\rangle\langle1|\rangle$ is $(2^N - 1) \times 1/2^N + 1 - 1/2^N = 2 - 2/2^N$. The trace distance is thus

$$\delta(\frac{1}{2^N}, \rho_b) = \frac{1}{2^N-1} \left( 1 - \frac{1}{2^N} \right) = \frac{1}{2^N}.$$  

Conclusion: for any $\varepsilon > 0$ there are entangled states at distance at most $2^{-N} + \varepsilon$ of the completely mixed state. Indeed, by the triangle inequality,

$$\delta(\frac{1}{2^N}, \rho_b) \leq \delta(\frac{1}{2^N}, \rho_\varepsilon) + \delta(\rho_b, \rho_\varepsilon) \leq 2^{-N} + \varepsilon.$$  

6.2 The $N$ Qubit Thermal State

The thermal state of one qubit is

$$\rho_\Theta = \left[ \begin{array}{cc} \frac{1}{2} & 0 \\ 0 & \frac{1}{2^N} \end{array} \right] = \frac{1 + \eta}{2} |0\rangle\langle0| + \frac{1 - \eta}{2} |1\rangle\langle1|.$$  

The thermal state of $N$ independent qudits (with the same $\eta$) is

$$\rho_\Theta^N = \rho_\Theta^\otimes N = \sum_{i \in \{0,1\}^N} \left( \frac{1 + \eta}{2} \right)^{N-|i|} \left( \frac{1 - \eta}{2} \right)^{|i|} |i\rangle\langle i|.$$  

where $|i|$ is the Hamming weight of the string $i$, i.e. the number of bits equal to 1 in $i$, each 1 giving a minus sign, and each 0 a plus sign. The thermal state is not only separable but it has an eigenbasis consisting of product states. The smallest eigenvalue is given by the eigenvector $|i\rangle = |1^N\rangle$, i.e. all qubits are 1 and it is

$$\lambda_{|1^N\rangle} = \left( \frac{1 - \eta}{2} \right)^N$$  

which is exponentially small with $N$.

6.2.1 Extrapolated States Close to the Thermal State.

Let us consider the extrapolated states

$$\varrho_t = (1-t)\rho_\Theta^N + t|1^N\rangle\langle1^N|$$

for $t < 0$ ($t = -p$ for some positive real number $p$). They are all separable and when the eigenvalue of $|1^N\rangle\langle1^N|$ becomes 0,
\( \rho_t \) is a void state. That happens when \((1-t)[(1-\eta)/2]^N + t = 0 \) i.e.
\[
t_b = -\frac{\lambda_{1|1^N}}{1-\lambda_{1|1^N}} = -\lambda_{1|1^N}^2 - \ldots
\]

a very small value, equal to \(-\lambda_{1|1^N} = -(1-\eta)/2)^N\) if we neglect terms of higher order. The trace distance between \(\rho_b\) and \(\rho_{\Theta}^N\) is
\[
\delta(\rho_b, \rho_{\Theta}^N) = \frac{1}{2} \text{tr} \left| (1-t_b) \rho_b^N + t_b |1^N\rangle\langle 1^N| - \rho_{\Theta}^N \right|
\]
\[
= \frac{|t_b|}{2} \text{tr} \left| \rho_{\Theta}^N - |1^N\rangle\langle 1^N| \right|
\]
The eigenvectors of \(\rho_{\Theta}^N - |1^N\rangle\langle 1^N|\) are those of \(\rho_{\Theta}^N\) and the eigenvalues are left unchanged except for the eigenvector \(|1^N\rangle\) whose eigenvalue of \(\lambda_{1|1^N}\) is decreased by 1 which implies that the sum of the absolute values of the eigenvalues is increased by \(1 - \lambda_{1|1^N}\)
\[
\delta(\rho_{\Theta}^N, \rho_b) = \frac{|t_b|}{2} \left( 2 - \lambda_{1|1^N} \right)
\]
\[
= \frac{1}{2} \left( 1 - \lambda_{1|1^N} \right) \left( 2 - \lambda_{1|1^N} \right)
\]
\[
= \left( \lambda_{1|1^N}^2 + \frac{\lambda_{1|1^N}}{1 - \lambda_{1|1^N}} \right)
\]
\[
= \lambda_{1|1^N} + \frac{1}{2} \lambda_{1|1^N}^2 + \frac{1}{2} \lambda_{1|1^N}^3 \ldots
\]

which is \(\lambda_{1|1^N}\) if we neglect terms of higher order. That distance is exponentially small with \(N\).

