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2006 J. Phys. A: Math. Gen. 39 617

(http://iopscience.iop.org/0305-4470/39/3/013)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **39** (2006) 617–636 doi:10.1088/0305-4470/39/3/013

Spectral conditions on the state of a composite quantum system implying its separability

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Received 12 June 2005, in final form 16 November 2005
Published 21 December 2005
Online at stacks.iop.org/JPhysA/39/617

Abstract
The separability modulus $\ell(\rho)$ of a state ρ of an arbitrary finite composite quantum system is the largest t in [0, 1] such that $t \cdot \rho + (1-t) \cdot \tau$ is separable, where τ is the normalized trace. The basic properties of ℓ, introduced by Vidal and Tarrach in another guise, are briefly established. With these properties, we obtain conditions on the spectrum of a state which imply that it is separable. As a consequence, we show that for any Hamiltonian H the thermal equilibrium states $e^{-H/T}/\mathrm{Tr}(e^{-H/T})$ are separable if T is large enough. Also, for F a unitarily invariant, convex continuous real-valued function on states, for which $F(\rho) > F(\tau)$ whenever $\rho \neq \tau$, there is a critical C_F such that $F(\rho) \leqslant C_F$ implies that ρ is separable, and for each possible $c > C_F$ there are entangled states ϕ with $F(\phi) = c$. This class includes all strictly convex unitarily invariant continuous functions, and also every non-trivial partial eigenvalue-sum. Some C_F are computed. General upper and lower bounds for C_F are given, and then improved for bipartite systems.

PACS numbers: 03.67.−a, 03.65.Ud

1. Introduction

Quantum state entanglement is a key feature of quantum information processing procedures [1]. This has fuelled the mathematical studies of entanglement in the last ten years or so.

Consider a finite level quantum system described by a complex Hilbert space $\mathcal{H}$ of finite dimension d. Let $\mathcal{B}(\mathcal{H})$ be the linear operators from $\mathcal{H}$ into itself equipped with the operator norm. An operator $a \in \mathcal{B}(\mathcal{H})$ is termed positive, written as $a \geqslant 0$, if $\langle\psi, a\psi\rangle \geqslant 0$ for all $\psi \in \mathcal{H}$. An application of polarization identity shows that $a \geqslant 0$ implies that a is self-adjoint. A *state* ρ on $\mathcal{B}(\mathcal{H})$ is a linear function $\rho : \mathcal{B}(\mathcal{H}) \to \mathbb{C}$ which is positive, that is, $a \geqslant 0$ implies $\rho(a) \geqslant 0$, and normalized $\rho(\mathbf{1}) = 1$, where $\mathbf{1}$ is the identity operator. It follows that $\rho(a^*) = \overline{\rho(a)}$. The state space $\mathcal{S}(\mathcal{H})$ or simply $\mathcal{S}$ is the set of all states. $\mathcal{S}$ is a convex subset of the set of linear functionals on $\mathcal{B}(\mathcal{H})$ which is compact with respect to the topology defined by the norm of linear functionals f given by $\|f\| = \sup\{|f(a)|/\|a\| : 0 \neq a \in \mathcal{B}(\mathcal{H})\}$. All continuity statements made in the present paper refer to this topology.

The extremal points $\mathrm{ext}(\mathcal{S})$ are precisely the pure states or vectorial states given by $\rho(a) = \langle\psi, a\psi\rangle$ for some unit vector $\psi \in \mathcal{H}$. We reserve the term 'pure' for these states. The decomposition of a mixed $\rho \in \mathcal{S}$ as a convex sum $\rho = \sum_{j=1}^{M} t_j \rho^{(j)}$, where $t_j > 0$, $\sum_{j=1}^{M} t_j = 1$ and the $\rho^{(j)}$ are pure states, is never unique; there are always uncountably many such decompositions with finite M. Among these convex decompositions into pure states, the *spectral decompositions* are those for which the pure states $\rho^{(j)}$ involved are pairwise orthogonal meaning that the associated vectors $\{\psi_j\}$ are pairwise orthogonal. For a spectral decomposition one has $M \leqslant d$ and the spectral decomposition is unique iff all the weights (non-zero eigenvalues of the density operator, see below) $t_j > 0$ involved are distinct.

Now there is a well-known (and in finite dimension elementary) representation theorem for states which states that every $\rho \in \mathcal{S}$ is given by $\rho(a) = \mathrm{Tr}(D_\rho a)$ where D_ρ is a unique density operator; that is, $D_\rho \geqslant 0$ and $\mathrm{Tr}(D_\rho) = 1$. The density operators $\mathcal{B}_1^+(\mathcal{H})$ clearly form a convex set which turns out to be compact with respect to the trace norm on $\mathcal{B}(\mathcal{H})$ given by $\|a\|_1 = \mathrm{Tr}(|a|)$. The formulae $\rho(a) = \mathrm{Tr}(D_\rho a)$, $\rho \in \mathcal{S}$, and $\rho_D(a) = \mathrm{Tr}(Da)$, $D \in \mathcal{B}_1^+(\mathcal{H})$, implement a bijective affine homeomorphism between the compact convex sets $\mathcal{S}$ and $\mathcal{B}_1^+(\mathcal{H})$. One has $\mathrm{ext}\big(\mathcal{B}_1^+(\mathcal{H})\big) = \{p \in \mathcal{B}(\mathcal{H}) : p = p^* = p^2, \mathrm{rank}(p) = 1\}$, i.e., the orthoprojectors onto the one-dimensional subspaces of $\mathcal{H}$. The spectral theorem applied to D_ρ provides a spectral decomposition of ρ. In what follows, we often identify ρ with the associated density operator.

Given $N \geqslant 2$ finite-dimensional Hilbert spaces $\mathcal{H}_j$ of dimension $d_j \geqslant 2$ ($j = 1, 2, \ldots, N$), the composite quantum system—whose constituents are the quantum systems described by $\mathcal{H}_j$—is described by the tensor product $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_N$ which has dimension $D = d_1 d_2 \cdots d_N$. Given a state $\rho \in \mathcal{S}$ we can define a state of $\mathcal{B}(\mathcal{H}_j)$ by

$$\rho^{[j]}(a) = \rho(\underbrace{\mathbf{1}_1 \otimes \mathbf{1}_2 \otimes \cdots \otimes \mathbf{1}_{j-1}}_{j-1 \text{ identity factors}} \otimes a \otimes \underbrace{\mathbf{1}_{j+1} \otimes \cdots \otimes \mathbf{1}_N}_{N-j \text{ identity factors}}), \qquad a \in \mathcal{B}(\mathcal{H}_j).$$

A state ρ is said to be a *product-state* if

$$\rho(a_1 \otimes a_2 \otimes \cdots \otimes a_N) = \rho^{[1]}(a_1)\rho^{[2]}(a_2) \cdots \rho^{[N]}(a_N),$$

for all $a_1 \in \mathcal{B}(\mathcal{H}_1)$, all $a_2 \in \mathcal{B}(\mathcal{H}_2), \ldots,$ and all $a_N \in \mathcal{B}(\mathcal{H}_N)$. Clearly, a product-state exhibits no correlations whatsoever among the constituent subsystems. The product-states in $\mathcal{S}$ are denoted by $\mathcal{S}^{\mathrm{prod}}$ and they are closed.

Given states ρ_j of $\mathcal{B}(\mathcal{H}_j)$, the map

$$(\rho_1 \otimes \rho_2 \otimes \cdots \otimes \rho_N)(a_1 \otimes a_2 \otimes \cdots \otimes a_N) = \rho_1(a_1)\rho_2(a_2) \cdots \rho_N(a_N),$$

$a_j \in \mathcal{B}(\mathcal{H}_j)$, admits a unique extension (by linearity and continuity) to a state of $\mathcal{B}(\mathcal{H})$ which is denoted by $\rho_1 \otimes \rho_2 \otimes \cdots \otimes \rho_N$. Thus, $\rho \in \mathcal{S}^{\mathrm{prod}}$ iff $\rho = \rho^{[1]} \otimes \rho^{[2]} \otimes \cdots \otimes \rho^{[N]}$.

We come to the basic definitions. Recall that the convex hull $\mathrm{co}(\mathcal{K})$ of a subset $\mathcal{K}$ of a convex set is the collection of all finite convex sums of elements of $\mathcal{K}$. A state $\rho \in \mathcal{S}$ is said to be *separable*, or *unentangled*, if it lies in the convex hull $\mathrm{co}(\mathcal{S}^{\mathrm{prod}})$ of the product-states. We write $\mathcal{S}^{\mathrm{sep}}$ for the separable states. Due to the finite dimension, $\mathcal{S}^{\mathrm{sep}} = \mathrm{co}(\mathcal{S}^{\mathrm{prod}})$ is a closed and thus compact subset of $\mathcal{S}$. The extremal points of $\mathcal{S}^{\mathrm{sep}}$, $\mathrm{ext}(\mathcal{S}^{\mathrm{sep}})$, are precisely the pure product-states $\mathrm{ext}(\mathcal{S}) \cap \mathcal{S}^{\mathrm{prod}}$. Thus in analysing the separability of a given $\rho \in \mathcal{S}$ one can restrict oneself to the convex decompositions of ρ into pure states. As mentioned, there are uncountably many such finite decompositions and, in general, the spectral decomposition(s) of a separable state are not decompositions into product-states. This is what makes the problem of deciding whether a state is separable or not a very subtle problem. A state is called *entangled* if it is not separable; that is, if it cannot be decomposed into a convex sum of (pure) product-states.

At present there are finite algorithms deciding whether a given state is entangled or not, only for two qubits ($N = 2$ with $d_1 = d_2 = 2$; Wootters' criterion [3], PPT criterion, [4]) and for $N = 2$ with $d_1 = 2$ and $d_2 = 3$ (PPT criterion, [4]). Gurvits [5] has shown that the separability problem is NP-hard in the category of computational complexity theory.

Here we present some very elementary arguments and basic facts which nevertheless allow us to isolate simple conditions on the spectrum of a density operator of an arbitrary finite composite quantum system guaranteeing that the state is separable. One of the basic ingredients of our arguments is not new: If τ is the normalized trace which is a product-state (hence separable) and ρ is any state, how large can t get before $t \cdot \rho + (1 - t) \cdot \tau$ becomes entangled? This question underlies the work of Życzkowski *et al* [6], Vidal and Tarrach [2], and other authors. Here we proceed backwards, in as much as we do not extend previous work, but use very elementary methods which require almost no precise information about entanglement to extract some general results, which seem to have been overlooked. We show that for any unitarily invariant, convex (or concave) real-valued function F on states, for which $F(\rho) = F(\tau)$ implies $\rho = \tau$, there exists a critical value C_F such that $F(\rho) \leqslant C_F$ ($F(\rho) \geqslant C_F$ in the concave case) implies that ρ is separable. The class of functions with this separating property includes all unitarily invariant strictly convex or concave continuous functions, and also the non-trivial partial eigenvalue-sums (which define the 'more mixed than' partial ordering of states [7]). Another simple result is that for any Hamiltonian of an arbitrary composite quantum system, there are finite critical temperatures $T_c^+ \geqslant 0$ and $T_c^- \leqslant 0$ such that the thermal equilibrium state $\exp(-H/T)/\operatorname{Tr}(\exp(-H/T))$ is separable if $T \geqslant T_c^+$ or $T \leqslant T_c^-$. With precise entanglement information, as is available or obtainable for $N = 2$, the results of this paper can be considerably improved and sharp bounds can be obtained for the critical values mentioned. Some results in this direction are obtained here, but work on this is in progress.

