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The structure of states and maps in quantum theory

SUDHAVATHANI SIMON[1], S P RAJAGOPALAN[2] and R SIMON[3,*]
[1]Department of Computer Science, Women's Christian College, Chennai 600 006, India
[2]Mohamed Sathak A.J. College of Engineering, Old Mahabalipuram Road, Egattur 603 103, India
[3]The Institute of Mathematical Sciences, CIT Campus, Taramani, Chennai 600 113, India
*Corresponding author. E-mail: simon@imsc.res.in

Abstract. The structure of statistical state spaces in the classical and quantum theories are compared in an interesting and novel manner. Quantum state spaces and maps on them have rich convex structures arising from the superposition principle and consequent entanglement. Communication channels (physical processes) in the quantum scheme of things are in one-to-one correspondence with completely positive maps. Positive maps which are not completely positive do not correspond to physical processes. Nevertheless they prove to be invaluable mathematical tools in establishing or witnessing entanglement of mixed states. We consider some of the recent developments in our understanding of the convex structure of states and maps in quantum theory, particularly in the context of quantum information theory.

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In classical theory, the statistical state space of a two-state system is a closed line segment, say between points A_1 and A_2. It is a convex set: the end or extremal points A_1, A_2 are the two pure states; and the interior points of the segment are mixed states, being convex or probabilistic sums of the extremal or pure states. Similarly, the state space for a three-state system is an equilateral triangle, the vertices A_1, A_2, A_3 being the three pure states. The state space is again a convex set, with three extremal points this time; every other point of the state space is a probabilistic sum of the extremals. For a four-state system, the state space is a regular tetrahedron, being a collection of all probabilistic sums

$$\sum_j p_j A_j, \quad p_j \geq 0, \quad \sum_j p_j = 1 \tag{1}$$

of the four pure states A_1, A_2, A_3, A_4, the vertices of the tetrahedron. Clearly, while for non-extremal points on the six edges and for the interior points of the four faces respectively two and three p_js in the convex sum realization are non-zero, all the p_js are non-zero for every genuine interior point. Further, the expansion coefficients

$\{p_j\}$ are unique for every point (Carathéodory theorem), consistent with the fact that pure states are mutually independent in the classical scheme.

Pure states in the quantum theory proliferate into a continuum because of the superposition principle. For instance, pure states of a two-level system are in one-to-one correspondence with points on the unit sphere S^2, called the Poincaré or Bloch sphere. Even though there are infinite number of pure states, the statistical state space is still finite-dimensional, owing to the fact that pure states in the quantum case are neither independent nor reliably distinguishable.

Statistical states of a d-level quantum system is described by $d\times d$ density matrices ρ, whose defining properties are Hermiticity, unit trace, and positivity:

$$\rho^\dagger = \rho, \quad \mathrm{tr}\,\rho = 1, \quad \rho \geq 0. \tag{2}$$

For a two-level system, ρ is necessarily of the form

$$\rho = \frac{1}{2}(1 + \mathbf{n}\cdot\boldsymbol{\sigma}), \quad \mathbf{n}\cdot\mathbf{n} \leq 1. \tag{3}$$

The state space is thus the (solid) unit ball in R^3 assumed to be centred at the origin. All boundary points are extremal and pure states, and this is as in the classical case. However, an interior point or mixed state can be written as a convex sum of extremal or pure states in an enormously large number of ways [1]. Indeed, much of the richness (or complexity) of problems related to quantum information can be traced to this proliferation of possible convex sum decompositions associated with a mixed state.

1. Three-level systems

The two-level system is special in the sense that for no $d > 2$ is the statistical state space of of a d-level quantum system has such a simple geometry as that of a sphere. Let us look at the case $d = 3$ in some detail. The λ-matrices

$$\lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$
$$\lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad \lambda_5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \quad \lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},$$
$$\lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad \lambda_8 = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}, \tag{4}$$

familiar as generators of the unimodular unitary group $SU(3)$ in the defining representation, form a set of Hermitian, traceless, orthogonal matrices:

$$\mathrm{tr}(\lambda_k\lambda_\ell) = 2\delta_{k\ell}, \quad k,\ell = 1,2,\ldots,8, \tag{5}$$

very much like the Pauli matrices. The structure of these matrices is described by the product property

$$\lambda_j \lambda_k = \frac{2}{3}\delta_{jk} + d_{jk\ell}\lambda_\ell + i f_{jk\ell}\lambda_\ell. \tag{6}$$

