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Wigner's theorem and the geometry of extreme positive maps

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Abstract

We consider transformation maps on the space of states which are symmetries in the sense of Wigner. By virtue of the convex nature of the space of states, the set of these maps has a convex structure. We investigate the possibility of a complete characterization of extreme maps of this convex body to be able to contribute to the classification of positive maps. Our study provides a variant of Wigner's theorem originally proved for ray transformations in Hilbert spaces.

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1. Introduction

Symmetries play a very important role in physics, as has been stressed by Wigner on several occasions [1–3]. The way symmetries are realized depends on the theory under consideration and more specifically, according to Felix Klein, on the corresponding geometric structure of the carrier space; these are 'kinematical' rather than 'dynamical' symmetries. It is well known that any description of physical systems requires the consideration of states and observables along with a pairing among them providing a real number with a computable probability [4]. In the Schrödinger–Dirac description of quantum mechanics one associates a Hilbert space with a quantum system, states are identified with rays of this space and observables are a derived concept—they are identified with self-adjoint operators, while symmetries are defined to be bijections among rays which preserve probability transitions.

In the C^*-algebraic approach to quantum mechanics, originated from the Heisenberg picture, observables are identified with real elements of this C^*-algebra, while states are a derived concept—they are identified with positive normalized functionals on the space of observables. The space of observables carries the structure of a Jordan algebra and this was the point of view of Kadison to define symmetries as Jordan-algebra isomorphisms [5, 6]. C^*-algebras are quite convenient to deal with the description of composite systems, the dual space of states turns out to have a rather involved geometrical structure. In particular, to take into account the distinction between separable and entangled states on the space of states, one is obliged to give up linear superposition in favor of convex combinations. This change of perspective introduces highly nontrivial problems, specific to the 'convex setting'. As shown elsewhere [7], in finite dimensions the space of states turns out to be a stratified manifold with faces of various dimensions.

The aim of this paper is to deal with symmetries as those transformations on the space of states which are appropriate for its geometrical structure. In doing so, we end up with yet another variant of the celebrated Wigner's theorem on the realization of symmetries as unitary or antiunitary transformations on the Hilbert space. The literature on this theorem, which is also available in textbooks [8, 9] in addition to the famous book by Wigner [10], is huge. We limit ourselves to a partial list trying to give a sampling of the various approaches which have been taken over the years [11–19].

This paper is organized in the following way. In section 2, we give a short geometrical description of the set of density states in a finite-dimensional Hilbert space. Density states form a convex body in the space of Hermitian operators. The set of affine maps which map a convex set K into itself, called simply positive maps, is also a convex set in the space of affine maps. Characterization of positive maps, e.g. by identifying the extremal ones, i.e. maps which cannot be decomposed into a nontrivial convex combination of other positive maps, can lead to a useful description of the underlying set K. Finding extreme points of such maps is, however, a difficult task, even if we know explicitly the extreme points of K. In section 3, we discuss and give examples of positive maps for which their extremality can be established upon analyzing the number of extreme points in the image. In section 4, we connect the obtained results to Wigner's theorem expressed in terms of positive maps which are bijective on pure states. Sections 5 and 6 are devoted to completely positive maps. In particular, we show again how the number of extreme points in their image establishes their form and extremality. We conclude with section 7 containing illustrative examples of extreme positive and completely positive maps in low dimensions.

2. Density states

Let $\mathcal{H}$ be a finite-dimensional Hilbert space, $\dim\mathcal{H} = n$, and let $gl(\mathcal{H})$ be the space of complex linear operators on $\mathcal{H}$. The space $gl(\mathcal{H})$ is canonically a Hilbert space itself with the Hermitian product $\langle A, B\rangle = \mathrm{Tr}(A^\dagger \circ B)$. As in [7], we shall treat the real linear space of Hermitian operators on $\mathcal{H}$ as the dual space, $\mathfrak{u}^*(\mathcal{H})$, of the Lie algebra (of antiHermitian operators), $\mathfrak{u}(\mathcal{H})$, of the unitary group $\mathcal{U}(\mathcal{H})$. We have the obvious decomposition $gl(\mathcal{H}) = \mathfrak{u}(\mathcal{H}) \oplus \mathfrak{u}^*(\mathcal{H})$ into real subspaces with a natural pairing between $\mathfrak{u}(\mathcal{H})$ and $\mathfrak{u}^*(\mathcal{H})$ given by

$$\langle A, T\rangle^* = \mathrm{i}\cdot\mathrm{Tr}(AT), \qquad (A, T) \in \mathfrak{u}^*(\mathcal{H}) \times \mathfrak{u}(\mathcal{H}), \tag{1}$$

and a scalar product induced on $\mathfrak{u}^*(\mathcal{H})$ by the Hermitian product and given by

$$\langle A, B\rangle_* = \mathrm{Tr}(AB), \qquad A, B \in \mathfrak{u}^*(\mathcal{H}). \tag{2}$$

We denote with$\|\cdot\|_*$ the corresponding norm.

The coadjoint action of $\mathcal{U}(\mathcal{H})$ on $\mathfrak{u}^*(\mathcal{H})$ reads

$$A \mapsto UAU^\dagger, \qquad A \in \mathfrak{u}^*(\mathcal{H}), \qquad U \in \mathcal{U}(\mathcal{H}). \tag{3}$$

We denote by $\mathcal{P}(\mathcal{H})$ the space of positive semi-definite operators from $gl(\mathcal{H})$, i.e. of those $\rho \in gl(\mathcal{H})$ which can be written in the form $\rho = T^\dagger T$ for a certain $T \in gl(\mathcal{H})$. It is a cone, since it is invariant with respect to the homotheties by λ with $\lambda \geqslant 0$. The set of density states $\mathcal{D}(\mathcal{H})$ is distinguished in the cone $\mathcal{P}(\mathcal{H})$ by the equation $\mathrm{Tr}(\rho) = 1$, so we will regard $\mathcal{P}(\mathcal{H})$ and $\mathcal{D}(\mathcal{H})$ as embedded in $u^*(\mathcal{H})$.

