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LETTER TO THE EDITOR

On the structure of the body of states with positive partial transpose

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Abstract
We show that the convex set of separable mixed states of the 2×2 system is a body of a constant height. This fact is used to prove that the probability of finding a random state to be separable equals twice the probability of finding a random boundary state to be separable, provided that the random states are generated uniformly with respect to the Hilbert–Schmidt (Euclidean) measure. An analogous property holds for the set of positive-partial-transpose states for an arbitrary bipartite system.

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The phenomena of quantum entanglement became crucial in the recent development of quantum information processing. In general, it is not easy to decide whether a given mixed quantum state is entangled or separable [1]. The situation gets simpler for the qubit–qubit and the qubit–qutrit systems, for which it is known that a state is separable if and only if its partial transpose is positive [2, 3]. However, even in the simplest case of the two-qubit system, the structure of the set of separable states is not fully understood. This 15-dimensional convex set $\mathcal{M}_S^{(4)}$ is known to contain the maximal ball inscribed in the set of all mixed states $\mathcal{M}^{(4)}$ [4]. Although some work has been done to estimate the volume of the set of separable states [5–9] and to describe its geometry [10, 11], the exact volume of the set of separable states is unknown even in this simplest case [12].

In order to elucidate properties of the set of separable states, Slater studied the probability that a random state be separable, inside the set of mixed states and at its boundary, using the Hilbert–Schmidt measure. For the two-qubit system, he found numerically that the ratio Ω between these two probabilities is close to 2 [13, 14]. The fact that it is more likely to find a separable state *inside* the total set of mixed states than on its boundary is consistent with the existence of the separable ball centred at the maximally mixed state.

We prove that for this system the ratio Ω *is* indeed equal to 2, provided we work in Euclidean geometry and use the measure induced by the Hilbert–Schmidt distance. Furthermore, we show that the space of two-qubit (or qubit–qutrit) separable states can be decomposed into pyramids of the same height. These results hold also for the convex set of states with positive partial transpose (PPT states) for any $K \times M$ bipartite system.

We will need some generalities about convex sets. Let $X \in \mathbb{R}^D$ be a convex body in $\mathbb{R}^D$ (in particular it is a closed, bounded set with nonempty interior) and ∂X its boundary. Let V denote the volume of X and A the ($(D-1)$-dimensional) area of ∂X, both computed with respect to the standard Euclidean geometry. For each body we define the dimensionless ratio

$$\gamma(X) := \frac{A(X)r(X)}{V(X)}, \tag{1}$$

where $r = r(X)$ is the radius of the maximal ball inscribed inside X. This ball is known as the insphere. Before we see why $\gamma(X)$ is interesting, we invoke some geometric definitions. A *face* of a convex body X is the intersection of X with an affine hyperplane which intersects ∂X, but does not separate (the interior of) X into two pieces. Such an affine plane is known as a *supporting hyperplane*. Such hyperplanes are important because any convex body equals the intersection of the half-spaces defined by its supporting hyperplanes. The *polar* Y° of a set $Y \subset \mathbb{R}^D$ is defined as the set $\{z : \langle z, y\rangle \leqslant 1 \text{ for all } y \in Y\}$. For additional background information, consult the literature [15, 16].

We can now formulate a lemma which is stated for bodies whose insphere is the unit ball (i.e., the ball of unit radius centred at the origin). However, this hypothesis is just a matter of convenience and can always be achieved by proper re-centring and re-scaling. Note that while, in general, there may be more than one inscribed ball with a maximal radius; this ambiguity cannot occur for bodies verifying the conditions of the lemma.

Lemma 1. *For a convex body X whose insphere is the unit ball, the following three conditions are equivalent:*

1. *every boundary point of X is contained in a face tangent to the inscribed ball;*
2. *$X = Y^\circ$, where Y is a closed subset of the unit sphere such that the convex hull of Y contains the origin in its interior;*
3. *$\gamma(X) = A/V = D$.*