Separating this product into commutator and anticommutator, we have

$$\begin{aligned}
\lambda_j \lambda_k - \lambda_k \lambda_j &= 2i f_{jk\ell}\lambda_\ell, \\
\lambda_j \lambda_k + \lambda_k \lambda_j &= \frac{4}{3}\delta_{jk} + 2 d_{jk\ell}\lambda_\ell.
\end{aligned} \tag{7}$$

The $SU(3)$ structure constants $f_{jk\ell}$ are totally antisymmetric in their indices, whereas $d_{jk\ell}$ are totally symmetric. The numerical values of their non-vanishing independent components are [2]

$$\begin{aligned}
& f_{123} = 1, \quad f_{458} = f_{678} = \frac{\sqrt{3}}{2}, \\
& f_{147} = f_{246} = f_{257} = f_{345} = f_{516} = f_{637} = \frac{1}{2}, \\
& d_{118} = d_{228} = d_{338} = -d_{888} = \frac{1}{\sqrt{3}}, \\
& d_{146} = d_{157} = -d_{247} = d_{256} = d_{344} = d_{355} = -d_{366} = -d_{377} = \frac{1}{2}, \\
& d_{448} = d_{558} = d_{668} = d_{778} = -\frac{1}{2\sqrt{3}}.
\end{aligned} \tag{8}$$

These λ matrices can be used to describe 3×3 density matrices in the form:

$$\rho = \frac{1}{3}(1 + \sqrt{3}\mathbf{n} \cdot \boldsymbol{\lambda}). \tag{9}$$

While Hermiticity of ρ is ensured by that of $\boldsymbol{\lambda}$ and reality of $\mathbf{n}$, unit trace is ensured by the $1/3$ factor, the λs being traceless. So only positivity remains to be taken care of. Since the state space is convex, the extremals being the pure states, it suffices to isolate those vectors $\mathbf{n} \in R^8$ which correspond to pure states. We expect these $\mathbf{n} \in R^8$ corresponding to pure states to form a four-parameter subset of the seven-parameter boundary of the state space.

Now a unit trace Hermitian matrix ρ is a pure state density operator if and only if it is a one-dimensional projection:

$$\rho \text{ is a pure state } \Leftrightarrow \ \rho^2 = \rho. \tag{10}$$

We define a star-product on vectors $\mathbf{n} \in R^8$ through

$$(\mathbf{n} * \mathbf{n})_j = \sqrt{3} d_{jk\ell} n_k n_\ell, \tag{11}$$

and compute

$$\rho^2 = \frac{1}{9}(1 + 2\mathbf{n} \cdot \mathbf{n} + 2\sqrt{3}\mathbf{n} \cdot \boldsymbol{\lambda} + \sqrt{3}\mathbf{n} * \mathbf{n} \cdot \boldsymbol{\lambda}). \tag{12}$$

It follows that ρ specified by $\mathbf{n}$ is a pure state if and only if the two conditions

$$\mathbf{n}\cdot\mathbf{n}=1, \quad \mathbf{n}*\mathbf{n}=\mathbf{n} \tag{13}$$

are met. While the first condition corresponds to the sphere S^7, the second one is a vector equation in R^8, i.e., it is a set of eight equations. Interestingly, it can be transcribed into a single scalar equation! This is a special feature of $d=3$ which does not hold for higher d.

This is easily seen by noting that for every unit vector $\mathbf{n}\in R^8$, the associated vector $\mathbf{n}*\mathbf{n}$ is a unit vector. It follows that the condition $\mathbf{n}*\mathbf{n}=\mathbf{n}$ is equivalent to the cubic scalar condition $\mathbf{n}*\mathbf{n}\cdot\mathbf{n}=1$. Thus we arrive at a complete characterization of CP^2, the family of all pure states of a three-level system:

$$CP^2=\{\mathbf{n}|\mathbf{n}\cdot\mathbf{n}=1, \quad \mathbf{n}*\mathbf{n}\cdot\mathbf{n}=1\}. \tag{14}$$

The enumeration of the extremals of our convex state space is thus complete: the state space of a three-level quantum system is the convex set in R^8 generated by these extremals. We may call it the Poincaré 'sphere' for this system.

Unlike the case of two-level system, the state space of the three-level system is far from being a sphere. To appreciate this, note that all density operators ρ which are singular as matrices constitute the boundary of the state space. Density matrices whose rank is two are precisely the non-extremal boundary points. The state space is contained within S^7, and the radius of the largest sphere contained in our state space is 1/2. Indeed, $\mathbf{n}=(0,0,0,0,0,0,0,-1)$, corresponding to $\rho=\mathrm{diag}(0,0,1)$, is an example of a state on S^7, while the rank-two density matrix $\mathrm{diag}(1/2,1/2,0)$ is also on the boundary at the 'opposite end', but it corresponds to $\mathbf{n}=(0,0,0,0,0,0,0,1/2)$, and hence sits on (the surface of) the sphere of radius 1/2.