The space $\mathcal{D}(\mathcal{H})$ is a convex set in the affine hyperplane $u_1^*(\mathcal{H})$ in $u^*(\mathcal{H})$, determined by the equation $\mathrm{Tr}(A) = 1$. The model vector space for $u_1^*(\mathcal{H})$ is therefore canonically identified with the space of Hermitian operators with trace 0. The space $\mathfrak{A}(u_1^*(\mathcal{H}))$ of affine maps of $u_1^*(\mathcal{H})$ can be canonically identified with the space of these linear maps $\Phi \in \mathcal{L}(u^*(\mathcal{H}))$ which preserve the trace.

It is known that the set of extreme points of $\mathcal{D}(\mathcal{H})$ coincides with the set $\mathcal{D}^1(\mathcal{H})$ of pure states, i.e. the set of one-dimensional orthogonal projectors $|x\rangle\langle x|$, and that every element of $\mathcal{D}(\mathcal{H})$ is a convex combination of points from $\mathcal{D}^1(\mathcal{H})$. The space $\mathcal{D}^1(\mathcal{H})$ of pure states can be identified with complex projective space $P\mathcal{H} \simeq \mathbb{C}P^{n-1}$ *via* the projection

$$\mathcal{H} \setminus \{0\} \ni x \mapsto \frac{|x\rangle\langle x|}{\|x\|^2} \in \mathcal{D}^1(\mathcal{H}),$$

which identifies the points of the orbits of the $\mathbb{C} \setminus \{0\}$-group action by complex homotheties.

If we choose an orthonormal basis $e_1, \ldots, e_n$ in $\mathcal{H}$, we can identify $u^*(\mathcal{H})$ with the real vector space $u^*(n)$ of Hermitian $n \times n$ matrices, $u_1^*(\mathcal{H})$ with the affine space of Hermitian $n \times n$ matrices with trace 1, $U(\mathcal{H})$ with the group $U(n)$ of unitary matrices, $\mathcal{D}(\mathcal{H})$ with $\mathcal{D}(n)$—the convex body of density $n \times n$ matrices, etc. Recall that the dimension of $u_1^*(n)$ is $n^2 - 1$ and the dimension of $u^*(n)$ is n^2.

Almost everything above can be repeated in the case when $\mathcal{H}$ is infinite dimensional if we assume that all the operators in question, i.e. operators from $gl(\mathcal{H})$ and $u^*(\mathcal{H})$, are Hilbert–Schmidt operators (see [20]). The positive semi-definite operators then, being of form $AA^\dagger$, are trace-class (nuclear) operators, so density states are trace-class operators with trace 1. There are some obvious minor differences with respect to finite dimensions; for instance, the convex set $\mathcal{D}(\mathcal{H})$ of density states is the closed convex hull of the set $\mathcal{D}^1(\mathcal{H})$ of pure states, rather than just the convex hull, etc.

3. Positive maps of convex sets

If K is a convex set in a locally convex topological vector space E, then the set $\mathrm{Pos}(K)$ of those continuous linear maps $\Phi : E \to E$ which map K into K is a convex set in the (real) vector space $\mathcal{L}(E)$ of all continuous linear maps from E into E. We will refer to elements of $\mathrm{Pos}(K)$ as *linear K-positive maps*, or simply *linear positive maps*, if K is determined.

If K is compact, then, due to the Krein–Milman theorem, it is the closed convex hull of the set K^0 of its *extreme points* (points which are not interior points of intervals included in K), $K = \overline{\mathrm{con}}(K^0)$. In this sense, compact convex sets K are completely determined by their extreme points.

However, it should be made clear from the beginning that the concepts of convex set, positive map, etc, are taken from the affine rather than the linear algebra and geometry. In an affine space $\mathbb{E}$, one can subtract points, $x = p - p'$, to get vectors of the model vector space $E = \mathbf{v}(\mathbb{E})$, or add a vector to a point, $p = p' + x$, to get another point, but there is no distinguished point that serves as the origin. More generally, in affine spaces we can take *affine combinations of points*, i.e. combinations $\sum_i \lambda_i p_i$ such that $\sum_i \lambda_i = 1$. If all λ_i are non-negative, the corresponding affine combination is just a *convex combination*. We say that points $p_0, \ldots, p_r \in \mathbb{E}$ are *affinely independent* if none is an affine combination of the others. This is the same as saying that $p_1 - p_0, \ldots, p_r - p_0 \in E$ are linearly independent vectors.

Convex sets in our approach will live in affine spaces. In this sense, the Krein–Milman theorem tells us something about compact convex sets in affine spaces modeled on locally convex linear spaces.

One can think that the problem is artificial, since by choosing a point in an affine space as the origin we end up in the model vector space. However, choosing a point is an additional piece of information put into the scheme which changes our setting. The situation is the same as in a gauge theory, where we can fix a gauge. But a fixed gauge has, in general, no physical interpretation, so we rather try to use gauge-invariant objects.

The second instance of affine space presence is the fact that in many situations, even when we work in a true linear space, it makes much more sense to admit that positive maps are affine. Note that affine maps on an affine hyperspace $\mathbb{E}$ of a linear space $\widehat{\mathbb{E}}$ come exactly from linear maps in $\widehat{\mathbb{E}}$ which preserve $\mathbb{E}$. On the other hand, every affine space (or even affine bundle) $\mathbb{E}$ can be canonically embedded in a linear space (vector bundle) $\widehat{\mathbb{E}}$ as an affine hyperspace (affine hyperbundle). We refer to [21, 22] for the corresponding theory with interesting applications to frame-independent formulations of some problems in analytical mechanics.