Before we prove this, let us observe that the equality $A/V = D$, from condition 3, is Archimedes' formula for the volume of a D-dimensional *pyramid* of unit height—where we define a pyramid as the convex hull of the base and the apex. Hence, it will be true that $\gamma(X) = D$ whenever the body can be decomposed into a union of disjoint pyramids of fixed height with apex at the centre of the inscribed ball. This is true for regular simplices, cubes and, more generally, for any polytope circumscribed around the unit ball, and hence verifying condition 1. The equality $A/V = D$ holds also for balls, which can be explained by the ball being a limit of an infinite sequence of polytopes. Thus, condition 1 can always be thought of as asserting such 'decomposability into pyramids', and we will refer to a body obeying it as a *body of constant height*. However, whenever the bases of pyramids (faces of X) are of dimension lower than $(D-1)$, the limiting procedures needed to prove equivalences will require some care. (For the body of $N \times N$ density matrices $D = N^2 - 1$, while the maximal faces have dimension $(D - 2N + 1)$.)

Proof of lemma 1 ($1 \Rightarrow 2$)**.** We first note that X equals the intersection of the half-spaces limited by supporting hyperplanes corresponding to faces tangent to the unit ball. Consider one such supporting hyperplane. Since it contains a tangent face, it has a common point with the unit sphere. On the other hand, it cannot cut the unit ball into two, since it is supporting to X and the unit ball is contained in X. Hence, the supporting hyperplane itself is tangent to the unit ball, and so the corresponding half-space is of the form $\{z : \langle z, y\rangle \leqslant 1\}$ for some $y \in S^{D-1}$. The set Y is the closure of the set of points y that arise this way. The condition on the convex hull of Y will be automatically satisfied as it is equivalent to boundedness of X.

$2 \Rightarrow 1$. First, if Y is a subset of the unit sphere, then the unit ball is inscribed into the polar of Y with every $y \in Y$ a contact point. A point lies on the boundary of $X = Y^\circ$ if and only if one of the inequalities that defines X as a polar body becomes an equality, i.e., if it belongs to the face $F_y := \{x \in X : \langle x, y\rangle = 1\}$ for some $y \in Y$. F_y is clearly contained in a hyperplane tangent to the unit ball and it contains the point of tangency (namely, y), so it is itself tangent to the unit ball. We have thus shown that every point of ∂X belongs to a face tangent to the unit ball, as required.

$1 \Rightarrow 3$. With an insphere $\mathbf{S}^{D-1}$ of radius 1 we can regard any one of its points $\omega \in \mathbf{S}^{D-1}$ as a unit vector, and we can define a positive real-valued function $r(\omega)$ such that $r(\omega)\omega \in \partial X$. Then

$$V(X) = \int_{\mathbf{S}^{D-1}} \mathrm{d}\omega \int_0^{r(\omega)} \mathrm{d}r\, r^{D-1} = \frac{1}{D} \int_{\mathbf{S}^{D-1}} \mathrm{d}\omega\, r(\omega)^D, \tag{2}$$

where $\mathrm{d}\omega$ is the usual measure on the unit sphere. Similarly, if $n(\omega)$ is the unit normal of X at the point lying 'above' ω,

$$A(X) = \int_{\mathbf{S}^{D-1}} \mathrm{d}\omega \frac{r(\omega)^{D-1}}{\langle \omega, n(\omega)\rangle}. \tag{3}$$

Here, and below, we rely on the fact that the normal of a convex body is uniquely defined, and continuous, almost everywhere. Whenever the normal $n(\omega)$ is uniquely determined, the face containing $r(\omega)\omega$ is also uniquely determined and hence perpendicular to $n(\omega)$. By assumption 1, that face, and the supporting hyperplane containing it, are tangent to the unit ball. This leads to the equality

$$\langle r(\omega)\omega, n(\omega)\rangle = 1 \tag{4}$$

or $\langle \omega, n(\omega)\rangle = 1/r(\omega)$; substituting this into (3) and comparing with (2) we obtain $V(X) = A(X)/D$.