Let r_{out} be the radius of the outer sphere, the smallest sphere containing the state space, and r_{in} be the radius of the inner sphere, the largest sphere contained in the state space. And let $\kappa=r_{\mathrm{in}}/r_{\mathrm{out}}$. We have just seen that $\kappa=1/2$ for a three-level quantum system. It is interesting that this ratio assumes the same value in the classical case as well: the inner circle and the outer circle of an equilateral triangle have radii in the ratio 1 : 2. Indeed, for a d-state system κ has the same value in the classical and quantum cases, for every d. The classical state space of a $(d+1)$-level system is a regular d-simplex, the convex set in R^d generated by $d+1$ extremal points, the distance between two points being the same for all pairs. It is not hard to see that $\kappa=1/d$ for a regular d-simplex. The tetrahedron is 3-simplex and $\kappa=1/3$. Thus we record, as an important aspect of the state space, the following theorem:

Theorem 1. *The radii of the inner and outer spheres of the convex state space of a d-level system are in the ratio* $1/(d-1)$. *This holds in the classical as well as quantum cases.*

2. *d*-Level systems

We may extend this Poincaré sphere kind of construction to higher values of d by noting that $d\times d$ Hermitian traceless matrices form a real vector space of dimension

$N_d \equiv d^2 - 1$. The structure of the convex state space $\Omega \in R^{N_d}$ of a d-level system thus obtained is no way close to a sphere. Considerable research has aimed at an understanding of its structure [3]. We may obtain a convenient Pauli or λ-like basis for this N_d-dimensional space in the following manner:

- Define σ_3-like diagonal traceless matrices $J_1, J_2, \ldots, J_{d-1}$ through

$$\begin{aligned} &J_1 = \text{diag}(1, -1, 0, 0, \ldots, 0),\\ &\sqrt{3}J_2 = \text{diag}(1, 1, -2, 0, \ldots, 0),\\ &\qquad\quad \ldots \quad \ldots \quad \ldots\\ &\sqrt{(d-1)(d-2)/2}J_{d-2} = \text{diag}(1, 1, \ldots, 1, -(d-2), 0),\\ &\sqrt{d(d-1)/2}J_{d-1} = \text{diag}(1, 1, \ldots, 1, 1, -(d-1)). \end{aligned}$$

- For each $1 \leq i_0 < j_0 \leq d$ define σ_1-like and σ_2-like matrices thus:

$$\begin{aligned} &(M(i_0, j_0))_{i,j} = \delta_{ii_0}\delta_{jj_0} + \delta_{ij_0}\delta_{ji_0},\\ &(N(i_0, j_0))_{i,j} = i(\delta_{ii_0}\delta_{jj_0} - \delta_{ij_0}\delta_{ji_0}). \end{aligned}$$

- Rename and relabel these $d^2 - 1$ matrices as $J_1, J_2, \ldots, J_{d^2-1}$.

There are thus $d(d-1)/2$ symmetric off-diagonal σ_1-type matrices, $d(d-1)/2$ antisymmetric (and hence purely imaginary) off-diagonal σ_2-type matrices and $d-1$ diagonal σ_3-type matrices. And these d^2-1 matrices form a complete orthonormal traceless set:

$$\text{tr}(J_k J_\ell) = 2\delta_{k\ell}, \quad k, \ell = 1, 2, \ldots, d^2 - 1. \tag{15}$$

We can again express the product structure of these J matrices through totally antisymmetric structure constants $f_{jk\ell}$ and totally symmetric $d_{jk\ell}$. Any $d \times d$ density operator can be written in the form