The organization of the paper is as follows. Section 2 and its subsections, where the composite structure is irrelevant, present some basic facts about global spectral properties of states and introduce a representation, the gap representation, of a state which turns out to be useful. In section 3, we turn to composite systems and, in section 3.1, we introduce and present basic material about the separability modulus of a state (the critical t of the above paragraph); this quantity has been studied extensively in another guise by Vidal and Tarrach [2]. In section 3.2 we obtain some simple spectral conditions which are sufficient for separability. The rest of the subsections of section 3 deal with the mentioned application to thermal states and unitarily invariant convex functions with the separation property. In section 4, we use available direct or indirect information about the modulus of separability for bipartite systems to make precise the results of section 3. The symbol □ indicates the end of a proof.

2. The global spectral properties of states

In this section, we consider states for some fixed d-dimensional Hilbert space $\mathcal{H}$ with $d \geqslant 2$ and abbreviate $\mathcal{B}_d = \mathcal{B}(\mathcal{H})$ and $\mathcal{S}_d = \mathcal{S}(\mathcal{H})$. We write τ_d for the state given by the normalized trace $\tau_d(a) = \operatorname{Tr}(a)/d$, $a \in \mathcal{B}_d$. We often identify the state with the density operator associated with it. For any self-adjoint operator $A \in \mathcal{B}_d$ write $\operatorname{spec}(A) = (a_1, a_2, \ldots, a_d)$ for the vector in $\mathbb{R}^d$ whose entries are the eigenvalues of A taking into account their multiplicities and numbered non-increasingly: $a_1 \geqslant a_2 \geqslant \cdots \geqslant a_d$.

2.1. The spectral simplex

If ρ is a state of $\mathcal{B}_d$ with $\mathrm{spec}(\rho) = (\lambda_1, \lambda_2, \ldots, \lambda_d)$ then $1 \geqslant \lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_d \geqslant 0$, and $\sum_{j=1}^{d} \lambda_j = 1$. We write $s_-(\rho)$ for the minimal eigenvalue of ρ; it satisfies $s_-(\rho) \leqslant 1/d$ there being equality iff $\rho = \tau_d$.

We introduce the set of all possible spec's of states

$$\mathcal{L}_d := \left\{ (\lambda_1, \lambda_2, \ldots, \lambda_d) : \lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_d \geqslant 0, \sum_{j=1}^{d} \lambda_j = 1 \right\},$$

and have that $\mathcal{L}_d$ is the image of $\mathcal{S}_d$ under the map spec. If $u \in \mathcal{B}_d$ is unitary and $\rho \in \mathcal{S}_d$, then ρ_u defined by $\rho_u(a) = \rho(u^* a u)$ is a state; and $\mathrm{spec}(\rho_u) = \mathrm{spec}(\rho)$. We say $\mathcal{K} \subseteq \mathcal{S}_d$ is unitarily invariant if $\rho \in \mathcal{K}$ implies $\rho_u \in \mathcal{K}$ for every unitary $u \in \mathcal{B}_d$. The map $\mathrm{spec} : \mathcal{S}_d \to \mathcal{L}_d$ is continuous (use singular value inequalities [8], or alternatively the second resolvent equation). The ordering required in the definition of the map spec prevents it form being affine; for example, if ρ_1, ρ_2 are pairwise orthogonal pure states then $\mathrm{spec}(\rho_1) = \mathrm{spec}(\rho_2) = (1, 0, \ldots, 0)$, $\mathrm{spec}(t \cdot \rho_1 + (1-t) \cdot \rho_2) = (\max\{t, 1-t\}, \min\{t, 1-t\}, 0, \ldots, 0)$.

The geometric structure of $\mathcal{L}_d$ is simple. It is a $(d-1)$-simplex, that is, a convex set with d extremal points such that the decomposition of every one of its points into a convex sum of extremal points is unique.

Proposition 1. *$\mathcal{L}_d$ is a compact convex subset of $\mathbb{R}^d$ and a $(d-1)$-simplex. The d extremal points are given by the vectors*

$$e^{(k)} = (\underbrace{1/k, 1/k, \ldots, 1/k}_{k \text{ times}}, 0, \ldots, 0), \qquad k = 1, 2, \ldots, d.$$

If $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_d) \in \mathcal{L}_d$ then $\lambda = \sum_{j=1}^{d} x_j e^{(j)}$, where

$$x_j = j(\lambda_j - \lambda_{j+1}), \qquad j = 1, 2, \ldots, d-1, \qquad x_d = d\lambda_d,$$

and $\sum_{j=1}^{d} x_j = 1$.

If $x_j \geqslant 0$ for $j = 1, 2, \ldots, d$ and $\sum_{j=1}^{d} x_j = 1$, then

$$\sum_{j=1}^{d} x_j e^{(j)} = \left(\sum_{k=1}^{d} x_k/k, \sum_{k=2}^{d} x_k/k, \ldots, \sum_{k=j}^{d} x_k/k, \ldots, x_d/d \right),$$

that is, the jth component of $\sum_{j=1}^{d} x_j e^{(j)}$ is $\sum_{k=j}^{d} x_k/k$.

Proof. Convexity and compactness are clear. We show that $e^{(k)}$ is extremal for each $k = 1, 2, \ldots, d$. Suppose $x, y \in \mathcal{L}_d$ and $0 < t < 1$. If $e^{(k)} = tx + (1-t)y$ then

$$x_j = y_j = 0, \qquad \text{for} \quad j = k+1, k+2, \ldots, d$$

and, thus $tx_j + (1-t)y_j = 1/k$ for $j = 1, 2, \ldots, k$, and $x_1 + x_2 + \cdots + x_k = y_1 + y_2 + \cdots + y_k = 1$. But then, for $j = 1, 2, \ldots, k-1$ we have

$$t(x_j - x_{j+1}) + (1-t)(y_j - y_{j+1}) = 0,$$

which implies $x_j = x_{j+1}$ and $y_j = y_{j+1}$ for all $j = 1, 2, \ldots, k-1$ and thus $x_j = y_j = 1/k$ for all $j = 1, 2, \ldots, k$. Hence $x = y = e^{(k)}$ proving that $e^{(k)}$ is extremal. In order to prove that there are no other extremal points it suffices to show that every $\lambda \in \mathcal{L}_d$ is a convex combination of these d extremal points. Now,

$$\sum_{j=1}^{d} x_j e^{(j)} = \left(\sum_{\ell=1}^{d} \frac{x_\ell}{\ell}, \sum_{\ell=2}^{d} \frac{x_\ell}{\ell}, \ldots, \sum_{\ell=k}^{d} \frac{x_\ell}{\ell}, \ldots, \frac{x_d}{d} \right);$$

and the equation $\sum_{j=1}^{d} x_j e^{(j)} = \lambda$ for arbitrary $\lambda \in \mathcal{L}_d$ can be solved for the x_j recursively giving

$$x_d = dx_d, \qquad x_j = j(\lambda_j - \lambda_{j+1}), \qquad j = 1, 2, \ldots, d-1,$$

which are unique. Clearly $x_j \geqslant 0$ for all $j = 1, 2, \ldots, d$ and

$$\sum_{j=1}^{d} x_j = d\lambda_d + \sum_{j=1}^{d-1} j(\lambda_j - \lambda_{j+1}) = d\lambda_d + \sum_{j=1}^{d-1} j\lambda_j - \sum_{\ell=2}^{d}(\ell - 1)\lambda_\ell$$
$$= dx_d + \sum_{j=1}^{d-1}(j - (j-1))\lambda_j - (d-1)\lambda_d = \sum_{j=1}^{d} \lambda_j = 1. \qquad \square$$

Recall the theory of majorization for vectors in $\mathcal{L}_d$ [7, 8]. The connections with entanglement are reviewed in [9]. Define the kth partial sum $\Sigma_k(\lambda)$ of $\lambda \in \mathcal{L}_d$ by $\Sigma_k(\lambda) = \sum_{j=1}^{k} \lambda_j$ $(k = 1, 2, \ldots, d)$, which is affine in λ. Agree that for $\lambda, \mu \in \mathcal{L}_d$, $\lambda \succ \mu$ means that $\Sigma_k(\lambda) \leqslant \Sigma_k(\mu)$ for every $k = 1, 2, \ldots, d$. We observe that $e^{(d)} \succ e^{(d-1)} \succ \cdots \succ e^{(2)} \succ e^{(1)}$. Now setting $\Sigma_k(\rho) = \Sigma_k(\mathrm{spec}(\rho))$, $k = 1, 2, \ldots, d$, these maps are convex continuous functions on $\mathcal{S}_d$. One says that the state ρ is more mixed (more chaotic) than the state ϕ, and writes $\rho \succ \phi$, if $\Sigma_k(\rho) \leqslant \Sigma_k(\phi)$ for $k = 1, 2, \ldots, d$. An intrinsic characterization is provided by Uhlmann's theorem: $\rho \succ \phi$ iff $\rho \in \mathrm{co}\{\phi_u : u \in \mathcal{B}_d \text{ unitary}\}$. Another very useful characterization which we will constantly use is

$$\rho \succ \phi \text{ iff } F(\rho) \leqslant F(\phi) \text{ for every unitarily invariant, convex continuous } F. \tag{1}$$

The non-increasing ordering of the components of a $\lambda \in \mathcal{L}_d$ imposes a number of bounds on the components of λ and on the partial sums $\Sigma_k(\lambda)$. These are particularly immediate if one uses the (baricentric) coordinates x_j, $\lambda = \sum_{j=1}^{d} x_j e^{(j)}$, of λ. The following is an example:

Lemma 1. *For $\lambda = (\lambda_1, \ldots, \lambda_d) \in \mathcal{L}_d$, one has the following:*

(i) $d^{-1} \leqslant \lambda_1 \leqslant 1$; with equality on the left-hand-side inequality iff $\lambda = e^{(d)}$, and on the right-hand-side inequality iff $\lambda = e^{(1)}$. For each $k \in \{2, \ldots, d\}$, $0 \leqslant \lambda_k \leqslant k^{-1}$ with equality on the left-hand-side inequality iff $\lambda \in \mathrm{co}(e^{(1)}, \ldots, e^{(k-1)})$, and on the right-hand-side inequality iff $\lambda = e^{(k)}$.

(ii) For each $k \in \{1, 2, \ldots, d\}$, $kd^{-1} \leqslant \Sigma_k(\lambda) \leqslant 1$. For $k < d$ one has equality on the left-hand-side inequality iff $\lambda = e^{(d)}$, and on the right-hand-side inequality iff $\lambda \in \mathrm{co}(e^{(1)}, \ldots, e^{(k)})$.