$3 \Rightarrow 1$. We first note that (by an elementary argument using convexity) the set $\Xi := \{\omega \in \mathbf{S}^{D-1} : r(\omega)\omega$ lies on a face of X tangent to the unit ball$\}$ is closed. If assumption 1 does not hold, the complement of Ξ in $\mathbf{S}^{D-1}$ is nonempty and it is an open subset of this sphere, hence of positive measure. By the same argument as in the preceding proof we have, almost everywhere in $\mathbf{S}^{D-1}\setminus\Xi$,

$$\langle \omega, n(\omega)\rangle > 1/r(\omega) \tag{5}$$

while still $\langle \omega, n(\omega)\rangle = 1/r(\omega)$ for $\omega \in \Xi$. Hence, from (2) and (3),

$$A(X) < \int_{\mathbf{S}^{D-1}} \mathrm{d}\omega\, r(\omega)^D = DV(X). \tag{6}$$

This concludes the proof. □

We can now easily establish:

Lemma 2. *Any intersection of two bodies of constant heights X_1, X_2, containing the same inscribed sphere, is a body of constant height.*

Proof. Let Y_j be the sets defined by $X_j = Y_j^\circ$ for $j = 1, 2$. Then $X_1 \cap X_2 = (Y_1 \cup Y_2)^\circ$ and of course $Y_1 \cup Y_2$ is a closed subset of the sphere, if each of the Y_j's was. Making use of property 2 we conclude that $X_1 \cap X_2$ is a body of constant height. □

We are going to use the above geometric concepts to investigate the set $\mathcal{M}^{(N)}$ of density matrices acting in the N-dimensional Hilbert space $\mathcal{H}_N$. An operator $\rho : \mathcal{H}_N \to \mathcal{H}_N$ belongs to $\mathcal{M}^{(N)}$ if it is Hermitian, $\rho = \rho^\dagger$, is (semi) positive definite, $\rho \geqslant 0$, and is normalized, $\mathrm{Tr}\,\rho = 1$. Due to the latter normalization condition the set $\mathcal{M}^{(N)}$ is compact and has dimensionality $D = N^2 - 1$. The sphere inscribed in $\mathcal{M}^{(N)}$ is centred at the maximally mixed state $\rho_* = 1/N$ and has the radius $r = 1/\sqrt{(N-1)N}$, if computed with respect to the Hilbert–Schmidt distance, $d_{\mathrm{HS}}^2(\rho, \sigma) = \mathrm{Tr}(\rho - \sigma)^2$. Observe that r is equal to the radius of the sphere inscribed inside the $(N-1)$-dimensional simplex Δ_{N-1} with edge lengths $\sqrt{2}$.

A recent analysis [17] of the volume and area of the set of mixed states shows that their ratio A/V is equal to $\sqrt{N(N-1)}(N^2-1)$. Therefore, the coefficient γ reads then

$$\gamma(\mathcal{M}^{(N)}) = r\frac{A}{V} = \frac{1}{\sqrt{(N-1)N}}\sqrt{N(N-1)}(N^2-1) = N^2 - 1 = D. \qquad (7)$$

This observation inspires us to propose:

Proposition 1. *The set $\mathcal{M}^{(N)}$ of mixed quantum states is a body of constant height.*

Indeed, it is immediate that condition 1 of lemma 1 holds. A density matrix lies on the boundary of $\mathcal{M}^{(N)}$ if and only if it has a zero eigenvalue. Such a matrix belongs to the face consisting of all density matrices with support in the subspace of the Hilbert space that is orthogonal to the corresponding eigenvector. (All such faces are maximal and isometric to $\mathcal{M}^{(N-1)}$.) The point of tangency of that face to the inscribed (Hilbert–Schmidt) ball will be a density matrix with one eigenvalue (corresponding to the same eigenvector as above) zero and all other eigenvalues equal. (As the set of pure states, both the set of maximal faces and the set Y of points of tangency have the structure of a complex projective space.) Of course, we can also derive the conclusion of proposition 1 from (7) and condition 3 of lemma 1, but such an argument would not be self-contained and, moreover, would obscure the matter.