$$\rho = \frac{1}{d}(1 + \sqrt{d(d-1)/2}\mathbf{n} \cdot \mathbf{J}), \tag{16}$$

the role of $\sqrt{3}$ in the three-level case being now played by $\sqrt{d(d-1)/2}$. Again we can define the star product on vectors $\mathbf{n} \in R^{d^2-1}$ using the totally symmetric $d_{jk\ell}$s, and obtain $\mathbf{n} \cdot \mathbf{n} = 1$, $\mathbf{n} * \mathbf{n} = \mathbf{n}$ as the two conditions for purity. But we cannot reduce these pure state condition to two scalar conditions, for in the present case we will have to ensure $\text{tr}\,\rho^4 = \text{tr}\,\rho^5 = \cdots = \text{tr}\,\rho^d = 1$ in addition to the earlier $\text{tr}\,\rho^2 = \text{tr}\,\rho^3 = 1$. Stated differently, $\mathbf{n} * \mathbf{n}$ is no more a unit vector for all $\mathbf{n} \in S^{d^2-1}$. The unit vector $\mathbf{n} = (0, 0, \ldots, 0, -1) \in S^{d^2-2}$ corresponds to the pure state $\rho = \text{diag}(0, 0, \ldots, 0, 1)$, but the vector $\mathbf{n} = (0, 0, \ldots, 0, 1/(d-1))$ of length $1/(d-1)$ too corresponds to a boundary point, for it represents the density operator $\rho = \text{diag}\left(\frac{1}{d-1}, \frac{1}{d-1}, \ldots, \frac{1}{d-1}, 0\right)$ which is of less than maximal rank. Thus, κ indeed equals $1/(d-1)$.

3. Positive maps and completely positive paps

Having looked at the convex structure of the state space in some detail, we now move forward to consider maps or transformations of the state space. Let $\mathcal{B}(\mathcal{H})$ be the complex linear space of linear operators acting on an underlying d-dimensional Hilbert space $\mathcal{H}$. (Since d is finite, these operators are necessarily bounded.) In particular, density operators of a d-level system are elements of $\mathcal{B}(\mathcal{H})$. A linear map (or simply map) M is a (complex) linear transformation $\mathcal{B}(\mathcal{H}) \rightarrow \mathcal{B}(\mathcal{H})$:

$$M\colon \rho \rightarrow \rho' = M(\rho)$$
$$\rho'_{ij} = \sum_{k,\ell=1}^{n} M_{ik,j\ell}\,\rho_{k\ell}. \tag{17}$$

Linear maps are sometimes called super-operators to underline the fact that they are operators on operators.

We know that any and every operator $\rho \in \mathcal{B}(\mathcal{H})$ obeying the defining conditions (i) $\rho^\dagger = \rho$, (ii) $\mathrm{tr}\,\rho = 1$ and (iii) $\rho \geq 0$ is a valid density operator, that every density operator describes a possible quantum state, and that the set of all density operators forms a convex set, the state space. Obviously, maps of interest to us should image this convex set into itself, and this leads to the notion of positive maps. A map M is said to be positive if, for every Hermitian positive input ρ, the output $M(\rho)$ is Hermitian positive. M is called trace preserving if $\mathrm{tr}\,M(\rho) = \mathrm{tr}\,\rho$ for all ρ. It is clear from the definition that positive maps on $\mathcal{B}(\mathcal{H})$ form a convex set. Examples of positive maps are easy to construct:

- Every unitary evolution $|\psi\rangle \rightarrow |\psi'\rangle = U|\psi\rangle$ of the state vector defines a map $U\colon \rho \rightarrow \rho' = U\rho U^\dagger$, which is manifestly positive.
- The defining properties of density operators are left unchanged under matrix transposition. That is, the transpose map $T\colon \rho \rightarrow \rho^{\mathrm{T}}$ (defined in any chosen basis) is positive.
- It is easy to verify that the reduction map $R\colon \rho \rightarrow \rho' = (d-1)^{-1}(\mathrm{tr}\,\rho - \rho)$ is positive.
- The map $A\colon \rho \rightarrow \rho' = A\rho A^\dagger$, for any operator A, preserves Hermiticity and positivity (it preserves trace if and only if A is unitary). It follows from the convexity of positive maps that $\rho \rightarrow \rho' = \sum_\alpha A_\alpha \rho A_\alpha^\dagger$ is a positive map, for any collection of operators $\{A_\alpha\}$. Clearly, this map will be trace preserving if and only if the collection $\{A_\alpha\}$ respects the resolution of identity $\sum_\alpha A_\alpha^\dagger A_\alpha = \mathrm{Id}$. It is also clear that this map is unital, i.e., it maps the identity matrix (the maximally mixed state) into identity, if and only if the collection is obedient to $\sum_\alpha A_\alpha A_\alpha^\dagger = \mathrm{Id}$.

Since any positive map on a system A takes its states into states, classical experience may prompt one to associate positive maps with valid evolutions or physical processes. There are, however, positive maps which acting on part of a composite system can map a density operator into something which is not. Clearly, such a positive map cannot represent any physical process. Therefore, the notion of positive maps needs to be further refined to isolate the ones which correspond to valid physical processes. It turns out that, in order to represent a valid evolution, a positive map should be completely positive.