Definition 1. *(a) Let $\mathbb{E}_i$ be a real affine space modeled on a locally convex topological real vector space $E_i = \mathbf{v}(\mathbb{E}_i), i = 1, 2$. We say that a map $\Phi : \mathbb{E}_1 \to \mathbb{E}_2$ is an affine map if there is a continuous linear map $v(\Phi) : E_1 \to E_2$ such that for any $p \in \mathbb{E}_1$ and any $x \in E_1$, we have $\Phi(p + x) = \Phi(p) + v(\Phi)(x)$, where $p \mapsto p + x$ is the natural action of E_1 on $\mathbb{E}_1$. The space of affine maps from $\mathbb{E}_1$ to $\mathbb{E}_2$ will be denoted by $\mathfrak{A}(\mathbb{E}_1, \mathbb{E}_2)$. If $\mathbb{E}_1 = \mathbb{E}_2 = \mathbb{E}$, for the space of affine maps on $\mathbb{E}$, i.e. for $\mathfrak{A}(\mathbb{E}, \mathbb{E})$, we will write briefly $\mathfrak{A}(\mathbb{E})$.*

(b) Let $\mathfrak{A}(\mathbb{E})$ be the space of all affine maps on $\mathbb{E}$ and let K be a convex set in $\mathbb{E}$. By positive maps on K (or simply positive maps if there is no ambiguity about K) we understand these affine maps $\Phi \in \mathfrak{A}(\mathbb{E})$ which map K into K. The set of all positive maps on K will be denoted by $\mathfrak{P}(K)$.

(c) By a convex body we will understand a compact convex set K with non-empty interior in a finite-dimensional Euclidean affine space $\mathbb{E}$.

Note that the set $\mathcal{D}(\mathcal{H})$ of density states for quantum systems with a finite number of levels is an example of a convex body, as it is canonically embedded in the Euclidean affine space $u_1^*(\mathcal{H})$ of Hermitian operators with trace 1—an affine hyperspace of $u^*(\mathcal{H})$.

It is easy to see that for a compact convex set K in a finite-dimensional affine space $\mathbb{E}$ the closed convex hull $\overline{\mathrm{con}}(K^0)$ is just the convex hull $\mathrm{con}(K^0)$ if only $K^0 \subset K$ is closed, and that the convex set of positive maps $\mathfrak{P}(K)$ is again a compact convex set, this time in $\mathfrak{A}(\mathbb{E})$. Note that $\mathfrak{A}(\mathbb{E})$ is canonically an affine space modeled on the vector space $\mathfrak{A}(\mathbb{E}, E)$ of affine maps from $\mathbb{E}$ into E. Moreover, if $\mathbb{E}$ is just a vector space, $\mathbb{E} = E$, the space $\mathfrak{A}(E)$ is a vector space with a canonical decomposition $\mathfrak{A}(E) = \mathcal{L}(E) \oplus E$, due to the fact that we can write any affine map $\Phi : E \to E$ uniquely in the form $\Phi(x) = v(\Phi)(x) + x_0$ for some $v(\Phi) \in \mathcal{L}(E)$ and $x_0 \in E$.

3.1. Fix-extreme positive maps

In general, it is not easy to find extreme points $\mathfrak{P}(K)^0$ of the convex set of positive maps $\mathfrak{P}(K)$, even if extreme points of the convex body K are explicitly known. This is exactly the case of the convex bodies $\mathfrak{P}(\mathcal{D}(\mathcal{H}))$ of positive maps in quantum mechanics.

On the other hand, extremality of some positive maps can be established relatively easily in the case of maps with many extreme points in the image, as each extreme point in the image fixes partially the map. This is based on the observation that, for $\Phi \in \mathfrak{P}(K)$, if $p_0 \in K^0$ is the image $p_0 = \Phi(p)$ for some $p \in K$, then $\Phi_i(p) = p_0$ for any Φ_i of a decomposition $\Phi = \sum_i \lambda_i \Phi_i$ into a convex combination of $\Phi_i \in \mathfrak{P}(K)$. Indeed, as $p_0 = \Phi(p) = \sum_i \lambda_i \Phi_i(p)$ is a decomposition of the extreme point p_0 into a convex combination of points $\Phi_i(p) \in K$, then $\Phi_i(p) = p_0$. This immediately implies the following.

Theorem 1. *Let K be a compact convex set in an n-dimensional real affine space. If a positive map $\Phi \in \mathfrak{P}(K)$ has $n + 1$ affinely independent extreme points in the image $\Phi(K)$ of K, then the map Φ is extreme positive, $\Phi \in \mathfrak{P}(K)^0$.*

Proof. Let $q_i \in K, i = 1, \ldots, n + 1$, be such that $p_i = \Phi(q_i)$ are extreme and affinely independent and assume that we have a decomposition $\Phi = t\Phi_0 + (1 - t)\Phi_1$ for certain $\Phi_0, \Phi_1 \in \mathfrak{P}(K)$ and $0 < t < 1$. According to the observation preceding the above theorem, $\Phi_0(q_i) = \Phi_1(q_i) = \Phi(q_i) = p_i$ for all $i + 1, \ldots, n + 1$. But an affine map from an n-dimensional affine space is completely determined by its values on $n + 1$ affinely independent points, so $\Phi_0 = \Phi_1 = \Phi$. □

The extreme positive maps Φ described in the above theorem (with $n + 1$ affinely independent extreme points in the image $\Phi(K)$) will be called *fix-extreme positive maps*.

Corollary 1. *For any convex body K, a positive map Ψ which has all extreme points in $\Psi(K)$ is extreme positive. In particular, the identity map is always an extreme positive map.*

3.2. Example: the closed unit ball in $\mathbb{R}^n$

Theorem 2. *Fix-extreme positive maps of unit balls in Euclidean vector spaces are orthogonal transformations.*

The proof of the above theorem will be based on the following lemma.

Lemma 1. *If the function $F : \mathbb{R}^n \to \mathbb{R}$,*

$$F(x_1, \ldots, x_n) = \sum_{i=1}^{n} (\alpha_i x_i + p_i)^2,$$

where $\alpha_i > 0$ and $p_i \in \mathbb{R}, i = 1, \ldots, n$, has on the unit sphere $S^{n-1} = \{x \in \mathbb{R}^n : \sum_i x_i^2 = 1\}$ local maxima at some $n+1$ affinely independent points $q_1, \ldots, q_{n+1} \in S^{n-1}$, then F is constant on S^{n-1}. In particular, $p_1 = \cdots = p_n = 0$ and $\alpha_1 = \alpha_2 = \cdots = \alpha_n$.