Let us now take the dimension N as a composite number, say $N = KM$, and consider operators acting on a composite Hilbert space $\mathcal{H}_N = \mathcal{H}_K \otimes \mathcal{H}_M$. Such a decomposition of the Hilbert space allows one to define *separable* states, as those represented as a convex sum of product states [18],

$$\rho_{\mathrm{sep}} = \sum_{j=1}^{L} q_j \rho_j^A \otimes \rho_j^B, \qquad (8)$$

where operators ρ^A and ρ^B act on Hilbert spaces $\mathcal{H}_K$ and $\mathcal{H}_M$, respectively, the weights are positive, $q_j > 0$, and sum to unity, $\sum_{j=1}^{L} q_j = 1$. A state which is not separable is called *entangled*. Any separable state has a positive partial transpose, $T_A(\rho) = (T \otimes \mathbb{1})\rho \geqslant 0$, and this criterion is sufficient if $N = 2 \times 2 = 4$ or $N = 2 \times 3 = 6$ [2, 3]. Thus the sets of separable states and PPT states (states with positive partial transpose) coincide in these cases and are equal to the intersection of $\mathcal{M}^{(N)}$ and its image $T_A(\mathcal{M}^{(N)})$—see figure 1. In any dimension $N = KM$, the sets $\mathcal{M}^{(N)}$ and $T_A(\mathcal{M}^{(N)})$ have the same shape, volume and surface area because the partial transpose T_A acts as a reflection with respect to the affine subspace of PPT-invariant states (which includes the maximally mixed state ρ_*).

Let us denote the volume and the area of the set of mixed states by $V_{\mathrm{tot}} = \mathrm{Vol}(\mathcal{M}^{(N)})$ and $A_{\mathrm{tot}} = \mathrm{Vol}(\partial\mathcal{M}^{(N)})$. Analogously V_{PPT} and A_{PPT} represent the volume and the area of the set of PPT states. The key result of this work will follow from

Theorem 1. *The set $\mathcal{M}_{\mathrm{PPT}}^{(N)}$ of PPT mixed quantum states is a body of constant height.*

Proof. The set $\mathcal{M}^{(N)}$ of mixed states is a body of constant height, and so is its image, $T_A(\mathcal{M}^{(N)})$. Both sets contain the same inscribed sphere of radius $r = 1/\sqrt{(N-1)N}$. Since the set of

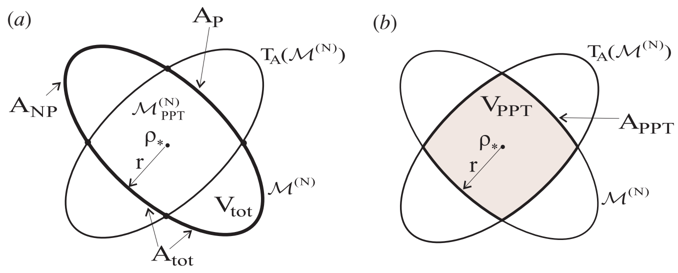

Figure 1. The set $\mathcal{M}^{(N)}_{\mathrm{PPT}}$ of PPT states arises as a common part of the set of mixed states $\mathcal{M}^{(N)}$ and its image $T_A(\mathcal{M}^{(N)})$ with respect to partial transpose. Its volume and area are denoted by V_{PPT} and A_{PPT}.

PPT states is an intersection of two bodies of constant height, $\mathcal{M}^{(N)}_{\mathrm{PPT}} = \mathcal{M}^{(N)} \cap T_A(\mathcal{M}^{(N)})$, the intersection lemma (lemma 2) implies that this set has constant height. □

The total area of the set $\mathcal{M}^{(N)}$ of mixed states can be divided into two parts: one part A_{P} containing PPT states, and the other part A_{NP} not containing PPT states—see figure 1(*a*). By definition $A_{\mathrm{tot}} = A_{\mathrm{NP}} + A_{\mathrm{P}}$. On the other hand, the surface of the set of PPT states is a union of two congruent parts: the part A_{P} described above, and its isometric image under T_A—see figure 1(*b*). Accordingly, it is possible to infer that the area A_{PPT} of the set $\mathcal{M}^{(N)}_{\mathrm{PPT}}$ equals $2A_{\mathrm{P}}$ once we establish that the area of the intersection of the two parts (the 'corners' of the set PPT on figure 1) is zero. This is indeed the case and is the content of the following.