Given a positive map M on $\mathcal{H}_{\rm B}$ (i.e., on $\mathcal{B}(\mathcal{H}_{\rm B})$), let us extend it to the map $\mathrm{Id}_{\rm A} \otimes M$ on the tensor product space $\mathcal{H}_{\rm A} \otimes \mathcal{H}_{\rm B}$, the Hilbert space of a composite system S=A+B:

$$\mathrm{Id}_{\rm A} \otimes M : \rho \rightarrow \rho'$$
$$\rho'_{\alpha i,\beta j} = \sum_{k,\ell} M_{ik,j\ell}\rho_{\alpha k,\beta\ell}. \tag{18}$$

Here the Greek indices on ρ correspond to basis vectors in the Hilbert space of the subsystem A, and the Roman indices to those of B. This trivial-looking extension is not all that trivial. Even though M is a positive map on $\mathcal{H}_{\rm B}$, the extension $\mathrm{Id}_{\rm A} \otimes M$ need not be a positive map on the extended Hilbert space $\mathcal{H}_{\rm A} \otimes \mathcal{H}_{\rm B}$, in spite of the fact that we are doing nothing to subsystem A. And this 'spooky action' leads to the notion of completely positive maps. A positive (P) map M is said to be completely positive (CP) if and only if all its trivial extensions are positive.

Of the four examples of positive maps we listed earlier, the first and the last are completely positive, but the second and third are not. Positive maps which are not completely positive are not objects of contempt in quantum information theory. It is their failure to be physical that empowers the transpose and reduction maps with the capacity to detect or witness entanglement.

It is again clear from the very definition that the set of all completely positive maps on a Hilbert space $\mathcal{H}$ (or more properly on $\mathcal{B}(\mathcal{H})$) is a convex set, a subset of the larger convex set of all positive maps. Indeed, this subset is fully characterized by a fundamental representation theorem.

Theorem 2. *All trace-preserving CP maps are of the form*

$$\rho \rightarrow \rho' = \sum_{\alpha} A_\alpha \rho A_\alpha^\dagger, \quad \sum_{\alpha} A_\alpha^\dagger A_\alpha = \mathrm{Id}. \tag{19}$$

That this kind of a map is CP and trace preserving is obvious. The non-trivial part therefore is the assertion that this is all. This result is at least as old as the 1961 work of Sudarshan and coworkers [4] but in the quantum information literature it has come to be known as the Kraus representation theorem [5].

If a positive map M on $\mathcal{H}_{\rm B}$ is not CP, then there exists at least one bipartite density operator $\rho_{\rm AB}$ such that $(\mathrm{Id}_{\rm A} \otimes M)\rho_{\rm AB}$ is not positive, and hence a non-state [6]. In that case, we say that M witnesses the inseparability of $\rho_{\rm AB}$. The converse is also true in the following sense [6]:

Theorem 3. *A bipartite density operator* $\rho_{\rm AB}$ *is separable if and only if* $(\mathrm{Id}_{\rm A} \otimes M)\rho_{\rm AB}$ *is a density operator, for every positive map* M *on* $\mathcal{B}(\mathcal{H})$.

This theorem suggests that separability of a given $\rho_{\rm AB}$ can be determined by running through all P maps which are not CP. And convexity of the set of all P maps further suggests that it is sufficient to run through just the extremal P maps. Unfortunately, while the CP maps are fully characterized by the representation theorem, complete characterization of the set of all P maps which are not CP continues to remain a difficult open problem.

The transpose map T is a P but not CP map of singular importance for two reasons. First, it is essentially the only such (i.e., P but not CP) map which maps the space of density operators on a Hilbert space onto itself. Second, when the dimensions of $\mathcal{H}_{\rm A} \otimes \mathcal{H}_{\rm B}$ are either 2×2 or 2×3, $\rho_{\rm AB}$ is separable if and only if $({\rm Id}_{\rm A} \otimes T)\rho_{\rm AB}$ is positive. That is, positivity under partial transpose (PPT) is a necessary and sufficient condition for separability in these dimensions [6,7]. (In the continuous variable case of infinite Hilbert space dimension, the transpose map can be viewed as momentum reversal, and positivity under partial transpose proves to be a necessary and sufficient condition for separability for all two-mode Gaussian states [8], but this is a result which holds only for Gaussian states.)