Proof. Let $\lambda = \sum_{j=1}^{d} x_j e^{(j)}$; one has $x_j \geqslant 0$ and $\sum_{j=1}^{d} x_j = 1$. Since $\lambda_k = \sum_{j=k}^{d} x_j/j$ one has

$$d^{-1} \sum_{j=k}^{d} x_j \leqslant \sum_{j=k}^{d} x_j/j \leqslant k^{-1} \sum_{j=k}^{d} x_j \leqslant k^{-1}.$$

One has $\Sigma_k(\lambda) = \sum_{j=1}^{k} x_j + k\sum_{j=k+1}^{d} x_j/j$ where the second sum is absent if $k = d$. Thus

$$kd^{-1} = kd^{-1}\left(\sum_{j=1}^{k} x_j + \sum_{j=k+1}^{d} x_j\right) \leqslant kd^{-1}\sum_{j=1}^{k} x_j + k\sum_{j=k+1}^{d} x_j/j$$
$$\leqslant \sum_{j=1}^{k} x_j + k\sum_{j=k+1}^{d} x_j/j \leqslant \sum_{j=1}^{k} x_j + k(k+1)^{-1}\sum_{j=k+1}^{d} x_j$$
$$= 1 - (k(k+1))^{-1}\sum_{j=k+1}^{d} x_j \leqslant 1.$$

The inequality $\Sigma_k(\lambda) \leqslant 1$ is strict unless $\sum_{j=k+1}^{d} x_j = 0$, that is to say, $\sum_{j=1}^{k} x_j = 1$, or $\lambda \in \mathrm{co}(e^{(1)}, \ldots, e^{(k)})$. The inequality $kd^{-1} \leqslant \Sigma_k(\lambda)$ is strict unless $k = d$, or $x_d = 1$. □

2.2. The gap representation of a state

Given a state ρ with $\mathrm{spec}(\rho) = (\lambda_1, \lambda_2, \ldots, \lambda_d) \in \mathcal{L}_d$ consider an orthonormal basis $\{\psi_j : j = 1, 2, \ldots, d\}$ of $\mathcal{H}_d$ consisting of eigenvectors ψ_j of the density matrix associated with ρ. Then $\rho = \sum_{j=1}^{d} \lambda_j \cdot \rho^{(j)}$, where the pure states $\rho^{(j)}$ are given by $\rho^{(j)}(a) = \langle \psi_j, a\psi_j \rangle$, $a \in \mathcal{B}_d$. This corresponds to a *spectral decomposition* into pairwise orthogonal pure states which is not unique if ρ has degenerate eigenvalues.

Proposition 2. *Let $\{\rho^{(j)} : j = 1, 2, \ldots, d\}$ be a maximal family of pairwise orthogonal pure states of $\mathcal{B}_d$. The set $\left\{\sum_{j=1}^{d} \lambda_j \cdot \rho^{(j)} : (\lambda_1, \lambda_2, \ldots, \lambda_d) \in \mathcal{L}_d\right\}$ is affinely homeomorphic to $\mathcal{L}_d$. Thus it is a compact convex subset of the state space of $\mathcal{B}_d$ and a $(d-1)$-simplex with the d extremal points given by the states*

$$\widehat{\rho}^{(j)} = j^{-1} \sum_{k=1}^{j} \rho^{(k)}, \qquad j = 1, 2, \ldots, d.$$

One has $\widehat{\rho}^{(d)} = \tau_d$, and

$$\sum_{j=1}^{d} \lambda_j \cdot \rho^{(j)} = \sum_{j=1}^{d-1} \mu_j(\lambda) \cdot \widehat{\rho}^{(j)} + d\lambda_d \cdot \tau_d, \tag{2}$$

where

$$\mu_j(\lambda) = j(\lambda_j - \lambda_{j+1}) \geqslant 0, \qquad j = 1, 2, \ldots, d-1, \tag{3}$$

and $\sum_{j=1}^{d-1} \mu_j(\lambda) = 1 - d\lambda_d$.

Proof. If $0 \leqslant t \leqslant 1$, and $\rho, \phi \in \left\{\sum_{j=1}^{d} \lambda_j \rho^{(j)} : (\lambda_1, \lambda_2, \ldots, \lambda_d) \in \mathcal{L}_d\right\}$ with $\mathrm{spec}(\rho) = \lambda$ and $\mathrm{spec}(\phi) = \mu$, we have

$$t \cdot \rho + (1-t) \cdot \phi = t \cdot \sum_{j=1}^{d} \lambda_j \cdot \rho^{(j)} + (1-t) \cdot \sum_{j=1}^{d} \mu_j \cdot \rho^{(j)} = \sum_{j=1}^{d} (t\lambda_j + (1-t)\mu_j) \cdot \rho^{(j)}$$

and thus $\mathrm{spec}(t \cdot \rho + (1-t) \cdot \phi) = t \cdot \mathrm{spec}(\rho) + (1-t) \cdot \mathrm{spec}(\phi)$. The converse is also true, and spec is an affine homeomorphism from $\left\{\sum_{j=1}^{d} \lambda_j \cdot \rho^{(j)} : (\lambda_1, \lambda_2, \ldots, \lambda_d) \in \mathcal{L}_d\right\}$ onto $\mathcal{L}_d$. Apply proposition 1. □

We call the representation of a state ρ given by (2) the *gap representation* of ρ due to formula (3) which involves the successive eigenvalue gaps. This representation is not unique in as much as the spectral decomposition is not unique when one has spectral degeneracies. But any multiplicities, if present, are automatically taken care of by the states $\widehat{\rho}^{(j)}$. Note that $\widehat{\rho}^{(j)}\widehat{\rho}^{(k)} = (1/\max\{j,k\})\widehat{\rho}^{(\min\{j,k\})}$. These algebraic equations are characteristic of a gap representation as follows:

Lemma 2. *If $k \in \{1, 2, \ldots, d\}$ and $\omega_1, \omega_2, \ldots, \omega_k$ are k distinct states with*

(i) for every $j \in \{1, 2, \ldots, k\}$ there is $s(j) \in \{1, 2, \ldots, d\}$ such that $j_1 \neq j_2$ implies $s(j_1) \neq s(j_2)$; i.e., s is an injection from $\{1, 2, \ldots, k\}$ into $\{1, 2, \ldots, d\}$,

(ii) $\omega_j\omega_m = (1/\max\{s(j), s(m)\})\omega_{s^{-1}(\min\{s(j),s(m)\})}$ for every $j, m \in \{1, 2, \ldots, k\}$,

then there is a maximal family $\{\rho^{(n)} : n = 1, 2, \ldots, d\}$ *of pairwise orthogonal pure states such that* $\omega_j = \widehat{\rho}^{(s(j))}$ *for every* $j = 1, 2, \ldots, k$.

Proof. The $s(j)$ are all distinct and the $s(j)\omega_j = P_{s(j)}$ are orthoprojectors of rank $s(j)$ which satisfy $P_{s(j)}P_{s(m)} = P_{\min\{s(j),s(m)\}}$. Renumerate the ω_j so that $1 \leqslant s(1) < s(2) < \cdots < s(k) \leqslant d$; then $P_{s(j)}P_{s(m)} = P_{s(\min\{j,m\})}$. Choose an orthonormal set $\{\psi_n : n = 1, 2, \ldots, s(1)\}$ spanning the range of $P_{s(1)}$, and then, successively, orthonormal sets $\{\psi_n : n = s(j)+1, \ldots, s(j+1)\}$ spanning the range of $P_{s(j+1)} - P_{s(j)}$, for $j = 1, 2, \ldots, k-1$. Finally, choose an orthonormal set $\{\psi_n : n = s(k) + 1, \ldots, d\}$ spanning the kernel of $P_{s(k)}$. Then if $\rho^{(n)}$ denotes the pure state associated with the vector ψ_n, $n = 1, 2, \ldots, d$, we have $\omega_j = \widehat{\rho}^{(s(j))}$. □

The gap representation has a number of features which turn out to be useful in the discussion of entanglement. The states $\widehat{\rho}^{(j)}$, which are the vertices of the $(d-1)$-simplex, obtained from different maximal families of pairwise orthogonal pure states are unitarily equivalent. For $j < d$ they have only two eigenvalues 0 (with multiplicity $d - j$) and $1/j$ (with multiplicity j). This will considerably simplify the discussion of their separability in composite systems.

2.3. *Unitarily invariant convex functions on* $\mathcal{S}$

Consider a real-valued function F defined on $\mathcal{S}_d$ which is unitarily invariant, convex, i.e., $F(t \cdot \rho + (1-t) \cdot \phi) \leqslant tF(\rho) + (1-t)F(\phi)$, for every $t \in [0, 1]$ and every $\rho, \phi \in \mathcal{S}_d$, and continuous. Let $F_+ := \sup\{F(\rho) : \rho \in \mathcal{S}_d\}$; by continuity and compactness there is a maximizer.

Proposition 3. *If* $F : \mathcal{S}_d \to \mathbb{R}$ *is a unitarily invariant convex function then:*

(i) For every $\rho \in \mathcal{S}_d$,

$$F(\tau_d) \leqslant F(\rho) \leqslant F_+. \tag{4}$$

Moreover $F(\rho) = F_+$ *for every pure state* ρ.

(ii) For each $c \in [F(\tau_d), F_+]$ *the level set* $\mathbb{L}_c := \{\rho \in \mathcal{S} : F(\rho) \leqslant c\}$ *is a compact, convex, unitarily invariant subset of* $\mathcal{S}$. *If* $\rho \succ \phi \in \mathbb{L}_c$ *then* $\rho \in \mathbb{L}_c$. *Moreover,* $\mathbb{L}_c \subseteq \mathbb{L}_b$ *if* $c < b$.

(iii) If F *is strictly convex then there is equality on the left-hand-side inequality of equation (4) iff* $\rho = \tau_d$; *and there is equality on the right-hand-side inequality of equation (4) iff* ρ *is pure. Moreover,* $\mathrm{ext}(\mathbb{L}_c) = \{\rho \in \mathcal{S} : F(\rho) = c\}$.

Proof. The reader is asked to verify the triviality of (i) and (ii) for a constant F. We thus assume that F is not constant.

Since, for every state ρ and every pure ϕ, one has $\tau_d \succ \rho \succ \phi$, inequality (4) follows from equation (1), and $F_+ = F(\phi)$. Suppose F is strictly convex and $\rho \neq \tau_d$ satisfies $F(\rho) = F(\tau_d)$, then $F(\tau_d) \leqslant F(t \cdot \rho + (1-t) \cdot \tau_d) < tF(\rho) + (1-t)F(\tau_d) = F(\tau_d)$, a contradiction. This and the definition of F_+ prove equation (4) and part of statement (iii); statement (ii) is clear.