6.2.3 Entangled States Close to the Thermal State

We have just proven that or any \(\epsilon > 0\), there are entangled states \(\epsilon\) such that \(\delta(\rho_b, \rho_{\epsilon}) \leq \epsilon\). By the triangle inequality (since the trace distance is a distance in the sense of metric spaces), the distance between those states \(\rho_\epsilon\) and \(\rho_{\Theta}^N\) is such that \(\delta(\rho_{\Theta}^N, \rho_\epsilon) \leq \delta(\rho_{\Theta}^N, \rho_b) + \delta(\rho_b, \rho_\epsilon) \leq \delta(\rho_{\Theta}^N, \rho_b) + \epsilon\), which implies that for any \(\epsilon > 0\) there are entangled states in a ball of trace-distance radius
\[
\epsilon + \left( \frac{1-\eta}{2} \right)^N + \frac{1}{2} \left( \frac{1-\eta}{2} \right)^{2N} + \frac{1}{2} \left( \frac{1-\eta}{2} \right)^{3N} \ldots
\]
around the thermal state \(\rho_{\Theta}^N\) of \(N\) qubits where \(\left( \frac{1-\eta}{2} \right)^N = \lambda_{1|1^N}\) is exponentially small in \(N\).

7 Discussion

We used extrapolation and interpolation to study the boundaries of some subsets of states and to make some connections between different notions of entanglement and quantum correlations. The majority of our results concern boundary separable states. We showed various classes of these states that play a significant role in quantum computing. In particular the classically correlated states in the computational basis and thermal states.

Our results are related to results on robustness against various types of noise. States near the boundary are generally more fragile than those far away from it. It is then interesting to note that although thermal states are not entangled they can become entangled by small fluctuation in the right direction, moreover the entanglement is distillable.

7.1 Discord and entanglement

While discord and entanglement are very different from an operational perspective (Modi et al 2012; Brodutch 2013), pure state entanglement and discord (for all states) share many similar mathematical properties (Modi et al 2012). Many of these appeared in the work above, in particular in the property of boundaries. All classical states are boundary classical (Corollary 23), similarly all pure product states are at the boundary of the set of entangled states (Corollary 19). This opens a number of interesting questions regarding operations on pure and mixed states. For example we showed in proposition 22 that mixing any classical state (and any classical state with respect to \(A\)) with an entangled state will make it discordant, similarly mixing a pure product state with an entangled state will make it entangled (Corollary 19). However the former is not an extension of the latter into mixed states since both take pure states to a mixed states. If one considers unitary operations on pure states there is come discrepancy. Universal entanglers (unitary operations that entangle all pure states) are known to exits only in higher dimensions (Chen et al 2008).
7.2 Quantum computing

It is currently an open question whether it is possible to efficiently simulate all quantum computations that produce (or consume) no entanglement [Boyer Brodutch and Mor 2017]. Surprisingly, it is not even clear if it is possible to simulate all quantum computation that produce (or consume) no discord. Boundary (classical or separable) states may play a critical role in these types of simulations since even small errors can cause the states to become discordant or entangled. This issue was pointed out for the case of discord free (concordant) computation in [Cable and Browne 2015] where the entire computation happens on the boundary (see also [Datta and Shaji 2011]).