Proof. We will use the method of Lagrange multipliers and consider the function

$$F_\lambda(x_1, \ldots, x_n) = \sum_{i=1}^{n} (\alpha_i x_i + p_i)^2 - \lambda \left(\sum_{i=1}^{n} x_i^2 \right).$$

Since q_j, $j = 1, \ldots, n+1$, are critical points of F, when restricted to the sphere, the coordinates $(x_1, \ldots, x_n)$ of each q_j solve the system of equations

$$\frac{\partial F_\lambda}{\partial x^i}(x) = \left(\alpha_i^2 - \lambda\right)x_i + p_i\alpha_i = 0, \qquad i = 1, \ldots, n, \tag{4}$$

$$\sum_{i=1}^{n} x_i^2 = 1.$$

Moreover, as at q_j we have local maxima, the second derivative of F_λ must be non-positive definite that yields $\alpha_i^2 - \lambda \leqslant 0$ for all i. We can assume that $\alpha_1 \geqslant \alpha_2 \geqslant \cdots \geqslant \alpha_n$, so $\lambda \geqslant \alpha_1^2$.

Assume first that $\lambda > \alpha_1^2$. Then,

$$x_i = \frac{p_i\alpha_i}{\lambda - \alpha_i^2} \tag{5}$$

and

$$G(\lambda) = \sum_{i=1}^{n} \frac{(p_i\alpha_i)^2}{\left(\lambda - \alpha_i^2\right)^2}$$

should be equal to 1. But the function $G(\lambda)$ is monotone with respect to $\alpha_1^2 < \lambda < +\infty$, so there is at most one solution (x, λ_0) of (4) with $\lambda_0 > \alpha_1^2$. There must be therefore at least n additional solutions with $\lambda = \alpha_1^2$. Let k be the number of the biggest α_i, i.e. $\alpha_1 = \alpha_2 = \cdots \alpha_k > \alpha_{k+1}$. We get easily from (4) that

$$b_1 = \cdots = b_k = 0. \tag{6}$$

Hence if $k = n$, then F is constantly α_1^2 on the sphere. It suffices to show now that $k < n$ is not possible. Indeed, if x is a solution of (4) with $\lambda = \alpha_1^2$, we get

$$x_i = \frac{p_i\alpha_i}{\alpha_1^2 - \alpha_i^2}, \qquad i = k+1, \ldots, n,$$

so we can have, together with the solution (5) corresponding to $\lambda > \alpha_1^2$, an affinely independent set of $n + 1$ solutions only if $k = n - 1$. But then, due to (6), the solution (5) must be

$$x = (0, \ldots, 0, sgn(p_n)), \tag{7}$$

so $p_n \neq 0$ and $G(\lambda)$ reduces to

$$G(\lambda) = \frac{(p_n\alpha_n)^2}{\left(\lambda - \alpha_n^2\right)^2}$$

and

$$G(\lambda_0) = \frac{(p_n\alpha_n)^2}{\left(\lambda_0 - \alpha_n^2\right)^2} = 1. \tag{8}$$

On the other hand, the solutions corresponding to $\lambda = \alpha_1^2$ must be of the form

$$\left(x_1, \ldots, x_{n-1}, \frac{p_n\alpha_n}{\alpha_1^2 - \alpha_n^2}\right),$$

so that we have solutions additional to (7) only if

$$\frac{(p_n\alpha_n)^2}{\left(\alpha_1^2 - \alpha_n^2\right)^2} < 1. \tag{9}$$

But, as $\lambda_0 > \alpha_1^2$, the latter contradicts (8):

$$1 = \frac{(p_n\alpha_n)^2}{\left(\lambda_0 - \alpha_n^2\right)^2} < \frac{(p_n\alpha_n)^2}{\left(\alpha_1^2 - \alpha_n^2\right)^2} < 1.$$

Now we can prove theorem 2. □

Proof. Let **B** be the unit ball in an n-dimensional Euclidean vector space E. Let us make an identification of E with $\mathbb{R}^n$ with the standard Euclidean norm

$$\|x\|^2 = \sum_{i=1}^{n} x_i^2.$$

Let Φ be a fix-extreme positive map of $\mathbf{B}$, i.e. $\Phi : \mathbb{R}^n \to \mathbb{R}^n$ is an affine map, $\Phi(x) = A(x)+p'$, where $A \in \mathcal{L}(\mathbb{R}^n)$ is a linear map of $\mathbb{R}^n$ such that $\Phi(\mathbf{B}) \subset \mathbf{B}$ and $\Phi(\mathbf{B})$ has $n + 1$ affinely independent points $\Phi(q'_1), \ldots, \Phi(q'_{n+1})$ in the unit sphere S^{n-1}. Of course, we can assume that $q'_1, \ldots, q'_{n+1}$ are extreme points of $\mathbf{B}$, so they lie on the sphere as well. In particular, the map (matrix) A is invertible.

Now we can apply the singular value decomposition to the matrix A in order to write it in the form $A = O_1 \circ T \circ O_2$, where O_1, O_2 are orthogonal matrices and T is a diagonal matrix with positive entries $\alpha_1, \ldots, \alpha_n > 0$ on the diagonal. Since we can write

$$\Phi(x) = A(x) + b' = O_1 \circ T \circ O_2(x) + b' = O_1(T \circ O_2(x) + b),$$

where $O_1(b) = b'$, and since the orthogonal maps preserve $\mathbf{B}$ and S^{n-1}, the map $\Phi_0(x) = T(x) + b$ has the same properties as Φ: it is a positive map of $\mathbf{B}$, $\Phi_0(\mathbf{B}) \subset \mathbf{B}$ and $\Phi_0(\mathbf{B})$ has $n + 1$ affinely independent points $\Phi_0(q_1), \ldots, \Phi_0(q_{n+1})$ on the unit sphere S^{n-1}, where $q_j = O_2^{-1}(q'_j)$ are points of the sphere, $j = 1, \ldots, n + 1$. This means that the function,

$$F(x) = \|\Phi_0(x)\|^2 = \sum_{i=1}^{n} (\alpha_i x_i + p_i)^2 ,$$

reduced to the unit sphere takes at $q_1, \ldots, q_{n+1}$ local maxima. Applying the above lemma we conclude that $b = 0$ and F is constant on the sphere, so that $\Phi_0 = T$ maps the unit sphere into the unit sphere. Hence, $T = I$ and $\Phi = O_1 \circ O_2$ is orthogonal. □

Remark 1. Theorem 2 can also be derived from the results of [23].