Suppose F is strictly convex. If $\rho \in \mathbb{L}_c$ but $\rho \notin \mathrm{ext}(\mathbb{L}_c)$, then $\rho = t \cdot \phi + (1-t) \cdot \omega$ with $0 < t < 1, \phi, \omega \in \mathbb{L}_c$ and $\phi \neq \omega$; thus $F(\rho) < tF(\phi) + (1-t)F(\omega) \leqslant c$. This proves $\{\rho : F(\rho) = c\} \subseteq \mathrm{ext}(\mathbb{L}_c)$. For $c = F_+$ we conclude that $F(\rho) = F_+$ implies that ρ is pure. It remains to show that $\mathrm{ext}(\mathbb{L}_c) \subseteq \{\rho : F(\rho) = c\}$. If $c = F(\tau_d)$ then $\mathbb{L}_{F(\tau_d)} = \{\tau_d\} = \{\rho : F(\rho) = F(\tau_d)\}$. We assume that $c > F(\tau_d)$ and $F(\rho) < c$ and show that ρ is not extremal in $\mathbb{L}_c$. Take any gap representation of ρ, then

$\rho = t_o \cdot \widehat{\rho}^{(1)} + (1 - t_o) \cdot \omega$ with $\mathrm{spec}(\omega) \in \mathrm{co}(e^{(2)}, \ldots, e^{(d)})$ and $t_o \in [0, 1]$. The map $[0, 1] \ni t \mapsto f(t) = F(t \cdot \widehat{\rho}^{(1)} + (1 - t) \cdot \omega$ is strictly convex since, for $u, t_1, t_2 \in [0, 1]$

$$\begin{aligned} f_\phi(ut_1 + (1-u)t_2) &= F((ut_1 + (1-u)t_2) \cdot \widehat{\rho}^{(1)} + (1 - (ut_1 + (1-u)t_2)) \cdot \omega) \\ &= F(u \cdot (t_1 \cdot \widehat{\rho}^{(1)} + (1 - t_1) \cdot \omega) + (1 - u) \cdot (t_2 \cdot \widehat{\rho}^{(1)} + (1 - t_2) \cdot \omega) \\ &\leqslant uF(t_1 \cdot \widehat{\rho}^{(1)} + (1 - t_1) \cdot \omega) + (1 - u)F(t_2 \cdot \widehat{\rho}^{(1)} + (1 - t_2) \cdot \omega) \\ &= uf(t_1) + (1 - u)f(t_2), \end{aligned}$$

and the inequality is strict if $0 < u < 1$ and $t_1 \neq t_2$ by the strict convexity of F and the fact that $t_1 \cdot \widehat{\rho}^{(1)} + (1-t_1) \cdot \omega \neq t_2 \cdot \widehat{\rho}^{(1)} + (1-t_2) \cdot \omega$. Moreover, if $1 \geqslant t_1 > t_2 \geqslant 0$ then $t_2 \cdot \widehat{\rho}^{(1)} + (1-t_2) \cdot \omega \succ t_1 \cdot \widehat{\rho}^{(1)} + (1 - t_1) \cdot \omega$ since this is equivalent to $(t_1 - t_2)(\Sigma_k(\widehat{\rho}^{(1)}) - \Sigma_k(\omega)) \geqslant 0$, and the latter follows from $\omega \succ \widehat{\rho}^{(1)}$. But then by equation (1), $f(t_2) = F(t_2 \cdot \widehat{\rho}^{(1)} + (1 - t_2) \cdot \omega) \leqslant F(t_1 \cdot \widehat{\rho}^{(1)} + (1 - t_1) \cdot \omega) = f(t_1)$ so that f_ϕ is non-decreasing. But a strictly convex, non-decreasing function must be increasing. Thus $F(\omega) = f(0) \leqslant f(t_o) = F(\rho) < c \leqslant F_+$; let t_* be the unique number in $[0, 1]$ such that $f(t_*) = c$ it follows that $t_o < t_*$ and thus $\rho = t_o \cdot \widehat{\rho}^{(1)} + (1 - t_o) \cdot \omega = (t_o/t_*) \cdot (t_* \cdot \widehat{\rho}^{(1)} + (1 - t_*) \cdot \omega) + (1 - (t_o/t_*)) \cdot \omega$ is not extremal in $\mathbb{L}_c$ since $f(0) = F(\omega) < c$ and $F(t_* \cdot \widehat{\rho}^{(1)} + (1 - t_*) \cdot \omega) = f(t_*) = c$. □

3. Spectral conditions implying separability

We return to the discussion of arbitrary compositions of finite quantum systems as described in the introduction. Given integers $d_1, d_2, \ldots, d_N$ all of which are larger or equal to 2, and N Hilbert spaces $\mathcal{H}_j$ of dimension d_j, consider $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_N$ which has dimension $D = d_1 d_2 \cdots d_N$. We identify $\mathcal{B} = \mathcal{B}(\mathcal{H})$ with $\mathcal{B}_{d_1} \otimes \mathcal{B}_{d_2} \otimes \cdots \otimes \mathcal{B}_{d_N}$. A state ρ of $\mathcal{B}$ is *separable* if it lies in the convex hull of the product-states of $\mathcal{B}$; otherwise it is called *entangled*. $\mathcal{S}^{\mathrm{sep}}$ denotes the separable states.

3.1. The separability modulus: generalities

We observe that $\tau_D = \tau_{d_1} \otimes \tau_{d_2} \otimes \cdots \otimes \tau_{d_N}$ so that $\tau \equiv \tau_D$ is a product-state, hence separable. τ is also the maximally mixed state of $\mathcal{B}$. Given any state ρ of $\mathcal{B}$ and any $t \in [0, 1]$, we let

$$\rho_t = (1 - t) \cdot \tau + t \cdot \rho.$$

We then ask ourselves: When is ρ_t separable?

Frequently, in what follows, we use the fact that if ω, φ are both separable states then $t \cdot \omega + (1 - t) \cdot \varphi$ is separable for every $t \in [0, 1]$ because $\mathcal{S}^{\mathrm{sep}}$ is convex.

We observe that if ρ is separable then ρ_t is separable for every $t \in [0, 1]$. In fact,

Lemma 3.

(i) ρ_t *is separable for every* $t \in [0, 1]$ *iff* ρ *is separable;*
(ii) if ρ_t *is separable for some* $t \in (0, 1]$ *then* ρ_s *is separable for every* $s \in [0, t]$*;*
(iii) if ρ_s *is entangled for some* $s \in (0, 1]$ *then* ρ_t *is entangled for every* $t \in [s, 1]$.

Proof. Statement (i) is clear. Suppose $0 \leqslant s \leqslant t \leqslant 1$, then $0 \leqslant s/t \leqslant 1$ and

$$\rho_s = s \cdot \rho + (1 - s) \cdot \tau = \frac{s}{t} \cdot (t \cdot \rho + (1 - t) \cdot \tau) + \left(1 - \frac{s}{t}\right) \cdot \tau = \frac{s}{t} \cdot \rho_t + \left(1 - \frac{s}{t}\right) \cdot \tau.$$

Under the hypotheses of (ii), ρ_s is separable as a convex sum of two separable states. Under the hypotheses of (iii), ρ_s would be separable if ρ_t were separable. □

The above allows us to introduce the *modulus of separability* of ρ (with respect to τ) as the number

$$\ell(\rho) = \sup\{t \in [0, 1] : \rho_t \text{ is separable}\}.$$

Vidal and Tarrach [2] have studied the quantity $\ell(\rho)^{-1} - 1$ which they called the *random robustness of entanglement*. Most of the results below are explicitly or implicitly given by them so the rest of this section is a streamlined exposition of the basic facts about ℓ that we need. For more information the reader should consult [2].

Lemma 4. *If $t \in [0, 1]$ then $\ell(\rho_t) = \min\{1, t^{-1}\ell(\rho)\}$ for every state ρ.*

Proof. A straightforward calculation gives $(\rho_t)_s = \rho_{ts}$. Suppose that $t > 0$, then

$$\begin{aligned}\ell(\rho_t) &= \sup\{s \in [0, 1] : (\rho_t)_s \text{ isseparable}\}\\ &= \sup\{s \in [0, 1] : \rho_{ts} \text{ is separable}\}\\ &= \sup\{r/t \in [0, 1] : \rho_r \text{ is separable}\}\\ &= t^{-1} \sup\{r \in [0, t] : \rho_r \text{ is separable}\}.\end{aligned}$$

If $t < \ell(\rho)$ the last supremum is t. If $\ell(\rho) \leqslant t$ the last supremum is $\ell(\rho)$. With the usual interpretation, the formula remains valid for $t = 0$ since $\rho_0 = \tau$ and $\ell(\tau) = 1$. □

Lemma 5. *$\rho_{\ell(\rho)}$ is separable.*

Proof. For $t < \ell(\rho)$ we have $\rho_{\ell(\rho)} - \rho_t = (\ell(\rho) - t) \cdot (\rho - \tau)$ and thus $\|\rho_{\ell(\rho)} - \rho_t\| = (\ell(\rho)-t)\|\rho-\tau\|$. Taking a sequence $\{t_n : n = 1, 2, \ldots\}$ with $t_n < \ell(\rho)$ and $\lim_{n\to\infty} t_n = \ell(\rho)$, we have $\rho_{t_n} \in \mathcal{S}^{\text{sep}}$ and $\lim_{n\to\infty} \rho_{t_n} = \rho_{\ell(\rho)}$ and hence $\rho_{\ell(\rho)}$ lies in the closure of $\mathcal{S}^{\text{sep}}$ which is closed. □

Corollary 1. *ρ_t is separable iff $t \leqslant \ell(\rho)$.*

Lemma 6. *If $0 < t_j \leqslant 1$ for $j = 1, 2, \ldots, M$ with $M \in \mathbb{N}$, and $\sum_{j=1}^{M} t_j = 1$, then*

$$\ell\left(\sum_{j=1}^{M} t_j \cdot \rho^{(j)}\right) \geqslant \min\{\ell(\rho^{(j)}) : j = 1, 2, \ldots, M\}$$

for any set of M states $\{\rho^{(j)} : j = 1, 2, \ldots, M\}$.

Proof. The following proof does not use the previous result. Let $\omega = \sum_{j=1}^{M} t_j \cdot \rho^{(j)}$; then

$$\omega_t = t \cdot \omega + (1 - t) \cdot \tau = \sum_{j=1}^{M} t_j (\rho^{(j)})_t.$$

If $t < t_o := \min\{\ell(\rho^{(j)}) : j = 1, 2, \ldots, M\}$, the states $(\rho^{(j)})_t$ are all separable and thus ω_t is separable; by definition of ℓ, $\ell(\omega) \geqslant t$. Taking the supremum with respect to $t < t_o$ one obtains the result. □

A substantial improvement of the above lower bound would be concavity of ℓ. Examples for two qubits show that this is not the case. However, $\rho \mapsto (1/\ell(\rho))$ turns out to be convex.