A second issue is related to the entangling power of mixed state quantum computers, where the initial state is fixed. Here we showed that the thermal states used in various mixed state models can become entangled after a small perturbation. However, we did not discuss the physical mechanism for such perturbations. In a follow up paper (Boyer Brodutch and Mor 2017) we explore perturbations due to unitary operations that are ε close to the identity. A question for future research involves the possible use of thermal states and some non-local operations to distill entanglement. This question is especially important in the setting of NMR quantum computing.

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References

Acín A, Augusiak R, Cavalcanti D, Hadley C, Korbicz JK, Lewenstein M, Masanes L, Piani M (2010) Unified framework for correlations in terms of local quantum observables. Phys Rev Lett 104:140,404, doi: [10.1103/PhysRevLett.104.140404]

Bengtsson I, Zyczkowski K (2006) Geometry of quantum states: an introduction to quantum entanglement. Cambridge University Press

Bennett CH, DiVincenzo DP, Fuchs CA, Mor T, Rains E, Shor PW, Smolin JA, Wootters WK (1999a) Quantum nonlocality without entanglement. Phys Rev A 59:1070–1091, doi: [10.1103/PhysRevA.59.1070]

Bennett CH, DiVincenzo DP, Mor T, Shor PW, Smolin JA, Terhal BM (1999b) Unextendible product bases and bound entanglement. Phys Rev Lett 82:5385–5388, doi: [10.1103/PhysRevLett.82.5385]

Boyer M, Mor T (2014) Extrapolated states, void states, and a huge novel class of distillable entangled states. In: Dediu AH, Lozano M, Martin-Vide C (eds) Theory and Practice of Natural Computing. Lecture Notes in Computer Science, vol 8890, Springer International Publishing, pp 107–118, doi: [10.1007/978-3-319-13749-0_10]

Boyer M, Brodutch A, Mor T (2017) Entanglement and deterministic quantum computing with one qubit [arXiv:1606.05283]

Braunstein SL, Caves CM, Jozsa R, Linden N, Popescu S, Schack R (1999) Separability of very noisy mixed states and implications for nmr quantum computing. Phys Rev Lett 83:1054–1057, doi: [10.1103/PhysRevLett.83.1054]

Brodutch A (2013) Discord and quantum computational resources. Phys Rev A 88:022,307, doi: [10.1103/PhysRevA.88.022307]

Brodutch A, Terno DR (2010) Quantum discord, local operations, and maxwell’s demons. Phys Rev A 81:062,103, doi: [10.1103/PhysRevA.81.062103]

Brunner N, Cavalcanti D, Pironio S, Scarani V, Wehner S (2014) Bell nonlocality. Rev Mod Phys 86:419–478, doi: [10.1103/RevModPhys.86.419]

Cable H, Browne D (2015) Exact and efficient simulation of concordant computation N. J. Phys. 17:113049 doi: [10.1088/1367-2630/17/11/113049]

Chen J, Duan R, Ji Z, Ying M, Yu J (2008) Existence of universal entangler. J Math Phys 49(1):012,103, doi: [10.1063/1.2829895]

Datta A, Shaji A (2011) Quantum Discord and Quantum Computing – An Appraisal Int. J. Quant. Info. 9:1787 doi: [10.1142/S0219749911008410]

Dur W, Vidal G, Cirac JI (2003) Three qubits can be entangled in two inequivalent ways. Phys Rev A 62:062,314, doi: [10.1103/PhysRevA.62.062314]

Ferraro A, Aolita L, Cavalcanti D, Cucchietti FM, Acín A (2010) Almost all quantum states have nonclassical correlations. Phys Rev A 81:052,318, doi: [10.1103/PhysRevA.81.052318]

Gühne O, Lütkenhaus N (2007) Nonlinear entanglement witnesses, covariance matrices and the geometry of separable states. J Phys: Conf Ser 67(1):012,004, doi: [10.1088/1742-6596/67/1/012004]

Groisman B, Kenigšberg D, Mor T (2007) “Quantumness” versus “classicality” of quantum states. arXiv:quant-ph/0703103