3.3. Example: an extreme map on the plane fixing two extreme points

In this section, we want to present a simple example of an extreme map in two dimensions which is a bijection on its two extreme points. To this end, let us consider the function on the interval $[-1, 1]$,

$$f(x) = \left(\frac{1-x}{2}\right)^2 \left(\frac{1+x}{2}\right)^{1/2} + 2\left(\frac{1-x}{2}\right)^{1/2} \left(\frac{1+x}{2}\right)^{5/2} + \frac{1-x^2}{4}. \quad (10)$$

The function f is concave, hence the subset S of the (x, y) plane bounded by its graph and the interval $[-1, 1]$ is convex. Let us perform a linear transformation of the (x, y) plane,

$$T : (x, y) \mapsto \left(-x, \frac{y}{2}\right). \quad (11)$$

Under this transformation, S is transformed into the set bounded by $[-1, 1]$ and the graph of

$$g(x) = \frac{1}{2} f(-x), \quad (12)$$

i.e.

$$g(x) = \frac{1}{2}\left(\frac{1+x}{2}\right)^2 \left(\frac{1-x}{2}\right)^{1/2} + \left(\frac{1+x}{2}\right)^{1/2} \left(\frac{1-x}{2}\right)^{5/2} + \frac{1-x^2}{8}. \quad (13)$$

Since $f(x) \geqslant g(x)$ for $x \in [-1, 1]$, we have $T(S) \subset S$. Moreover, T is a bijection on two extremal points, $(x, y) = (-1, 0)$ and $(x, y) = (1, 0)$, of S. Observe also that T is an extreme mapping in the sense that for an arbitrary $\alpha \geqslant 1$ there is $x \in [-1, 1]$ such that $f(x) - \alpha g(x) < 0$, i.e. the linear transformation

$$T_\alpha : (x, y) \mapsto \left(-x, \alpha\frac{y}{2}\right) \quad (14)$$

does not map S into S.

The above-described properties of f and g can be established by straightforward calculations. We illustrate them in figures 1–3.

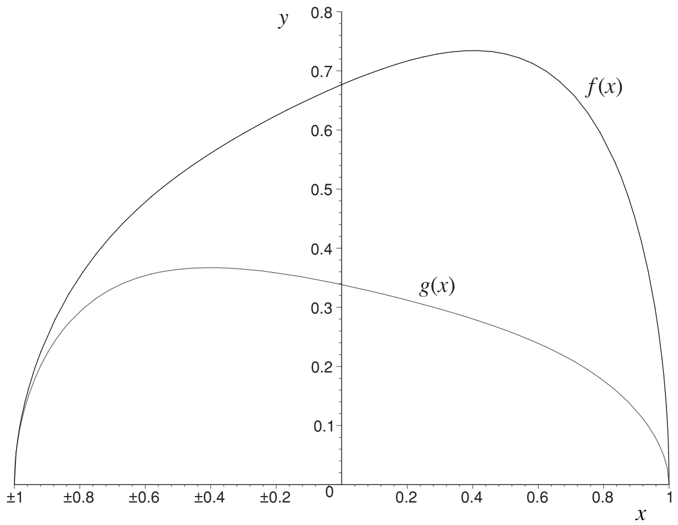

Figure 1. Functions $f(x)$ and $g(x)$.

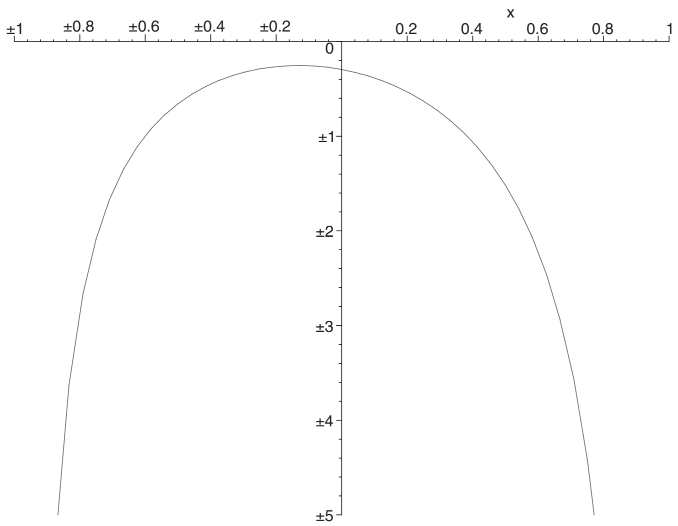

Figure 2. Second derivative of f.

4. Positive maps bijective on pure states—a version of Wigner's theorem

Before we formulate a version of Wigner's theorem [14], let us comment on complex antilinear and antiunitary maps in a Hilbert space. A map $A : \mathcal{H} \to \mathcal{H}$ we call *antilinear* if $A(\alpha x + \beta y) = \bar{\alpha} x + \bar{\beta} y$, where $\bar{\alpha}$ denotes the complex conjugation of $\alpha \in \mathbb{C}$. An antilinear map $U : \mathcal{H} \to \mathcal{H}$ we call *antiunitary* if $\langle Ux|Uy\rangle = \langle y|x\rangle$ for all $x, y \in \mathcal{H}$. The adjoint $A^\dagger$ of an antilinear map is an antilinear map defined *via* the identity

$$\langle Ax|y\rangle = \langle A^\dagger y|x\rangle.$$

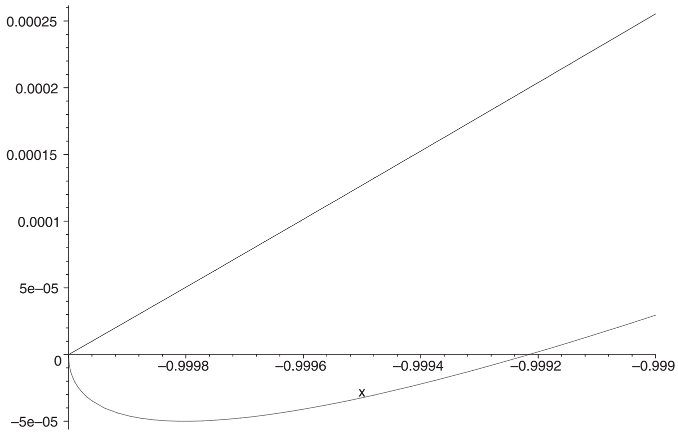

Figure 3. Functions $f - g$ (upper curve) and $f(x) - 1.01 \cdot g(x)$ (lower curve) in the vicinity of $x = -1$.