But this happy state of affairs with the Peres–Horodecki separability criterion does not extend beyond these low dimensions. In higher dimensions there exist states which are PPT, and yet are inseparable. The first examples of states of this type were constructed by Horodecki [9]. We reproduce here his example in 3×3 dimensions:

$$\rho = \frac{1}{8a+1}\begin{bmatrix} a & 0 & 0 & 0 & a & 0 & 0 & 0 & a \\ 0 & a & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & a & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & a & 0 & 0 & 0 & 0 & 0 \\ a & 0 & 0 & 0 & a & 0 & 0 & 0 & a \\ 0 & 0 & 0 & 0 & 0 & a & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1+a}{2} & 0 & \frac{\sqrt{1-a^2}}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & a & 0 \\ a & 0 & 0 & 0 & a & 0 & \frac{\sqrt{1-a^2}}{2} & 0 & \frac{1+a}{2} \end{bmatrix}. \tag{20}$$

Obviously, a is a positive scalar.

It should be added that the inseparability of this PPT entangled state was demonstrated not by exhibiting a positive map which witnesses its inseparability, but through what has come to be known as the range criterion [9]. Clearly, if a state is separable, its partial transpose must also be a separable state. If $\rho_{\rm AB}$ is of rank r and its partial transpose $\rho_{\rm AB}^{T_{\rm B}}$ is of rank r', then a necessary condition for separability is that $\rho_{\rm AB}$ should have at least r linearly independent product states in its range, and its partial transpose should have at least r' such states in its range. Horodecki showed that his PPT state fails this range criterion, and thus established its inseparability.

Several examples of PPT entangled states have been constructed since the work of Horodecki [10,11]. Of particular interest are the states based on the notion of unextendible product basis (UPB) [12]. In any Hilbert space, a given partial basis can always be extended into a full basis. And in any bipartite Hilbert space there exists a large supply of product bases. However, given a partial product basis, there may not exist any product vector which is orthogonal to all product vectors in the partial basis. Such partial bases cannot be extended, and hence are called UPBs. Associated with every UPB there exists a PPT entangled state, and its inseparability is easily established through the range criterion.

Because of the special status of the transpose map, those maps which are manufactured from the transpose map and CP maps are called decomposable maps. These maps are of the form $C_1 + C_2 T$, where C_1 and C_2 are CP maps and T is the transpose map. Clearly, to witness PPT entanglement we need non-decomposable maps. The first example of a non-decomposable map was constructed by Choi [13], and Kossakowski has recently presented generalizations of this map [14]. Another interesting non-decomposable map based on UPBs was constructed by Terhal [15]. In what follows we present a new class of PPT entangled states, and employ the Choi map to witness their inseparability.

Trace preserving unital positive maps assume a particularly simple form [16] in the R^{d^2-1} description we have been extensively using in this paper. It is clear from the linearity of the association

$$\rho = \frac{1}{d}\left(\mathrm{Id} + \sum_{k=1}^{d^2-1} n_k J_k\right) \tag{21}$$

between $d \times d$ Hermitian unit-trace matrices and points in R^{d^2-1} that linear maps which preserve trace, Hermiticity, and unity are in one-to-one correspondence with real linear homogeneous transformations in R^{d^2-1}, represented by $(d^2-1)\times(d^2-1)$ real matrices M:

$$\begin{aligned} &M\colon \mathbf{n} \to \mathbf{n}' = M\mathbf{n}, \\ &n'_k = \sum_{\ell=1}^{d^2-1} M_{k\ell} n_\ell, \quad k = 1, 2, \ldots, d^2-1. \end{aligned} \tag{22}$$

This is simply a transcription of eq. (17) to the present unit preserving (unital) case. Unitary evolutions fit precisely into this form, with $M \in SO(d^2-1)$ being the real matrix obtained from the given unitary matrix $\in SU(d)$ in going over to the adjoint representation. It is clear that M is a positive map if it images the state space $\Omega \subset R^{d^2-1}$ into itself. Unitary evolutions correspond to rotations in R^{d^2-1}. Note that such rotations form a (d^2-1)-parameter family, and hence is a proper subset of $\mathcal{O}(d^2-1)$, the $(d^2-1)(d^2-1)/2$-parameter orthogonal group, for $d \geq 3$. The transpose map simply inverts the signatures of the $d(d-1)/2$ coordinates corresponding to the σ_2-like matrices, and hence is an element of $\mathcal{O}(d^2-1)$. It is an improper rotation for $d = 2, 3, 6, 7, \ldots$ and a proper rotation for $d = 4, 5, 8, 9, \ldots$.