Consider

$$L := \inf\{\ell(\rho) : \rho \in \mathcal{S}\};$$

due to lemma 6, the infimum can be taken over the pure states. Moreover, $L < 1$ since there are entangled pure states. L has been computed in various cases [2, 10, 11]. For our purposes it would suffice to know that $L > 0$, and Życzkowski *et al* [6] give an elegant proof of this. Rungta [10], for $d_1 = d_2 = \cdots = d_N$ (using the methods of [11]) obtained (to handle the case of distinct dimensions d_j we just embed $\mathcal{B}_{d_j}$ in $\mathcal{B}_d$ by adding the necessary rows and columns of zeros)

$$L \geqslant \frac{1}{1+d^{2N-1}}, \qquad d = \max\{d_1, d_2, \ldots, d_N\},$$

while Vidal and Tarrach [2] obtained

$$L \geqslant \frac{1}{(1+D/2)^{N-1}}.$$

The second bound is exact for $N = 2$ while the Rungta bound is poor for this case. As N increases, the first bound eventually exceeds the second one and becomes the better lower bound on L. The best lower bounds for L can be obtained using the results of Gurvits and Barnum [12–14] on the separable balls around the trace in the Frobenius norm $X \to \|X\|_2 = \sqrt{\mathrm{Tr}(X^*X)}$; for example, from corollary 3 of [13],

$$L \geqslant \frac{2}{2^{N/2}\sqrt{D(D-1)}}.$$

Proposition 4. *$1/\ell$ is convex.*

Proof. Convexity of $1/\ell$ is

$$\ell(t\cdot\rho^{(1)} + (1-t)\cdot\rho^{(2)})^{-1} \leqslant t\ell(\rho^{(1)})^{-1} + (1-t)\ell(\rho^{(2)})^{-1},$$

or equivalently

$$\ell(t\cdot\rho^{(1)} + (1-t)\cdot\rho^{(2)}) \geqslant \frac{\ell(\rho^{(1)})\ell(\rho^{(2)})}{t\ell(\rho^{(2)}) + (1-t)\ell(\rho^{(1)})}.$$

Put $\ell_j := \ell(\rho^{(j)})$ and $s = \ell_1\ell_2/(t\ell_2 + (1-t)\ell_1)$. Observe that $s \geqslant 0$ and $s \leqslant \ell_1\ell_2/\max\{\ell_1, \ell_2\} = \min\{\ell_1, \ell_2\} \leqslant 1$. Thus, by corollary 1, convexity is proved if we show that $(t\cdot\rho^{(1)} + (1-t)\cdot\rho^{(2)})_s$ is separable. But

$$\begin{aligned}(t\cdot\rho^{(1)} + (1-t)\cdot\rho^{(2)})_s &= s\cdot(t\cdot\rho^{(1)} + (1-t)\cdot\rho^{(2)}) + (1-s)\cdot\tau \\ &= \left(\frac{\ell_1\ell_2 t}{t\ell_2 + (1-t)\ell_1}\right)\cdot\rho^{(1)} + \left(\frac{\ell_1\ell_2(1-t)}{t\ell_2 + (1-t)\ell_1}\right)\cdot\rho^{(2)} + (1-s)\cdot\tau.\end{aligned}$$

Put

$$r := \left(\frac{\ell_2 t}{t\ell_2 + (1-t)\ell_1}\right);$$

which is in $[0, 1]$. Then

$$1 - r = \left(\frac{\ell_1(1-t)}{t\ell_2 + (1-t)\ell_1}\right), \qquad (1-s) = 1 - r\ell_1 - (1-r)\ell_2,$$

so that

$$\begin{aligned}(t\cdot\rho^{(1)} + (1-t)\cdot\rho^{(2)})_s &= r\ell_1\cdot\rho^{(1)} + (1-r)\ell_2\cdot\rho^{(2)} + (1 - r\ell_1 - (1-r)\ell_2)\cdot\tau \\ &= r\cdot(\ell_1\cdot\rho^{(1)} + (1-\ell_1)\cdot\tau) + (1-r)\cdot(\ell_2\cdot\rho^{(2)} + (1-\ell_2)\cdot\tau) \\ &= r\cdot(\rho^{(1)})_{\ell_1} + (1-r)\cdot(\rho^{(2)})_{\ell_2},\end{aligned}$$

which is separable by lemma 5. □

The convexity of $1/\ell$ gives an improvement on the lower bound of lemma 6:

Corollary 2. *If* $0 < t_j \leqslant 1$ *for* $j = 1, 2, \ldots, M$ *with* $M \in \mathbb{N}$*, and* $\sum_{j=1}^{M} t_j = 1$*, then*

$$\ell\left(\sum_{j=1}^{M} t_j \cdot \rho^{(j)}\right) \geqslant \left(\sum_{j=1}^{M} \frac{t_j}{\ell(\rho^{(j)})}\right)^{-1} \geqslant \min\{\ell(\rho^{(j)}) : j = 1, 2, \ldots, M\}$$

for any set of N states $\{\rho^{(j)} : j = 1, 2, \ldots, M\}$*. There is equality on the right-hand-side inequality iff all* $\ell(\rho^{(j)})$ *are equal.*

Although the convexity bound is saturated when all $\rho^{(j)}$ are separable it is a rather poor bound when at least one of the $\rho^{(j)}$ is entangled as we will see below.

Proposition 5. ℓ *is upper semi-continuous.*

Proof. We have to show that the sets $\mathcal{K}_x = \{\rho : \ell(\rho) \geqslant x\}$ are closed for every real x. These sets are empty for $x > 1$ and are the whole space of states for $x \leqslant 0$. Otherwise, for $x \in (0, 1]$ we have $\rho_x \in \mathcal{S}^{\text{sep}}$ for every $\rho \in \mathcal{K}_x$. If the sequence $\{\rho^{(n)} : n = 1, 2, \ldots\} \subset \mathcal{K}_x$ converges to ρ then the sequence $\left\{\rho_x^{(n)} : n = 1, 2, \ldots\right\}$ is in $\mathcal{S}^{\text{sep}}$ and converges to ρ_x. Thus, since $\mathcal{S}^{\text{sep}}$ is closed, ρ_x is separable and thus $\ell(\rho) \geqslant x$ so $\rho \in \mathcal{K}_x$. □

Thus $\rho \mapsto E(\rho) := (1/\ell(\rho)) - 1$ is a bona fide measure of entanglement in as much as it is convex and lower semi-continuous, and it is zero iff ρ is separable. As mentioned, Vidal and Tarrach [2] have studied E extensively and computed it in a number of particular cases.

Upper semi-continuity of ℓ and compactness of $\mathcal{S}$ imply that there exists a state ρ such that $\ell(\rho) = L$. Any state with this property will be called *maximally entangled* and is automatically pure (the relationship with other notions of what a maximally entangled pure state is, needs yet to be explored).

3.2. Putting the gap representation to work

We can now use the gap representation to obtain our weakest result of the type described by the title of the paper:

Theorem 1. *If* $s_-(\rho) \geqslant (1 - L)/D$ *then* ρ *is separable. For every* s *with* $0 \leqslant s < (1 - L)/D$ *there is an entangled state* ϕ *such that* $s_-(\phi) = s$.

Proof. Let $\text{spec}(\rho) = (\lambda_1, \lambda_2, \ldots, \lambda_D)$; if the condition on $\lambda_D = s_-(\rho)$ is met the gap representation gives

$$\begin{aligned}
\rho &= \sum_{j=1}^{D-1} \mu_j(\lambda) \cdot \widehat{\rho}^{(j)} + Ds_-(\rho) \cdot \tau \\
&= (1 - Ds_-(\rho)) \cdot \underbrace{\left(\sum_{j=1}^{D-1} \frac{\mu_j(\lambda)}{1 - Ds_(\rho)} \cdot \widehat{\rho}^{(j)}\right)}_{\phi} + Ds_-(\rho) \cdot \tau \\
&= (1 - Ds_-(\rho)) \cdot \phi + Ds_-(\rho) \cdot \tau = \phi_{1-Ds_-(\rho)};
\end{aligned}$$

but $1 - Ds_-(\rho) \leqslant L$ and thus $(1 - Ds_-(\rho)) \leqslant \ell(\phi)$ which implies that $\rho = \phi_{1-Ds_-(\rho)}$ is separable.

Take any maximally entangled state ω, then ω_t is separable iff $t \leqslant L$, and, because ω is pure, $s_-(\omega_t) = (1-t)/D$. For any $s \in [0, (1-L)/D)$ the state ω_{1-Ds} is entangled and $s_-(\omega_{1-Ds}) = s$. □

We observe that, in the language of section 2.1, the theorem states that

$$\{\rho : \Sigma_{D-1}(\rho) \leqslant (D+L-1)/D\} \subseteq \mathcal{S}^{\mathrm{sep}}.$$

An immediate improvement of the weak result above would follow if it were true that *every state* ρ *with* $\mathrm{spec}(\rho) = e^{(D-1)}$ *is separable*. This has been proved for $N = 2$, $d_1 = 2$ and $d_2 = 2, 3$ by [6] (see also appendix A of [15] for a more direct approach), and in general for $N = 2$ by Gurvits and Barnum [12] (see the following section 4). How the separability of ρ with $\mathrm{spec}(\rho) = e^{(D-1)}$ can be used to improve theorem 1 is shown in appendix B.

Another useful feature of the gap representation is that it provides an improvement on the convexity bound of corollary 2 obtained from any spectral decomposition of a state:

Lemma 7. *Let* $\mathrm{spec}(\rho) = (\lambda_1, \lambda_2, \ldots, \lambda_D) \in \mathcal{L}_D$ *and*

$$\rho = \sum_{j=1}^{D} \lambda_j \cdot \rho^{(j)} = \sum_{j=1}^{D-1} \mu_j(\lambda) \cdot \widehat{\rho}^{(j)} + D\lambda_D \cdot \tau$$

be a gap representation. Then

$$\ell(\rho) \geqslant \left(\sum_{j=1}^{D-1} \frac{j(\lambda_j - \lambda_{j+1})}{\ell(\widehat{\rho}^{(j)})} + D\lambda_D \right)^{-1} \geqslant \left(\sum_{j=1}^{D} \frac{\lambda_j}{\ell(\rho^{(j)})} \right)^{-1}.$$

Proof. Let us abbreviate $\ell(\rho^{(j)}) = \ell_j$ and $\ell(\widehat{\rho}^{(j)}) = \widehat{\ell}_j$. Applying corollary 2 to the gap representation and observing that $\widehat{\ell}_D = 1$ we get

$$\ell(\rho) \geqslant \left(\sum_{j=1}^{D-1} \frac{\mu_j(\lambda)}{\widehat{\ell}_j} + D\lambda_D \right)^{-1}.$$

The other inequality is equivalent to

$$\sum_{j=1}^{D} \frac{\lambda_j}{\ell_j} \geqslant \sum_{j=1}^{D-1} \frac{\mu_j(\lambda)}{\widehat{\ell}_j} + D\lambda_D,$$

which we now prove. Another application of corollary 2 gives

$$1/\widehat{\ell}_j \leqslant j^{-1} \sum_{k=1}^{j} (1/\ell_j), \qquad j = 1, 2, \ldots, D;$$

thus

$$\begin{aligned}
\sum_{j=1}^{D-1} \frac{\mu_j(\lambda)}{\widehat{\ell}_j} + D\lambda_D &\leqslant \sum_{j=1}^{D-1} \frac{\mu_j(\lambda)}{j} \left(\sum_{k=1}^{j} (1/\ell_k) \right) + \lambda_D \left(\sum_{k=1}^{D} (1/\ell_k) \right) \\
&= \sum_{j=1}^{D-1} (\lambda_j - \lambda_{j+1}) \left(\sum_{k=1}^{j} (1/\ell_j) \right) + \lambda_D \left(\sum_{k=1}^{D} (1/\ell_k) \right) = \sum_{j=1}^{D} \lambda_j / \ell_j.
\end{aligned}$$

□

3.3. An application to thermal states

Given any self-adjoint $h \in \mathcal{B}$ and $\beta \in \mathbb{R}$ consider the (thermal equilibrium) state ρ_β given by the density operator

$$\rho_\beta = \begin{cases} \tau & \text{if} \quad \beta = 0 \\ \exp(-\beta h)/\operatorname{Tr}(\exp(-\beta h)) & \text{if} \quad \beta \neq 0. \end{cases}$$

One has $\lim_{\beta\to 0} \rho_\beta = \tau$ and the expectation is that for $|\beta|$ sufficiently small one will have separability of ρ_β. This is indeed the case.