Any linear (antilinear) map $A : \mathcal{H} \to \mathcal{H}$ induces a linear (resp., antilinear) map $M_A : gl(\mathcal{H}) \to gl(\mathcal{H})$ which on one-dimensional maps $|x\rangle\langle y|$ takes the form $M_A(|x\rangle\langle y|) = |Ax\rangle\langle Ay|$. For linear A we can easily represent the map M_A as $M_A(\rho) = A\rho A^\dagger$, while with antilinear maps the situation is a little bit more complicated.

If an orthonormal basis is chosen, then in the Hilbert space $\mathcal{H}$ we can define a complex conjugation

$$C : \mathcal{H} \to \mathcal{H}, \qquad C^2 = I, \qquad C\left(\sum_i a_i e_i\right) = \sum_i \bar{a}_i e_i.$$

Instead of Cx we will write simply $\bar{x}$. It is clear that $\langle x|y\rangle = \langle \bar{y}|\bar{x}\rangle$. If A is a complex linear map, then $\widetilde{A} = A \circ C$ is antilinear and *vice versa*. Since any continuous complex linear (antilinear) map $A : \mathcal{H} \to \mathcal{H}$ is represented by a (possibly infinite) matrix (a_{ij}), where $A(e_i) = \sum_j a_i^j e_j$, also the transposition $A \mapsto A^T$ is well defined,

$$A^T(e_i) = \sum_j a_j^i e_j,$$

and we extend it to the whole $\mathcal{H}$ by complex linearity (antilinearity). For linear A the adjoint map $A^\dagger$ can then be written as

$$A^\dagger = C \circ A^T \circ C,$$

so that $C \circ A \circ C = A^T$ for the linear Hermitian $A = A^\dagger$. If A is antilinear then $\widetilde{A} = A \circ C$ is linear, so

$$|Ax\rangle\langle Ay| = |\widetilde{A}\bar{x}\rangle\langle \widetilde{A}\bar{y}| = \widetilde{A} \circ |\bar{x}\rangle\langle \bar{y}| \circ (\widetilde{A})^\dagger.$$

But, as easily seen,

$$|\bar{x}\rangle\langle \bar{y}| = C \circ |x\rangle\langle y| \circ C,$$

so that, for Hermitian ρ,

$$M_A(\rho) = \widetilde{A}\rho^T(\widetilde{A})^\dagger. \tag{15}$$

Wigner's theorem (compare with [14]) can now be formulated as follows.

Theorem 3. *Let $\psi : \mathcal{D}^1(\mathcal{H}) \to \mathcal{D}^1(\mathcal{H})$ be a bijection of pure states in a Hilbert space $\mathcal{H}$ preserving the transition probabilities*

$$\langle\psi(\rho_1)|\psi(\rho_2)\rangle_* = \langle\rho_1|\rho_2\rangle_*. \tag{16}$$

Then, there is a unitary $U : \mathcal{H} \to \mathcal{H}$ such that

$$\psi(\rho) = U\rho U^\dagger \quad \text{for all pure states } \rho \tag{17}$$

or

$$\psi(\rho) = U\rho^T U^\dagger \quad \text{for all pure states } \rho, \tag{18}$$

where $\rho \mapsto \rho^T$ is the transposition associated with a choice of an orthonormal basis in $\mathcal{H}$.

The standard versions of Wigner's theorem usually consider (unit) vectors of the Hilbert space rather than pure states. But if x, y are unit vectors representing pure states ρ_1 and ρ_2, respectively, then

$$\langle\rho_1, \rho_2\rangle_* = |\langle x, y\rangle|^2,$$

so that preserving $|\langle x, y\rangle|$ is the same as preserving $\langle\rho_1, \rho_2\rangle_*$. Moreover, any unitary (or antiunitary) action in the Hilbert space, $x \mapsto Ux$, induces on pure states $\rho = |x\rangle\langle x|$ the action (17) or (18). We will call the maps (17) and (18) defined on pure states or on $u^*(\mathcal{H})$ *Wigner maps*. The Wigner maps on $u^*(\mathcal{H})$ can be abstractly characterized as follows.

Theorem 4. *A linear map $\psi : u^*(\mathcal{H}) \to u^*(\mathcal{H})$ is a Wigner map if and only if it is positive and orthogonal.*

Proof. The Wigner maps are clearly positive and orthogonal, so let us assume that ψ has these properties. For all Hermitian ρ_1, ρ_2 we have therefore (16) and we know that $\psi(\rho)$ is positive semi-definite if ρ is. The map ψ is orthogonal, therefore invertible, and its inverse ψ^{-1} is orthogonal as well. Let us observe that ψ^{-1} is also a positive map. Take a pure state ρ and suppose that $\psi^{-1}(\rho)$ has the spectral decomposition $\psi^{-1}(\rho) = \rho_+ - \rho_-$ into a difference of positive semi-definite operators ρ_+, ρ_- which are orthogonal, $\langle\rho_+|\rho_-\rangle_* = 0$. Then ρ is a difference of orthogonal positive semi-definite operators $\rho = \psi(\rho_+) - \psi(\rho_-)$ and, as ρ is a pure state, $\psi(\rho_-)$ (thus ρ_-) must be 0. A similar argument shows that the image $\psi(\rho)$ of any pure state ρ is a positive semi-definite operator which is not decomposable into a sum of orthogonal positive semi-definite operators, so $\psi(\rho)$ is a pure state up to a constant factor. Since

$$\mathrm{Tr}(\psi(\rho)^2) = \langle\psi(\rho)|\psi(\rho)\rangle = \langle\rho|\rho\rangle = 1,$$

this factor equals 1, and we conclude that ψ induces a bijection on pure states. □

We will now prove a theorem which extends Wigner's theorem and relates it to the problem of extreme positive maps.