Lemma 3. *The $(D-1)$-dimensional area of the intersection of the boundary $\partial\mathcal{M}^{(N)}$ with its image under T_A is zero.*

Before we prove this, we need to recall some basic facts about the boundary $\partial\mathcal{M}^{(N)}$. First of all any density matrix can be written as

$$\rho = UEU^{\dagger}, \tag{9}$$

where U is a unitary matrix and E is diagonal. As indicated in the comments following proposition 1, $\partial\mathcal{M}^{(N)}$ consists exactly of those density matrices that have a zero eigenvalue. Further, after disregarding the density matrices with multiple eigenvalues (a subset of dimension $(D-2)$, and hence of surface measure zero), the remaining 'generic' part of $\partial\mathcal{M}^{(N)}$ is a smooth manifold which—because of equation (9)—is naturally diffeomorphic to the Cartesian product of the open simplex $\Lambda := \left\{(0, \lambda_2, \ldots, \lambda_N) : 0 < \lambda_2 < \cdots < \lambda_N, \sum_{j=2}^{N} \lambda_j = 1\right\}$ and the flag manifold $\mathrm{Fl}^{\mathbb{C}}_N = U(N)/U(1)^N$. The first component is just the ordered sequence of eigenvalues of the matrix, while the second component is the set of unitary matrices with those matrices that commute with E 'divided out'; the second component is in fact given by the corresponding sequence of eigenspaces. (A more detailed analysis of the stratification of $\mathcal{M}^{(N)}$ can be found in [11].) Moreover, as is well known (cf, e.g., [17]), this diffeomorphism transforms the surface measure to a product measure of the type $f(\lambda)\, \mathrm{d}\lambda \otimes \mathrm{d}u$, where $\mathrm{d}\lambda$ is the Lebesgue measure on Λ, $f(\lambda)$—a positive continuous function on Λ, and $\mathrm{d}u$ is the invariant measure on $\mathrm{Fl}^{\mathbb{C}}_N$ induced by the action of $U(N)$.

The heuristic idea behind the proof that follows is that the area of intersection is zero if the normals of the two hypersurfaces are distinct in 'nearly all' places where they intersect. However, some care is needed in order to ensure that this argument works.

Proof of lemma 3. We will first prove a weaker statement, namely, that the intersection $\partial\mathcal{M}^{(N)} \cap T_A(\partial\mathcal{M}^{(N)})$ has empty interior (relative to $\partial\mathcal{M}^{(N)}$).

We shall argue by contradiction. Assume that the intersection *does have* nonempty interior. Then the subset C_{gen} of the intersection consisting of density matrices ρ verifying

- ρ and $T_A(\rho)$ belong to the generic part of $\partial\mathcal{M}^{(N)}$
- the pure states corresponding to the eigenvectors of ρ and $T_A(\rho)$ are *not* separable

also has a nonempty interior since each of the above two conditions is satisfied outside a (closed) set of dimension $< D-1$. Let ρ_0 be an interior point of C_{gen}. We now recall that the first eigenvector (of eigenvalue zero) of a generic boundary density matrix ρ corresponds to the pure state which is normal to $\partial\mathcal{M}^{(N)}$ at ρ. Thus, by our assumption, the normal to $\partial\mathcal{M}^{(N)}$ at $T_A(\rho_0)$ corresponds to an entangled state and, consequently, its image under T_A—which is the normal to $T_A(\partial\mathcal{M}^{(N)})$ at ρ_0—corresponds to a trace 1 matrix which is not positive definite. (This is because for all entangled *pure* states their negativity is positive [20, 21], so the PPT criterion is necessary and sufficient for separability of pure states.) In particular, the (unique) normals to $T_A(\partial\mathcal{M}^{(N)})$ and $\partial\mathcal{M}^{(N)}$ at ρ_0 are *distinct*. This implies that, in sufficiently small neighbourhoods of ρ_0, the intersection of $T_A(\partial\mathcal{M}^{(N)})$ and $\partial\mathcal{M}^{(N)}$ is a $(D-2)$-dimensional object and so ρ_0 cannot be an interior point of the intersection and *a fortiori* of C_{gen}, a contradiction.