Gurvits L (2003) Classical deterministic complexity of edmonds’ problem and quantum entanglement. In: Proceedings of the Thirty-fifth Annual ACM Symposium on Theory of Computing, ACM, New York, NY, USA, STOC ’03, pp 10–19, doi: [10.1145/780542.780545]

Henderson L, Vedral V (2001) Classical, quantum and total correlations. J Phys A: Math Gen 34(35):6899, doi: [10.1088/0305-4470/34/35/315]

Horodecki M, Horodecki P, Horodecki R (1997) Inseparable two spin-1/2 density matrices can be distilled to a singlet form. Phys Rev Lett 78:574–577, doi: [10.1103/PhysRevLett.78.574]

Horodecki P (1997) Separability criterion and inseparable mixed states with positive partial transposition. Phys Lett A 232(5):333 – 339, doi: [10.1016/S0375-9601(97)00416-7]

Horodecki R, Horodecki P, Horodecki M, Horodecki K (2009) Quantum entanglement. Rev Mod Phys 81:865–942, doi: [10.1103/RevModPhys.81.865]

Kraus B, Lewenstein M, Cirac JI (2002) Characterization of distillable and activatable states using entanglement witnesses. Phys Rev A 65:042,327, doi: [10.1103/PhysRevA.65.042327]

Mølgaard K, Paterek T, Son W, Vedral V, Williamson M (2010) Unified view of quantum and classical correlations. Phys Rev Lett 104:080,501, doi: [10.1103/PhysRevLett.104.080501]

Mølgaard K, Brodutch A, Cable H, Paterek T, Vedral V (2012) The classical-quantum boundary for correlations: Discord and related measures. Rev Mod Phys 84:1655–1707, doi: [10.1103/RevModPhys.84.1655]

Ollivier H, Zurek WH (2001) Quantum discord: A measure of the quantumness of correlations. Phys Rev A 88:017,901, doi: [10.1103/PhysRevA.88.017901]

Peres A (1996) Separability criterion for density matrices. Phys Rev Lett 77:1413–1415, doi: [10.1103/PhysRevLett.77.1413]
Appendix

A The Peres Entanglement Criterion

Here are a few relevant remarks using the notations of the main article.

A.1 Transpose and partial transpose

Given a Hilbert space $\mathcal{H}$ and a basis $\{i\}$ (we always assume finite dimensional systems), the transpose is defined by linearity on basis operators $|i\rangle_1|j\rangle_2$ by $T(|i\rangle_1|j\rangle_2) = |j\rangle_1|i\rangle_2$. It follows that for any linear operator $L$, $(i_1|T(L)|i_2) = (i_2|L|i_1)$. If $\rho$ is a state and $\rho = \sum \lambda_i |i\rangle_1\langle i|_1|j\rangle_2$, one can check that $\rho = \sum \lambda_i |i\rangle_1\langle i|_1|j\rangle_2$ with $|i\rangle_1\langle i|_1|j\rangle_2$, $|j\rangle_2$ being the complex conjugate of $a_i$. It follows that $T(\rho)$ is also a state, with same eigenvalues as $\rho$.

Given a compound system described by $\mathcal{H}_A \otimes \mathcal{H}_B$, the partial transpose with respect to the $A$ system is simply the operator $(T \otimes I)(\rho) = |i\rangle_1\langle i|_1|j\rangle_2$ on basis elements. It also follows that for any operator $L$ on $\mathcal{H}_A \otimes \mathcal{H}_B$, $(i_1|j_2)(T \otimes I)(L)|i_1j_2\rangle = (|i_1\rangle_1|j_2\rangle)(L)|i_1j_2\rangle$.