Let $u^*_f(\mathcal{H})$ be the linear subspace of $u^*(\mathcal{H})$ consisting of Hermitian finite-rank operators. For $K_1, K_2 \subset u^*_1(\mathcal{H})$ we say that a map $\psi : K_1 \to K_2$ is *affine* if ψ is the restriction on K_1 of a trace-preserving linear map $\Phi : \langle K_1\rangle \to \langle K_2\rangle$ from the linear span $\langle K_1\rangle$ of K_1 in $u^*(\mathcal{H})$ into the linear span $\langle K_2\rangle$ of K_2 in $u^*(\mathcal{H})$, $\Phi(K_1) \subset K_2$.

Theorem 5. *Let $\psi : \mathcal{D}^1(\mathcal{H}) \to \mathcal{D}^1(\mathcal{H})$ be a bijective map. The following are equivalent:*

- *ψ is affine;*
- *ψ preserves transition probabilities between pure states;*
- *ψ is a Wigner map.*

If any (or all) of these cases is satisfied, there is a unique continuous affine extension $\Psi : u_1^*(\mathcal{H}) \to u_1^*(\mathcal{H})$ *of* ψ *which is extreme positive,* $\Psi \in \mathfrak{P}(\mathcal{D}(\mathcal{H}))^0$.

Proof. $(a) \Rightarrow (b)$. Since $u_f^*(\mathcal{H})$ is spanned by the set $\mathcal{D}^1(\mathcal{H})$ of pure states, let $\Phi : u_f^*(\mathcal{H}) \to u_f^*(\mathcal{H})$ be the (unique) linear trace-preserving map on the space $u_f^*(\mathcal{H})$ of finite-rank Hermitian operators inducing ψ on $\mathcal{D}^1(\mathcal{H})$. Since Φ maps convex combinations into convex combinations, Φ maps finite-rank density states into finite-rank density states, so Φ is a positive map. We will prove that Φ is a linear isomorphism on $u_f^*(\mathcal{H})$. This follows from the fact that Φ preserves the rank, i.e. induces a bijection on $\mathcal{D}^k(\mathcal{H})$ for each $k = 1, 2, \ldots$.

To see the latter, let us remark that the rank, $\mathrm{rank}(\rho)$, of $\rho \in u_f^*(\mathcal{H})$ is defined as a minimal number of pure states whose linear combination is ρ, so that, as Φ is linear and is a bijection on pure states, $\mathrm{rank}(\Phi(\rho)) \leqslant \mathrm{rank}(\rho)$. Conversely, if $\rho \in \mathcal{D}(\mathcal{H})$ is of rank k, then it is a convex combination of some pure states $\rho_1, \ldots, \rho_k$, thus the image by Φ of a convex combination of pure states $\Phi^{-1}(\rho_1), \ldots, \Phi^{-1}(\rho_k)$. This shows that $\mathcal{D}^k(\mathcal{H}) \subset \Phi(\mathcal{D}^k(\mathcal{H}))$. The linear map Φ induces a bijection on $\mathcal{D}^1(\mathcal{H})$, so assume inductively that it induces a bijection on $\mathcal{D}^l(\mathcal{H})$ for $l \leqslant k$. Let now $\rho \in u_f^*(\mathcal{H})$ be of rank $k+1$, $\rho \in \mathcal{D}^{k+1}(\mathcal{H})$, with the spectral decomposition $\rho = \sum_{i=0}^k \lambda_i \rho_i$, with $\lambda_i > 0$, $\sum_i \lambda_i = 1$ and $\rho_i = |x_i\rangle\langle x_i|$ being pairwise orthogonal pure states, $\langle x_i|x_j\rangle = 0, i \neq j$. We must show that the rank of $\Phi(\rho)$ is $k+1$.

Suppose the contrary. Hence, according to the inductive assumption, $\rho' = \Phi(\rho)$ is of rank k. As $\rho = \lambda_0\rho_0 + \widetilde{\rho}$, where $\widetilde{\rho} = \sum_{i=1}^k \lambda_i \rho_i$, thus $\widetilde{\rho}' = \Phi(\widetilde{\rho})$ is of rank k, the image of $\Phi(\rho_0) = |x_0'\rangle\langle x_0'|$, thus x_0' belongs to the image of $\widetilde{\rho}'$. Consider the spectral decomposition $\widetilde{\rho}' = \sum_{i=1}^k \lambda_i'\rho_i'$, with $\lambda_i' > 0$, $\sum_i \lambda_i' = 1$, and $\rho_i' = |x_i'\rangle\langle x_i'|$ being pairwise orthogonal pure states, $\langle x_i'|x_j'\rangle = 0, i \neq j$. Let $\mathcal{H}_0$ (resp., $\mathcal{H}_0'$) be the subspace in $\mathcal{H}$ spanned by the vectors $x_1, \ldots, x_k$ (resp., $x_1', \ldots, x_k'$) and let $\mathcal{D}^1(\mathcal{H}_0)$ (resp., $\mathcal{D}^1(\mathcal{H}_0')$) be the set of all pure states of $\mathcal{H}_0$ (resp., $\mathcal{H}_0'$), i.e. those pure states from $\mathcal{D}^1(\mathcal{H})$ which are represented by unit vectors from $\mathcal{H}_0$ (resp., $\mathcal{H}_0'$). It is now clear that $\rho_0' = \Phi(\rho_0) \in \mathcal{D}^1(\mathcal{H}_0')$. Note that pure states η from $\mathcal{D}^1(\mathcal{H}_0')$ can be characterized as such pure states which added to $\widetilde{\rho}'$ do not change the rank, $\mathrm{rank}(\widetilde{\rho}' + \eta) = \mathrm{rank}(\widetilde{\rho}') = k$. According to the inductive assumption, this implies that $\mathrm{rank}(\widetilde{\rho} + \Phi^{-1}(\eta)) = k$ as well, but

$$\mathrm{rank}(\widetilde{\rho} + \Phi^{-1}(\rho_0')) = \mathrm{rank}(\widetilde{\rho} + \rho_0) = \mathrm{rank}(\rho) = k + 1,$$

which is a contradiction.