Proposition 6. *There are real numbers $\beta_c^\pm$ with $\beta_c^- < 0 < \beta_c^+$ such that ρ_β is separable for $\beta \in [\beta_c^-, \beta_c^+]$, and if I is any interval that contains $[\beta_c^-, \beta_c^+]$ properly, then there is $\beta' \in I$ such that $\rho_{\beta'}$ is entangled.*

Proof. Assume $\beta \neq 0$ and put $Z(\beta) = \operatorname{Tr}(\mathrm{e}^{-\beta h}) = \sum_{j=1}^{D} \mathrm{e}^{-\beta\epsilon_j}$, where $\operatorname{spec}(h) = (\epsilon_1, \ldots, \epsilon_D)$. Take $\beta > 0$; then $Z(\beta) \leqslant D\,\mathrm{e}^{-\beta s_-(h)}$ where $s_-(h)$ is the minimal eigenvalue of h. Now $s_-(\rho_\beta) = \mathrm{e}^{-\beta s_+(h)} Z(\beta)^{-1} \geqslant D^{-1} \exp(-\beta(s_+(h) - s_-(h)))$, where $s_+(h)$ is the maximal eigenvalue of h. If

$$\exp\{-\beta(s_+(h) - s_-(h))\} \geqslant (1 - L),$$

the hypothesis of theorem 1 is met and we conclude that ρ_β is separable. But $s_+(h) > s_-(h)$ unless h is a multiple of $\mathbf{1}$ in which case $\rho_\beta = \tau$ for every β. Thus, ρ_β will be separable if

$$\beta \leqslant \beta_o := \frac{-\ln(1 - L)}{s_+(h) - s_-(h)}.$$

An analogous argument in the case $\beta < 0$ shows that ρ_β is separable if $\beta \geqslant -\beta_o$. Define

$$\beta_c^+ = \sup\{\beta > 0 : \rho_\gamma \text{ is separable for every } \gamma \in [0, \beta]\},$$
$$\beta_c^- = \inf\{\beta < 0 : \rho_\gamma \text{ isseparable for every } \gamma \in [\beta, 0]\};$$

then $\beta_c^- < -\beta_o < 0 < \beta_o < \beta_c^+$. Moreover, since $\beta \to \rho_\beta$ is continuous $\rho_{\beta_c^\pm}$ is separable as a limit of separable states. □

Observe that $\beta_c^+ = \infty$ and $\beta_c^- = -\infty$ are possible, for example, when all spectral orthoprojectors of h are products.

A beautiful result of Uhlmann and Wehrl [7, 16] states that $\beta \to \rho_\beta$ is $\succ$-decreasing for positive β ($\succ$-increasing for negative β): $\rho_{\beta_1} \succ \rho_{\beta_2}$ if $0 \leqslant \beta_1 < \beta_2$. The limit $\beta \to \pm\infty$ of ρ_β is the state $\rho_{\pm\infty} = P_\mp/m_\mp$ where P_- (respectively P_+) is the orthoprojection onto the eigenspace of the minimal eigenvalue $s_-(h)$ (respectively the maximal eigenvalue $s_+(h)$) of the Hamiltonian and m_- (respectively m_+) is its multiplicity. If ρ_∞ is entangled (e.g., $m_- = 1$ and the ground-state vector is not a product-vector), then $\beta_c^+ < \infty$. What happens above β_c^+? This is considered in [17].

3.4. Unitarily invariant convex functions as separability detectors

We use the definitions and notation of 2.3. A function F on the state space of a composite system is said to be *good* if $F(\rho) = F(\tau)$ implies that $\rho = \tau$. In particular, F cannot be constant. By proposition 3, every unitarily invariant strictly convex continuous function is good. Also, any kth eigenvalue partial sum Σ_k with $k < D$ is good by lemma 1.

If $F : \mathcal{S} \to \mathbb{R}$ is unitarily invariant, convex and continuous, the numbers

$$C_L^+ = F(L \cdot \phi + (1 - L) \cdot \tau), \qquad \phi \text{ pure};$$
$$C_L^- = F(L \cdot \omega + (1 - L) \cdot \tau), \qquad \operatorname{spec}(\omega) = e^{(D-1)},$$

are well defined. To see that $C_L^- \leqslant C_L^+$, take an ω with $\mathrm{spec}(\omega) = e^{(D-1)}$ and take any gap representation of ω; the state $\widehat{\rho}^{(1)}$ is pure and $\omega \succ \widehat{\rho}^{(1)}$ so that $C_L^- = F(L\cdot\omega + (1-L)\cdot\tau) \leqslant F(L\cdot\rho^{(1)} + (1-L)\cdot\tau) = C_L^+$. Also $C_L^- = F(L\cdot\omega + (1-L)\cdot\tau) \geqslant F(\tau)$ because of proposition 3, with strict inequality if F is good; and $C_L^+ \leqslant LF(\phi) + (1-L)F(\tau) = LF_+ + (1-L)F(\tau) \leqslant F_+$, with strict inequality for non-constant F. The reason for introducing these numbers is

Theorem 2. *If $F : \mathcal{S} \to \mathbb{R}$ be a unitarily invariant, convex, continuous and good function, then there is a number C_F in $\left[C_L^-, C_L^+\right]$ such that $\mathbb{L}_c \subset \mathcal{S}^{\mathrm{sep}}$ for every $c \in [F(\tau), C_F]$, whereas for every $c' \in (C_F, F_+]$ there is an entangled state ρ with $F(\rho) = c'$.*

There is of course a version of the above for unitarily invariant, concave, continuous and good functions, i.e., entropies that deserve their name. The statement is then $\{\rho : F(\rho) \geqslant c\} \subseteq \mathcal{S}^{\mathrm{sep}}$ if $c \geqslant C_F$. The above result shows that every unitarily invariant continuous and good function on $\mathcal{S}$ which is convex or concave provides us with a separability detector. The list of separability detectors includes, apart from the kth partial sums for $k = 1, 2, \ldots, D-1$, the von Neumann entropy $S(\rho) = \mathrm{Tr}(\rho\ln(\rho))$, the Rényi entropies, the functions $F(\rho) = \mathrm{Tr}(\rho^q)$ with $q > 0$, etc.

The rest of this section is devoted to the proof of this theorem, and to the computation of the bounds $C_L^\pm$ for some especially interesting F.

By proposition 3, the level sets $\mathbb{L}_c$ are closed and convex for every $c \in [F(\tau), F_+]$ and not empty since $\tau \in \mathbb{L}_c$ always. The basic observation is

Lemma 8. *If F is good and $\tau \neq \rho \in \mathcal{S}$, then the map $[0, 1] \ni t \mapsto f_\rho(t) = F(t\cdot\rho + (1-t)\cdot\tau)$ is increasing, and convex.*

Proof. f_ρ is constant for $F(\rho) = F(\tau)$; otherwise, by convexity of F, it is convex and, by goodness, it assumes its minimal value $F(\tau)$ precisely at $t = 0$. It follows that the map is increasing. □

Let ρ be a maximally entangled state; then it is pure and $F(L\cdot\rho + (1-L)\cdot\tau) = C_L^+$. By the above lemma, for every $F_+ \geqslant c > C_L^+$ there is a (unique) $t > L$ such that $F(t\cdot\rho + (1-t)\cdot\tau) = f_\rho(t) = c$ and $t\cdot\rho + (1-t)\cdot\tau$ is entangled. This shows that for every $c > C_L^+$, $\mathbb{L}_c$ is not contained in $\mathcal{S}^{\mathrm{sep}}$ but contains an entangled state ϕ with $F(\phi) = c$.

Let $C = \{c \in [F(\tau), F_+] : \mathbb{L}_c \subseteq \mathcal{S}^{\mathrm{sep}}\}$. Then C is not empty because $\mathbb{L}_{F(\tau)} = \{\tau\} \subseteq \mathcal{S}^{\mathrm{sep}}$. Put $C_F = \sup(C)$ $\left(\leqslant C_L^+\right)$, and $\mathbb{K} = \cup_{c\in C}\mathbb{L}_c$.

We first show that $C_F \geqslant C_L^-$. Suppose that $\rho \in \mathbb{L}_{C_L^-}$ then $\rho = t\cdot\phi + (1-t)\cdot\tau = \phi_t$ with $t \in [0, 1]$ and $\mathrm{spec}(\phi) \in \mathrm{co}(e^{(1)}, \ldots, e^{(D-1)})$ in a gap representation. If $t = 0$ then $\rho = \tau$ which is separable. If $0 < t < 1$, let $\sigma = \widehat{\rho}^{(D-1)}$ then $\sigma \succ \phi$ and thus $t\cdot\sigma + (1-t)\cdot\tau \succ t\cdot\phi + (1-t)\cdot\tau = \rho$, which implies

$$\begin{aligned} f_\phi(t) &= F(t\cdot\phi + (1-t)\cdot\tau) = F(\rho) \leqslant C_L^- \\ &= F(L\cdot\sigma + (1-L)\cdot\tau) \leqslant F(L\cdot\phi + (1-L)\cdot\tau) = f_\phi(L). \end{aligned}$$

The lemma then implies that $t \leqslant L$ and thus $\rho = \phi_t$ is separable.

We now show that $\mathbb{K} = \mathbb{L}_{C_F}$. By the definitions of $\mathbb{K}$ and C_F, $\mathbb{K} \subseteq \mathbb{L}_{C_F}$ and since $\mathbb{L}_{C_F}$ is closed, the closure $\overline{\mathbb{K}}$ of $\mathbb{K}$ is contained in $\mathbb{L}_{C_F}$. Also, $\mathbb{K} \subseteq \mathcal{S}^{\mathrm{sep}}$, and since $\mathcal{S}^{\mathrm{sep}}$ is closed, $\overline{\mathbb{K}} \subseteq \mathcal{S}^{\mathrm{sep}}$. The claim is proved by showing that $\mathbb{L}_{C_F} \subseteq \overline{\mathbb{K}}$. Suppose $\tau \neq \rho \in \mathbb{L}_{C_F}$. Then for every $0 \leqslant t < 1$, $F(t\cdot\rho + (1-t)\cdot\tau) = f_\rho(t) < F(\rho) \leqslant C_F$ by the lemma, so for such t $t\cdot\rho + (1-t)\cdot\tau \in \mathbb{K}$. Take an increasing sequence $\{t_n\}$ in $[0, 1)$ with $\lim_{n\to\infty} t_n = 1$. Then $\rho_n = t_n\cdot\rho + (1-t_n)\cdot\tau \in \mathbb{K}$ and $\lim_{n\to\infty}\rho_n = \rho$ so that $\rho \in \overline{\mathbb{K}}$. This proves that C_F satisfies the required properties and $C_F \leqslant C_L^+$. This completes the proof of the theorem.

We will see that the bound C_L^- is very poor and needs to be substantially improved in order to pin down C_F (cf, section 4). This requires detailed information about the least separability modulus of the states $\widehat{\rho}^{(j)}$ as one goes through the maximal families of pairwise orthogonal pure states.