A.2 The Peres Criterion

A state $\rho$ of a bipartite system $\mathcal{H}_A \otimes \mathcal{H}_B$ is said to be separable if it can be written in the form

$$\rho = \sum_i p_i \rho_i^A \otimes \rho_i^B,$$

where $p_i \geq 0$, $\sum_i p_i = 1$ (6)

where the $\rho_i^A$ (resp. $\rho_i^B$) are states of $\mathcal{H}_A$ (resp. $\mathcal{H}_B$); if $\rho$ is not separable, it is said to be entangled. If $\rho$ is given by (6), then

$$(T \otimes I)(\rho) = \sum_i p_i (T(\rho_i^A)) \otimes \rho_i^B$$

and since the $T(\rho_i^A)$ are states, this implies that $(T \otimes I)(\rho)$ is itself a state (and separable). This implies in turn that $(T \otimes I)(\rho)$ must be positive semi-definite.

A.3 Checking for positivity

An operator $P$ is positive semi-definite if it is Hermitian and if for all pure states $|\psi\rangle$, $\langle \psi|P|\psi\rangle \geq 0$ (iff $P$ has no negative eigenvalue). For any state $\rho$ of $\mathcal{H}_A \otimes \mathcal{H}_B$, $(T \otimes I)(\rho)$ is always Hermitian. To prove that it is not positive semi-definite, we need only find a $|\psi\rangle$ such that $\langle \psi|(T \otimes I)(\rho)|\psi\rangle < 0$. The partial transpose however depends on the basis chosen for $\mathcal{H}_A$. We now show (using our notations) that whether $(T \otimes I)(\rho)$ is positive semi-definite or not does not depend on the choice of that basis. Indeed, let $\{e_i\}$ be any orthonormal basis of $\mathcal{H}_A$. Then $\rho$ can always be written (in a unique way) as $\rho = \sum_i |e_i\rangle\langle e_i| \otimes \rho_{ij}$ where the $\rho_{ij}$ are operators of $\mathcal{H}_B$. Let $T_\rho$ be the transpose operator in the basis $e$ i.e. $T_\rho(|e_i\rangle\langle e_i|) = |e_i\rangle\langle e_i|$. Then

$$(T_\rho \otimes I)(\rho) = \sum_i T_\rho(|e_i\rangle\langle e_i|) \otimes \rho_{ij} = \sum_i |e_i\rangle\langle e_i| \otimes \rho_{ij}$$

$$(T \otimes I)(\rho) = \sum_i T(|e_i\rangle\langle e_i|) \otimes \rho_{ij} = \sum_i |e_i\rangle\langle e_i| \otimes \rho_{ij}$$

The $|\psi_i\rangle$ also form an orthonormal basis of $\mathcal{H}_A$. Now let $|\Psi_i\rangle = \sum_i |e_i\rangle |\psi_i\rangle$ be any pure state of $\mathcal{H}_A \otimes \mathcal{H}_B$. Then $|\Psi_i\rangle = \sum_i |\psi_i\rangle |\psi_i\rangle$ is also a pure state and

$$\langle \Psi_i|(T \otimes I)(\rho)|\Psi_i\rangle = \sum_j \langle \psi_j| \otimes |\psi_j\rangle = \sum_j \langle \psi_j| \otimes |\psi_j\rangle$$

A.4 Proof of Lemma [11]

Proof Let us assume $P$ is positive semidefinite: $P = \sum \lambda_i |\psi_i\rangle\langle \psi_i|$ with $\lambda_i \geq 0$. If $\langle \psi_i|P|\psi_i\rangle = 0$, then $\sum \lambda_i |\psi_i\rangle\langle \psi_i|$ is positive semidefinite. The partial transpose is defined by linearity on basis elements $|i\rangle_1|j\rangle_2$ by $T(|i\rangle_1|j\rangle_2) = |j\rangle_1|i\rangle_2$. It follows that $T(\rho)$ is also a state, with same eigenvalues as $\rho$.

B Distillability

Note that the Peres Criterion is not a characterization. If the partial transpose of $\rho$ is positive semi-definite, $\rho$ may still be entangled. Furthermore, if a state $\rho_{\text{out-ent}}$ is entangled and admits a positive partial transpose then it is not distillable (namely, one cannot distill a single state out of many copies of $\rho_{\text{out-ent}}$ via local operations and classical communication). Such states are said to have “bound entanglement”. A characterization of distillable states can be found in (Horodecki, 2009).