Since $\partial\mathcal{M}^{(N)} \cap T_A(\partial\mathcal{M}^{(N)})$ is closed, the above argument does show that it is a rather 'thin' set ('nowhere dense' in topological parlance). However, this is not sufficient for our purposes because intersections of convex surfaces may be rather complicated; in particular, they may be of positive area in spite of having empty (relative) interior. To correct this shortcoming, we need to choose $\rho_0 \in C_{\mathrm{gen}}$ to be a Lebesgue point of (the indicator function of) C_{gen} rather than an interior point of C_{gen}. Then, for every sufficiently regular sequence (N_k) of neighbourhoods of ρ_0 (relative to $\partial\mathcal{M}^{(N)}$) which shrinks to ρ_0, the ratios of the areas of $N_k \cap C_{\mathrm{gen}}$ and of N_k tend to 1 (this is just a reformulation of the definition of a Lebesgue point). By the Lebesgue differentiation theorem, almost all points of a measurable set have this property (see, e.g., [19], theorem 3.21). Accordingly, if we assume that $\partial\mathcal{M}^{(N)} \cap T_A(\partial\mathcal{M}^{(N)})$, hence C_{gen}, has strictly positive area, then such a choice of $\rho_0 \in C_{\mathrm{gen}}$ is possible and we are led to a contradiction in the same way as earlier. □

The ratio between the probabilities of finding a PPT state in the interior of $\mathcal{M}^{(N)}$ and at its boundary is defined by [13]

$$\Omega \equiv \frac{p_V}{p_A} := \frac{V_{\mathrm{PPT}}/V_{\mathrm{tot}}}{A_{\mathrm{P}}/A_{\mathrm{tot}}} = \frac{V_{\mathrm{PPT}}A_{\mathrm{tot}}}{V_{\mathrm{tot}}A_{\mathrm{P}}}. \tag{10}$$

The above quantity allows us to formulate the main result of the work.

Theorem 2. *For any bipartite $K \times M$ system the ratio (10) is equal to 2.*

Proof. By theorem 1 the set of PPT states has constant height; hence $\gamma\left(\mathcal{M}_{\mathrm{PPT}}^{(KM)}\right) = rA_{\mathrm{PPT}}/V_{\mathrm{PPT}} = D$. For any fixed system of the size $N = KM$, the sets $\mathcal{M}^{(N)}$ and $\mathcal{M}_{\mathrm{PPT}}^{(N)}$ have the same dimensionality D and the same radius r of the inscribed ball, so that

$$\frac{A_{\mathrm{tot}}}{V_{\mathrm{tot}}} = \frac{A_{\mathrm{PPT}}}{V_{\mathrm{PPT}}}. \tag{11}$$

Lemma 3 implies $A_{\mathrm{P}} = A_{\mathrm{PPT}}/2$. Substituting this relation into (10) and making use of (11) we find

$$\Omega = \frac{V_{\mathrm{PPT}}A_{\mathrm{tot}}}{V_{\mathrm{tot}}A_{\mathrm{PPT}}/2} = 2, \tag{12}$$

which concludes the proof. □

The relation $\Omega = 2$ is thus established for any bipartite system. In the simplest cases of 2×2 and 2×3 systems any PPT state is separable [3]. Hence, for such systems, equation (12) describes the ratio between the probabilities of finding a separable state inside the set of mixed states and at its boundary.

The value $\Omega = 2$ is consistent with the numerical data obtained in [13, 14] for the Hilbert–Schmidt measure. Since our reasoning hinges directly on the Euclidean geometry, it does not allow one to predict any values of analogous ratios computed with respect to the Bures measure [22], nor other measures. On the other hand, the result obtained is valid also for the set of real density matrices, for which the complex flag manifold $\mathrm{Fl}_N^{\mathbb{C}}$ has to be replaced by the real flag manifold, $\mathrm{Fl}_N^{\mathbb{R}} = \mathrm{O}(N)/\mathrm{O}(1)^N$. The set of real density matrices is often used as an attractive toy model, since its dimensionality $D_R = N(N+1)/2 - 1$ is smaller than $D = N^2 - 1$ of the full set of complex states.

The geometry of the 15-dimensional set of separable states of two qubits is not easy to describe. In this work, we have established a concrete rigorous result in this direction, proving that this set is 'pyramid decomposable' and hence is a body of constant height. This is also true for the set of positive-partial-transpose states for an arbitrary bipartite system. We hope that these properties will be useful for further investigation of the geometry of the set of separable states. Although in this work we have concentrated on the bipartite case only, one could try to obtain similar results for a general class of multipartite systems, for which some estimates of the volume of the set of separable states or PPT states are known [8, 9, 23, 24].

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