Theorem 1 states that the critical value of the $(D-1)$th partial eigenvalue-sum is $1-(1-L)/D$. Let us denote the critical value of the kth partial eigenvalue-sum Σ_k function by $C[k]$. The computation of $C_L^{\pm}$ for the kth partial sums is immediate, and one gets

Proposition 7. *For* $k = 1, 2, \ldots, D-1$, $k\left(\frac{L}{D-1} + \frac{1-L}{D}\right) \leqslant C[k] \leqslant k\frac{1-L}{D} + L$.

Note that the bounds coalesce for $k = D-1$ to $C[D-1] = 1-(1-L)/D$ recovering theorem 1.

The unitarily invariant strictly convex function $F(\rho) = \mathrm{Tr}(\rho^2)$ is among the simplest separability detectors as it does not require spectral information to be calculated. $C_L^{\pm}$ can be easily computed leading to

Proposition 8. *The critical value* C_F *for the trace of the square satisfies* $\frac{D-1+L^2}{D(D-1)} \leqslant C_F \leqslant \frac{L^2(D-1)+1}{D}$.

Proof. For any ρ, we have $(t\cdot\rho + (1-t)\cdot\tau)^2 = t^2\cdot\rho^2 + 2t(1-t)\cdot\rho\tau + (1-t)^2\tau^2 = t^2\cdot\rho^2 + (2t(1-t)/D)\cdot\rho + ((1-t)^2/D)\tau$; hence $F(t\cdot\rho + (1-t)\cdot\tau) = t^2F(\rho) + (1-t^2)/D$. If ρ is pure $F(\rho) = 1$ and thus $C_L^+ = L^2 + (1-L^2)/D$. If $\mathrm{spec}(\rho) = e^{(D-1)}$ and $F(\rho) = (D-1)^{-1}$, whence $C_L^- = F(L\cdot\rho + (1-L)\cdot\tau) = (L^2/(D-1)) + (1-L^2)/D$. □

Similar calculations can be carried out for other $F's$, for example, the von Neumann entropy.

4. Bipartite systems

For $N = 2$ detailed entanglement information is available or obtainable. Notably, the results of Vidal and Tarrach [2] imply (recall $D = d_1d_2$)

$$L = 2/(2+D). \tag{5}$$

We can thus specify the characteristic parameters and bounds entering the results obtained in section 3.

Proposition 9. *For* $N = 2$, *one has*

(i) $k(D+1)/(D+2)(D-1) \leqslant C[k] \leqslant (k+2)/(D+2)$ *for* $k = 1, 2, \ldots, D-2$ *and* $C[D-1] = (D+1)/(D+2)$.

(ii) The critical value C_F *for* $F(\rho) = \mathrm{Tr}(\rho^2)$ *satisfies*

$$\frac{D(D+3)}{(D-1)(2+D)^2} \leqslant C_F \leqslant \frac{D+8}{(2+D)^2}.$$

(iii) The critical value C_S *of the von Neumann entropy satisfies*

$$\ln(2+D) - \frac{3}{2+D}\ln(3) \leqslant C_S \leqslant \ln(D+2) - \frac{D+1}{D+2}\ln\left(\frac{D+1}{D-1}\right).$$

But for the trace of the square (item (ii) in the above result), Gurvits and Barnum do much better [12]:

Proposition 10 (Gurvits and Barnum)**.** *For $N = 2$,*

(i) $\mathrm{Tr}(\rho^2) \leqslant 1/(D-1)$ *implies that ρ is separable; Moreover, for any c with $1/(D-1) < c \leqslant 1$ there is an entangled state ω with $\mathrm{Tr}(\omega^2) = c$;*

(ii) if $\mathrm{Tr}(\rho^2) > 1/(D-1)$ *then*

$$\ell(\rho) \geqslant \frac{1}{\sqrt{(D-1)(D\,\mathrm{Tr}(\rho^2)-1)}}.$$

Thus the critical value of C_F for $F = \mathrm{Tr}(\cdot^2)$ is $1/(D-1)$ for $N = 2$. Moreover, if $\mathrm{spec}(\rho) = e^{(D-1)}$ then $\mathrm{Tr}(\rho^2) = 1/(D-1)$ so that ρ is separable.

This new bit of separability information immediately leads to the following improvement on the lower bound for the critical value of theorem 2:

Proposition 11. *If F is either a unitarily invariant, strictly convex continuous function or one of $\Sigma_k(\cdot)$ for $k = 1, 2, \ldots, D-1$, on the states of a bipartite system, then*

$$C_F \geqslant \inf_{t\in[0,1]} \{F(t\cdot\sigma + (1-t)L\cdot\omega + (1-t)(1-L)\cdot\tau\},$$

where $\mathrm{spec}(\sigma) = e^{(D-1)}$, $\mathrm{spec}(\omega) = e^{(D-2)}$ *with* $\omega\sigma = \omega/(D-1)$.

This is proved in appendix B.

The computation of the above infimum is often quite straightforward. In the case of the partial eigenvalue-sums it is easily done and leads to the following improvement of proposition 9:

Proposition 12. *For $N = 2$, $kD/(D^2-4) \leqslant C[k] \leqslant (k+2)/(D+2)$ for $k = 1, \ldots, D-3$, and $C[D-2] = D/(D+2)$.*

We can also improve theorem 1 as follows:

Theorem 3. *For a bipartite system, if* $\mathrm{spec}(\rho) = (\lambda_1, \ldots, \lambda_D)$ *and* $3\lambda_D + (D-1)\lambda_{D-1} \geqslant 1$ *then ρ is separable. For each $s \in [0, 1)$ there are entangled states with $3\lambda_D + (D-1)\lambda_{D-1} = s$.*

This is a consequence of proposition 13 of appendix B, proposition 10 and equation (5). Note that the map G defined on states of a (bipartite) system via $\mathrm{spec}(\rho) = (\lambda_1, \ldots, \lambda_D)$ by $G(\rho) = 3\lambda_D + (D-1)\lambda_{D-1} = 3 + (D-4)\Sigma_{D-1}(\rho) - (D-1)\Sigma_{D-2}(\rho)$ is unitarily invariant and continuous, but is not expected to be convex or concave.

5. Final comments

With no other specific entanglement information other than $1 > L > 0$ we have obtained conditions on the spectrum of a state which guarantee its separability. These conditions are either direct restrictions on the spectrum or are hidden in the critical level set of unitarily invariant, convex, good continuous functions. Only the spectrum is needed to compute the values of such functions. We have also exemplified how more detailed entanglement information leads to less restrictive spectral conditions.

The problem of improving the results, in particular the bounds on C_F, seems worthy of pursuit. Exact values of L for $N > 2$ are not available. Further progress would come if something precise can be said about the following. It is not difficult to show that there are entangled states ρ with $\mathrm{spec}(\rho) = e^{(2)}$, and Gurvits and Barnum have shown that $\mathrm{spec}(\rho) = e^{(D-1)}$ implies the separability of ρ in bipartite ($N = 2$) systems. Where in the spectral chain $e^{(D-1)} \succ e^{(D-2)} \succ \cdots \succ e^{(2)}$ is the cut separable/entangled? The solution of this problem will enhance the use of the gap representation to deal with entanglement problems.

For a fixed compositum, call $\mathcal{F}$ the collection of the unitarily invariant, convex, good continuous functions on the state space. Take an $F \in \mathcal{F}$ and apply the F-test: reject the state ρ if $F(\rho) \leqslant C_F$. You are left with the states passing the test $\{\rho : F(\rho) > C_F\}$; this includes all pure states, in particular the pure product-states. Take another $G \in \mathcal{F}$ and do the G-test on $\{\rho : F(\rho) > C_F\}$ which outputs $\{\rho : F(\rho) > C_F\} \cap \{\rho : G(\rho) > C_G\}$. When you exhaust $\mathcal{F}$ you are left with $\cap_{F\in\mathcal{F}}\{\rho : F(\rho) > C_F\}$ which still contains all pure states, hence all pure separable states. Does one have $\cap_{F\in\mathcal{F}}\{\rho : F(\rho) > C_F\} = \{\rho \text{ is entangled}\} \cup \{\rho \text{ is a pure separable state}\}$? To put it another way: If ρ is separable but not pure, is there an $F \in \mathcal{F}$ such that $F(\rho) \leqslant C_F$? As the analysis of entanglement in thermal equilibrium states shows [17], the answer to the questions is unfortunately no: there are separable, mixed states that cannot be detected by $\mathcal{F}$.

Acknowledgments

I should like to thank O A Nagel for discussions, and O Osenda for suggesting a look at thermal states. L Gurvits pointed out the relevance of his results with H Barnum [12–14] which I was unaware of; these results are responsible for the extension of the applications of section 4 as presented previously in [15].

Appendix A. Proof of theorem 3 and proposition 11

Both results below are proved under the hypothesis that

$$\text{if} \quad \operatorname{spec}(\rho) = e^{(D-1)}, \quad \text{then } \rho \text{ is separable.} \tag{A.1}$$

This has been proved (proposition 10) for $N = 2$ by Gurvits and Barnum [12].

Proposition 13. *Assume (A.1). Then, if* $\operatorname{spec}(\rho) = (\lambda_1, \lambda_2, \ldots, \lambda_D)$ *and*

$$\left(1 - \frac{(1-L)(D-1)}{D}\right)\lambda_D + \frac{(1-L)(D-1)}{D}\lambda_{D-1} \geqslant (1-L)/D; \tag{A.2}$$

it follows that ρ is separable. Moreover, for every $s \in [0, (1-L)/D)$ there is an entangled state ρ where the left-hand side of (A.2) is equal to s.

Before proving this, we observe that the left-hand side of inequality (A.2) is larger than or equal to λ_D, so we recover theorem 1.

Proof. Take any gap representation $\rho = \sum_{j=1}^{D} t_j \widehat{\rho}^{(j)}$. Let $t = t_{D-1}$, and $s = \sum_{j=1}^{D-2} t_j$; then $t + s = 1 - t_D$.

If $t = 0$ then

$$\rho = \sum_{j=1}^{D-2} t_j \cdot \widehat{\rho}^{(j)} + (1-s)\cdot\tau = s\cdot\omega + (1-s)\cdot\tau, \tag{A.3}$$

where

$$\omega = \sum_{j=1}^{D-2} \frac{t_j}{s} \cdot \widehat{\rho}^{(j)}, \qquad \text{if} \quad s > 0.$$

If $1 > t > 0$, then

$$\rho = t\cdot\sigma + (1-t)\cdot(r\cdot\omega + (1-r)\cdot\tau) \tag{A.4}$$

where $r = s/(1-t)$, ω is as above when $s > 0$, and $\sigma = \widehat{\rho}^{(D-1)}$ is separable by (A.1). If $t = 1$, then $\rho = \sigma$ is separable.

If now $s \leqslant L(1-t)$, we have the following alternatives: (1) $t = 0$ and $s \leqslant L$, in which case equation (A.3) implies that ρ is separable; (2) $1 > t > 0$ and $r \leqslant L$ in which case equation (A.4) implies that ρ is separable; and (3) $t = 1$ in which case $\rho = \sigma$ is separable. Thus $s \leqslant L(1-t)$ implies that ρ is separable.