Here is the lemma as we use it, as stated in (Kraus et al., 2002).

Lemma 25 (Kraus et al., 2002; Horodecki, 2009) A state $\rho$ of $\mathcal{H}_A \otimes \mathcal{H}_B$ is distillable if and only if there exists a positive integer $N$ and a state $|\Psi\rangle = |e_1\rangle f_1 + |e_2\rangle f_2$ such that

$$\langle J|T \otimes I(\rho^{\otimes N})|\Psi\rangle < 0,$$

where $|e_1, e_2\rangle$ (resp. $\{f_1, f_2\}$) are two unnormalized orthogonal vectors of $\mathcal{H}_A^{\otimes N}$ (resp. $\mathcal{H}_B^{\otimes N}$).

C Proof of Proposition [14] using matrices

When the states $|i\rangle$ are put in lexicographic order, the partial transpose $(T \otimes I)$ corresponds to transposing blocks in the block matrix, whereas $(I \otimes T)$ corresponds to transposing each of the blocks individually. The matrix of Proposition [14] is a $3 \times 3$ block matrix, with $3 \times 3$ blocks.

We first calculate for both $\rho_0$ and $\rho_1$ the entries $(11, 11)$ and $(01, 10)$ (row 01, column 10 of their matrix). Those are $(11|\rho_0|11) = 0$, and $\langle 01|\rho_1|10\rangle = 0 = \langle 11|\rho_0|11\rangle = 0$ and $\langle 10|\rho_1|10\rangle = 1/2$ for $\rho_1$. Those values were obtained in the main text. The matrices for $\rho_0$ and $\rho_1$ are then the following (useless entries being kept blank).

| 00 | 01 | 02 | 10 | 11 | 12 | 20 | 21 | 22 |
|----|----|----|----|----|----|----|----|----|
| 0  |   |   |    |   |   |    |    |   |
|    |   | 0  |    |    |   |    |    |   |
| 10 |   |    |    |    |    |    |    |   |
| 11 |   |    |    |    |    |    |    |   |
| 12 |   |    |    |    |    |    |    |   |
| 20 |   |    |    |    |    |    |    |   |
| 21 |   |    |    |    |    |    |    |   |
| 22 |   |    |    |    |    |    |    |   |
Then, the $3 \times 3$ block matrix is transposed, giving respectively for $(T \otimes I)(\rho_0)$ and $(T \otimes I)(\rho_1)$ the matrices:

$$
\begin{pmatrix}
00 & 01 & 02 & 10 & 11 & 12 & 20 & 21 & 22 \\
01 & 00 & 1/2 & 0 & 0 & 0 & 0 & 0 & 0 \\
10 & 11 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
12 & 20 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
21 & 22 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
$$

The matrix of $(T \otimes I)(\rho_\varepsilon) = (1 - \varepsilon)(T \otimes I)(\rho_0) + \varepsilon(T \otimes I)(\rho_1)$ is then

$$
\begin{pmatrix}
00 & 01 & 02 & 10 & 11 & 12 & 20 & 21 & 22 \\
01 & 00 & 1/2 & 0 & 0 & 0 & 0 & 0 & 0 \\
10 & 11 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
12 & 20 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
21 & 22 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
$$

We see clearly that the matrix of $(T \otimes I)(\rho_\varepsilon)$ has a 0 diagonal entry for which there is a non zero entry on the corresponding row (or corresponding column). That implies that the matrix is not positive semi-definite and consequently that $\rho_\varepsilon$ is entangled.

Of course, the blank values in the density operator for $\rho_1$ could take any value without affecting the result; in fact any density operator $\rho_1$ such that $\langle 11 | \rho_1 | 11 \rangle = 0$ and $\langle 01 | \rho_1 | 10 \rangle \neq 0$ could have been used instead to give entangled states that arbitrarily close to $\rho_0$. 