Given a $(d^2-1)\times(d^2-1)$ real matrix M, testing if M maps Ω into itself is in general non-trivial. However, for a particular class of matrices such a test is quite simple [16]:

Theorem 4. *Every map represented by a matrix of the form $M = (d-1)^{-1}R$, where $R \in \mathcal{O}(d^2-1)$, the orthogonal group of proper and improper rotations in R^{d^2-1}, is positive.*

Proof. $R \in \mathcal{O}(d^2-1)$ images the out-sphere of Ω into itself, and the scale factor $(d-1)$ images the out-sphere into the in-sphere. This completes the proof in view of the following facts: (1) There is no state outside the out-sphere and (2) every point in the in-sphere is a valid state.

It is seen that the reduction map is precisely a map of this type, with $R \in \mathcal{O}^{d^2-1}$ representing inversion about the origin in R^{d^2-1}, this inversion being a proper or improper rotation depending on whether d is odd or even. The point being made is that the price one pays in terms of the contraction factor $(d-1)$ with respect to the reduction map is high enough that one has earned, through it, the freedom to do any proper or improper $\mathcal{O}(d^2-1)$ rotation. In particular, this scale factor allows one to perform any permutation of the diagonal elements of the density matrix, since such a permutation corresponds to a proper or improper rotation among the σ_3-like coordinates. We shall demonstrate presently the usefulness of precisely such permutations [16].

4. A new class of inseparable PPT states and associated indecomposable maps

Let us specialize our considerations to the case $d=3$. Consider the following bipartite density operator in 3×3 dimensions [16]:

$$\rho=\rho_0+\epsilon\mathrm{Id},$$

$$\rho_0=\begin{bmatrix} 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1\\ 0 & a & 0 & 1 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & a^{-1} & 0 & 0 & 0 & 1 & 0 & 0\\ 0 & 1 & 0 & a^{-1} & 0 & 0 & 0 & 0 & 0\\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1\\ 0 & 0 & 0 & 0 & 0 & a & 0 & 1 & 0\\ 0 & 0 & 1 & 0 & 0 & 0 & a & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & a^{-1} & 0\\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \end{bmatrix}, \tag{23}$$

where ϵ is a small positive parameter. We have suppressed a normalization constant $3(1+a+a^{-1})$ in the definition of ρ_0, and this does not affect our considerations below.

It is readily seen that rank of ρ_0 is 4. Further, ρ_0 is symmetric under partial transpose, and hence ρ_0 is either separable or PPT entangled. Peres–Horodecki criterion cannot distinguish between these two possibilities. And the reduction criterion of separability is known to be subordinate to the Peres–Horodecki criterion [17].

Closer examination shows that there is no product state in the range of ρ_0, if $a\neq 1$. The range criterion thus establishes the inseparability of ρ_0 for $a\neq 1$. But our ultimate interest is in ρ; it has full rank, and hence the range criterion offers no help in deciding its separability property.

We are thus forced to look for a suitable non-decomposable map. Consider the following map on the space of density operators of a system whose Hilbert space dimension is 3:

$$M\colon \begin{bmatrix} \rho_{11} & \rho_{12} & \rho_{13}\\ \rho_{21} & \rho_{22} & \rho_{23}\\ \rho_{31} & \rho_{32} & \rho_{33} \end{bmatrix} \rightarrow \frac{1}{2}\begin{bmatrix} \rho_{11}+\rho_{22} & -\rho_{12} & -\rho_{13}\\ -\rho_{21} & \rho_{22}+\rho_{33} & -\rho_{23}\\ -\rho_{31} & -\rho_{32} & \rho_{33}+\rho_{11} \end{bmatrix}. \tag{24}$$

This corresponds to the reduction map followed by $2\pi/3$ rotation in the (λ_3, λ_8) plane, and hence is a positive map in view of Theorem 4.

We will now let the extension $\mathrm{Id}_3 \otimes M$, where Id_3 is the three-dimensional unit map, act on ρ_0:

$$(\mathrm{Id}_3 \otimes M)\rho_0 = \begin{bmatrix} 1+a & 0 & 0 & 0 & -1 & 0 & 0 & 0 & -1 \\ 0 & a+\frac{1}{a} & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{a}+1 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & \frac{1}{a}+1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 1+a & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & a+\frac{1}{a} & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & a+\frac{1}{a} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & \frac{1}{a}+1 & 0 \\ -1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 1+a \end{bmatrix}.$$

Again we have suppressed an inessential multiplicative factor of 1/2. We see that $(\mathrm{Id}_3 \otimes M)\rho_0$ is not positive. Indeed, the column vector $(1,0,0,0,1,0,0,0,1)^{\mathrm{T}}$ is an eigenvector of $(\mathrm{Id}_3 \otimes M)\rho_0$ with eigenvalue $(a-1)$, which is negative for $a < 1$. This establishes the inseparability of ρ_0 for $a < 1$. Since no decomposable map could witness the inseparability of the PPT state ρ_0, we have the following theorem.