But since $s = 1 - t - t_D$ this inequality is equivalent to $(1-L)(1-t) \leqslant t_D$. In the notation of proposition 2, $t_j = \mu_j(\lambda)$ is given by (3). Thus, we get $(1-L)(1-(D-1)(\lambda_{D-1} - \lambda_D) \leqslant D\lambda_D$ which is (A.2).

Take a maximally entangled state ϕ which is pure and suppose $0 \leqslant s < (1-L)/D$, then $1 \geqslant 1 - sD > L$ and the state $\phi_{1-sD} = (1-sD) \cdot \phi + sD \cdot \tau$ is entangled and has $\mathrm{spec}(\phi_{1-sD}) = (1 - sD + s, s, s, \ldots, s)$; we see that the left-hand side of (A.2) is equal to s.

□

The improvement on the lower bound for the critical value of a unitarily invariant, convex, good continuous function is the following:

Proposition 14. *Assume (A.1). If F is either a unitarily invariant strictly convex, continuous function, or one of the $\Sigma_k(\cdot)$ with $k = 1, 2, \ldots, D-1$, then its critical value is not below the number*

$$\inf_{t\in[0,1]} \{F(t \cdot \sigma + (1-t)L \cdot \omega + (1-L)(1-t) \cdot \tau)\},$$

where $\mathrm{spec}(\omega) = e^{(D-2)}$, $\mathrm{spec}(\sigma) = e^{(D-1)}$, *with* $\omega\sigma = \omega/(D-1)$.

Proof. Consider a unitarily invariant, convex continuous function F. Refer to the previous proof, whose notation t, s, r, ω, σ we keep. We have

$$\rho = t \cdot \sigma + (1-t) \cdot (r \cdot \omega + (1-r) \cdot \tau) = t \cdot \sigma + s \cdot \omega + (1-t-s) \cdot \tau)$$

with $s = r(1-t) \leqslant (1-t)$. Note that $\mathrm{spec}(\omega) \in \mathrm{co}(e^{(1)}, \ldots, e^{(D-2)})$.

The first observation is that $t' \cdot \sigma + (1-t')r' \cdot \widehat{\rho}^{(D-2)} + (1-r')(1-t') \cdot \tau \succ t' \cdot \sigma + (1-t')r' \cdot \omega + (1-r')(1-t') \cdot \tau$ for all $t', r' \in [0, 1]$; indeed this is equivalent to $(1-t')r'(\Sigma_k(\omega) - \Sigma_k(\widehat{\rho}^{(D-2)})) \geqslant 0$ for $k = 1, 2, \ldots, D$; and this is satisfied because $\widehat{\rho}^{(D-2)} \succ \omega$. □

The other basic observation here is

Lemma 9. *Suppose F satisfies the hypothesis of the proposition and $0 \leqslant t' < 1$. Then the map $[0, 1-t'] \ni s' \mapsto f_{\omega,\sigma}(s'; t') = F(s' \cdot \omega + t' \cdot \sigma + (1-t'-s') \cdot \tau)$ is increasing and convex.*

Proof. If $s_1, s_2 \in [0, 1-t']$ and $u \in [0, 1]$ then $us_1 + (1-u)s_2 \in [0, 1-t']$ and

$$\begin{aligned}
&(us_1 + (1-u)s_2) \cdot \omega + t' \cdot \sigma + (1 - (us_1 + (1-u)s_2) - t') \cdot \tau \\
&\qquad = u \cdot (s_1. \cdot \omega + t' \cdot \sigma + (1 - s_1 - t') \cdot \tau) \\
&\qquad\quad + (1-u) \cdot (s_2. \cdot \omega + t' \cdot \sigma + (1 - s_2 - t') \cdot \tau)
\end{aligned}$$

so that

$$\begin{aligned}
&f_{\omega,\sigma}(us_1 + (1-u)s_2; t') \\
&\qquad = F((us_1 + (1-u)s_2) \cdot \omega + t' \cdot \sigma + (1 - (us_1 + (1-u)s_2) - t') \cdot \tau) \\
&\qquad = F(u \cdot (s_1 \cdot \omega + t' \cdot \sigma + (1 - s_1 - t') \cdot \tau)
\end{aligned}$$

$$\begin{aligned}&+(1-u)\cdot(s_2\cdot\omega+t'\cdot\sigma+(1-s_2-t')\cdot\tau))\\ &\leqslant uF(s_1\cdot\omega+t'\cdot\sigma+(1-s_1-t')\cdot\tau)\\ &\quad+(1-u)F(s_2\cdot\omega+t'\cdot\sigma+(1-s_2-t')\cdot\tau)\\ &=uf_{\omega,\sigma}(s_1;t')+(1-u)f_{\omega,\sigma}(s_2;t'),\end{aligned}$$

so $f_{\omega,\sigma}(\cdot;t')$ is convex. Moreover, if F is strictly convex then the inequality is strict for $0<u<1$ and $s_1\neq s_2$ by proposition 3, since $s_1\cdot\omega+t'\cdot\sigma+(1-s_1-t')\cdot\tau\neq s_2\cdot\omega+t'\cdot\sigma+(1-s_1-t')\cdot\tau$.

We now prove that $f_{\omega,\sigma}(\cdot;t')$ is increasing. If $0\leqslant s_1<s_2\leqslant(1-t')$, then $s_1\cdot\omega+t'\cdot\sigma+(1-s_1-t')\cdot\tau\succ s_2\cdot\omega+t'\cdot\sigma+(1-s_2-t')\cdot\tau$ because the partial sums Σ_k satisfy $(k=1,2,\ldots,D)$

$$\Sigma_k(s'\cdot\omega+t'\cdot\sigma+(1-t'-s')\cdot\tau)=s'\Sigma_k(\omega)+t'\Sigma_k(\sigma)+(1-t'-s')\Sigma_k(\tau),$$

and

$$\Sigma_k(s_1\cdot\omega+t'\cdot\sigma+(1-s_1-t')\cdot\tau)\leqslant\Sigma_k(s_2\cdot\omega+t'\cdot\sigma+(1-s_2-t')\cdot\tau)$$

is equivalent to

$$(s_2-s_1)\Sigma_k(\omega)\geqslant(s_2-s_1)\Sigma_k(\tau),$$

which is always satisfied because $\tau\succ\rho$ for every state ρ. Equation (1) implies that

$$F(s_1\cdot\omega+t\cdot\sigma+(1-s_1-t)\cdot\tau)\leqslant F(s_2\cdot\omega+t'\cdot\sigma+(1-s_2-t')\cdot\tau),\quad\text{or}$$
$$f_{\omega,\sigma}(s_1;t')\leqslant f_{\omega,\sigma}(s_2;t').$$

But as a non-decreasing convex function, $f_{\omega,\sigma}(\cdot;t')$ must be constant up to a certain $s_*\leqslant 1$ and increasing for $s\geqslant s_*$. We have

$$s_*=\sup\{s'\in[0,1]:f_{\omega,\sigma}(s';t')=f_{\omega,\sigma}(0,;t')\}.$$

If now F is strictly convex then $s_*=0$. Suppose $F=\Sigma_k(\cdot)$ for some $k=1,2,\ldots,D-1$. Then $f_{\omega,\sigma}(s_*;t')=f_{\omega,\sigma}(0;t')$ is equivalent to $s_*(\Sigma_k(\omega)-k/D)=0$ and lemma 1 implies that $s_*=0$. □

Put H for the infimum that is claimed to be a lower bound for C_F, and assume that $F(\rho)\leqslant H$. If $t=1$ we have $\rho=\sigma$ which is separable. Otherwise, by the definition of H and the first observation,

$$\begin{aligned}f_{\omega,\sigma}(s;t)=F(\rho)\leqslant H&\leqslant F(t\cdot\sigma+(1-t)L\cdot\widehat{\rho}^{(D-2)}+(1-t)(1-L)\cdot\tau)\\ &\leqslant F(t\cdot\sigma+(1-t)L\cdot\omega+(1-t)(1-L)\cdot\tau)=f_{\omega,\sigma}(L(1-t);t).\end{aligned}$$

And, by the lemma, $s\leqslant L(1-t)$ which implies $r\leqslant L$ and the separability of ρ follows from (A.3) or (A.4). Thus $C_F\geqslant H$. This proves the claim.

A detailed analysis of the proof above suggests the introduction of a condition on unitarily invariant convex functions which we propose in appendix B.

Appendix B. *k*-good functions

Suppose F is a unitarily invariant, convex continuous function. Take an arbitrary maximal family $\{\rho^{(j)}:j=1,2,\ldots,d\}$ of pairwise orthogonal pure states. F is determined by its values in $\left\{\sum_{j=1}^{d}\lambda_j\rho^{(j)}:\lambda\in\mathcal{L}_d\right\}$. Fix $k\in\{1,2,\ldots,d-1\}$ and suppose $\mathrm{spec}(\omega)\in\mathrm{co}(e^{(1)},e^{(2)},\ldots,e^{(d-k)})$. For $t_1,t_2,\ldots,t_{k-1}\in[0,1]$ with $t=t_1+t_2+\cdots+t_{k-1}\leqslant 1$ consider $f(s)=F(s\cdot\omega+\sum_{j=1}^{k-1}t_j\cdot\widehat{\rho}^{(d-k+j)}+(1-t-s)\cdot\tau)$, for $s\in[0,1-t]$, which is convex.

Now, if $1-t \geqslant s > s' \geqslant 0$, it follows that $s' \cdot \omega + \sum_{j=1}^{k-1} t_j \cdot \widehat{\rho}^{(d-k+j)} + (1-t-s') \cdot \tau \succ s \cdot \omega + \sum_{j=1}^{k-1} t_j \cdot \widehat{\rho}^{(d-k+j)} + (1-t-s) \cdot \tau$, and by equation (1), f is non-decreasing. We say that F is *k-good* if $f(s) > f(0)$ for $s > 0$. By the convexity of f this is equivalent to saying that f is increasing.

The proof of the last proposition of the previous appendix will in fact work if F is 2-good.

Proposition 15. *If F is a unitarily invariant, convex , continuous function then it is good iff it is 1-good. If F is unitarily invariant, continuous and either strictly convex or one of the $\Sigma_k(\cdot)$ for some $k = 1, 2, \ldots, d-1$, then F is p-good for every $p = 1, 2, \ldots, d-1$.*

Proof. 1-goodness is $F(s \cdot \rho + (1-s) \cdot \tau) > F(\tau)$ for $s > 0$ for every ρ with $\mathrm{spec}(\rho) \in \mathrm{co}(e^{(1)}, \ldots, e^{(d-1)})$. This property follows iff F is good.

No matter what p is, if F is strictly convex, the map f will be strictly convex and it then follows that it is increasing.

If $F = \Sigma_k$ for some $k = 1, 2, \ldots, d-1$, then, for any $p = 1, 2, \ldots, d-1$, $f(s) = f(0)$ is equivalent to $s(\Sigma_k(\omega) - \Sigma_k(\tau)) = 0$ for $\mathrm{spec}(\omega) \in \mathrm{co}(e^{(1)}, \ldots, e^{(d-p)})$; which implies $s = 0$ by lemma 1. □

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