Theorem 5. *The positive map M described in eq.* (24) *is indecomposable.*

In the case $a > 1$, inseparability of ρ_0 is not witnessed by the map M in eq. (24). We may use in its place the positive map

$$M' : \begin{bmatrix} \rho_{11} & \rho_{12} & \rho_{13} \\ \rho_{21} & \rho_{22} & \rho_{23} \\ \rho_{31} & \rho_{32} & \rho_{33} \end{bmatrix} \rightarrow \frac{1}{2} \begin{bmatrix} \rho_{11}+\rho_{33} & -\rho_{12} & -\rho_{13} \\ -\rho_{21} & \rho_{22}+\rho_{11} & -\rho_{23} \\ -\rho_{31} & -\rho_{32} & \rho_{33}+\rho_{22} \end{bmatrix}, \tag{25}$$

corresponding to the reduction map followed by $-2\pi/3$ rotation in the (λ_3, λ_8) plane, to witness the inseparability of ρ_0. We will thus find that $(\mathrm{Id}_3 \otimes M')\rho_0$ has a negative eigenvalue $(a^{-1} - 1)$. Thus we conclude with the following theorem.

Theorem 6. *The positive map M' described in eq.* (25) *is indecomposable.*

Now we turn our attention to $\rho = \rho_0 + \epsilon\mathrm{Id}$, a mixture of ρ_0 with the maximally mixed state. Since ρ_0 is PPT, so is ρ. Indeed, the eigenvalues of the partial transpose of ρ are bounded from below by the positive constant ϵ. We consider the case $a > 0$; the case $a < 0$ can be handled through a similar procedure.

The fact that $(\mathrm{Id}_3 \otimes M)\rho_0$ has an eigenvalue $(a-1)$ implies that $(\mathrm{Id}_3 \otimes M)\rho$ has an eigenvalue $(a-1)+2\epsilon$, which is negative for sufficiently small values of ϵ, and hence the PPT state ρ is inseparable for such values of ϵ.

We may proceed one step further and explore a neighbourhood of ρ. Let Q be an arbitrary Hermitian traceless $d^2 \times d^2$ matrix, with $\mathrm{tr}\, Q^2 \leq 1$. That is, Q is in the unit ball in $R^{d^4-1} = R^{80}$. Its eigenvalues λ are necessarily in the range $-1 < \lambda < 1$. Tighter bounds, with ± 1 replaced by $\pm 1/\sqrt{2}$, are possible, but are not required for our purpose. Let $Q^{T_{\rm B}}$ be the partial transpose of Q. Clearly, $\mathrm{tr}\,(Q^{T_{\rm B}})^2 = \mathrm{tr}\,Q^2$ and hence the eigenvalues of $Q^{T_{\rm B}}$ obey similar bounds.

Now consider $\rho' = \rho + \epsilon' Q$, where ϵ' is a positive number. Since the smallest eigenvalue of the partial transpose of ρ is ϵ, the smallest eigenvalue of the partial transpose of $\rho + \epsilon' Q$ is not less than $\epsilon - \epsilon'$, and hence ρ' is PPT for $\epsilon' < \epsilon$. The fact that $(\mathrm{Id}_3 \otimes M)\rho$ has an eigenvalue $(a-1) + 2\epsilon$ implies that $(\mathrm{Id}_3 \otimes M)\rho'$ has an eigenvalue $\leq (a-1) + 2\epsilon + \epsilon'$, and we can thus choose $\epsilon \geq \epsilon' > 0$ such that this eigenvalue is negative for all Q in the unit ball. We have thus established the following fact.

Theorem 7. *The state* $\rho = \rho_0 + \epsilon \mathrm{Id}$, *for sufficiently small* $\epsilon > 0$, *has a neighbourhood of states all of which are PPT and inseparable. Their inseparability is witnessed by the indecomposable map* M *or* M' *depending on whether* $a < 1$ *or* $a > 1$.

Finally, we may turn this argument inside out. Staying with the expression $(\mathrm{Id}_3 \otimes M)\rho'$, instead of examining it over a neighbourhood of ρ, for fixed M, we can explore a small neighbourhood of M in the convex set of positive maps, with ρ' fixed at $\rho' = \rho$. We will find, by virtue of continuity, that $(\mathrm{Id}_3 \otimes M)\rho$ has a negative eigenvalue for this entire neighbourhood of positive maps. Thus we arrive at the following theorem.

Theorem 8. *The indecomposable map* M *(and similarly* M'*) has a neighbourhood consisting of indecomposable positive maps.*

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