Since we know now that Φ induces bijections on each $\mathcal{D}^k(\mathcal{H})$, $k = 1, 2, \ldots$, it is easy to conclude that it is a rank-preserving isomorphism, so that Φ^{-1} is also a positive map. Indeed, as $\mathcal{D}^1(\mathcal{H})$ spans $u_f^*(\mathcal{H})$, it is clearly 'onto'. It is also injective, since $\Phi(\lambda\rho - \lambda'\rho') = 0$, where $\lambda, \lambda' > 0$ and $\rho, \rho' \in \mathcal{D}(\mathcal{H})$ are density states of finite ranks, implies (Φ is positive) that $\Phi(\rho) = \Phi(\rho') = 0$, thus $\rho = \rho' = 0$, as Φ preserves the rank of density states.

To finish the proof, we will need the following lemma.

Lemma 2. *Let* $\rho \in \mathcal{D}(\mathcal{H})$ *be a density state of a finite rank k. Then the square of the Hilbert–Schmidt norm* $\|\rho\|_*^2 = \mathrm{Tr}(\rho^2)$ *can be characterized as the maximum of the expressions* $\sum_{i=1}^k \lambda_i^2$ *over all decompositions* $\rho = \sum_{i=1}^k \lambda_i \rho_i$ *of* ρ *as a convex combination of k pure states* $\rho_1, \rho_2, \ldots, \rho_k$. *This maximum is associated with the spectral decomposition.*

Proof. As

$$\mathrm{Tr}(\rho^2) = \sum_i \lambda_i^2 + 2\sum_{i\neq j} \lambda_i\lambda_j \,\mathrm{Tr}(\rho_i\rho_j) \tag{19}$$

and

$$\sum_{i\neq j} \lambda_i\lambda_j \,\mathrm{Tr}(\rho_i\rho_j) \geqslant 0, \tag{20}$$

we have

$$\|\rho\|_*^2 \geqslant \sum_{i=1}^{k} \lambda_i^2. \tag{21}$$

Moreover, we have equality in (21) if and only if we have equality in (20), so as all $\lambda_i > 0$, if and only if $\langle\rho_i|\rho_j\rangle_* = \mathrm{Tr}(\rho_i\rho_j) = 0$ for all $i \neq j$. This corresponds to the spectral decomposition. □

The above lemma implies that the map Φ preserves the Hilbert–Schmidt norm of density states. Indeed, if we use the spectral decomposition to write ρ as a convex combination $\rho = \sum_{i=1}^{k} \lambda_i\rho_i$ of pure states, then $\Phi(\rho)$ can be expressed as a convex combination of pure states $\Phi(\rho) = \sum_{i=1}^{k} \lambda_i\Phi(\rho_i)$ with the same coefficients, so that $\|\Phi(\rho)\|_*^2 \geqslant \sum_i \lambda_i^2 = \|\rho\|_*^2$. But we can apply the above consideration to Φ^{-1} instead of Φ and get $\|\Phi^{-1}(\eta)\|_*^2 \geqslant \|\eta\|_*^2$ for any density state of rank k, in particular for $\eta = \Phi(\rho)$. We get therefore $\|\Phi(\rho)\|_*^2 = \|\rho\|_*^2$.

Let us now take two pure states ρ_1, ρ_2 and consider $\rho = \frac{1}{2}(\rho_1 + \rho_2)$. Since, according to (19),

$$\|\rho\|_*^2 = \tfrac{1}{2}(1 + \langle\rho_1|\rho_2\rangle_*)$$

and

$$\|\rho\|_*^2 = \|\Phi(\rho)\|_*^2 = \|\tfrac{1}{2}(\Phi(\rho_1) + \Phi(\rho_1))\|_*^2,$$

we have

$$\tfrac{1}{2}(1 + \langle\rho_1|\rho_2\rangle_*) = \tfrac{1}{2}(1 + \langle\Phi(\rho_1)|\Phi(\rho_2)\rangle_*),$$

thus

$$\langle\rho_1|\rho_2\rangle_* = \langle\Phi(\rho_1)|\Phi(\rho_2)\rangle_* = \langle\psi(\rho_1)|\psi(\rho_2)\rangle_*,$$

so ψ preserves transition probabilities between pure states.

$(b) \Rightarrow (c)$ is Wigner's theorem.

$(c) \Rightarrow (a)$ is obvious.

Moreover, ψ has an obvious unique continuous extension $\Psi : u_1^*(\mathcal{H}) \to u_1^*(\mathcal{H})$, $\Psi(\rho) = U\rho U^\dagger$ or $\Psi(\rho) = U\rho^T U^\dagger$. Since Ψ is positive and has all extreme points in its image, it is extreme positive according to the obvious infinite-dimensional version of corollary 1. □

If the dimension of the Hilbert space $\mathcal{H}$ is n, then the dimension of the affine space $u_1^*(\mathcal{H})$ of Hermitian operators with trace 1 equals $n^2 - 1$, and we know from the general theory (theorem 1) that a positive map $\Phi \in \mathfrak{P}(\mathcal{D}(\mathcal{H}))$ possessing n^2 pure states in the image $\Phi(\mathcal{D}(\mathcal{H}))$ of $\mathcal{D}(\mathcal{H})$ is extreme positive (we called such positive maps fix-extreme). We finish this section with the following conjecture motivated by theorem 2.

Conjecture 1. *Any fix-extreme positive map $\Phi \in \mathfrak{P}(\mathcal{D}(\mathcal{H}))^0$ is a Wigner map.*

5. Completely positive maps acting on pure states

A linear map $A : u^*(\mathcal{H}) \to u^*(\mathcal{H})$ is called *completely positive* (CP) if $A \otimes I_N : u^*(\mathcal{H}) \otimes M_N \to u^*(\mathcal{H}) \otimes M_N$, where M_N is the algebra of complex $N \times N$ matrices, is positivity-preserving for all N. It was shown by Choi [24] and Kraus [25] that each CP map admits a representation in the so-called Kraus form

$$A\rho = \sum_{i=1}^{s} V_i^\dagger \rho V_i, \tag{22}$$

where V_k are operators acting on $\mathcal{H}$.

Definition 2. *We say that a CP operator (22) acting on Hermitian operators of a Hilbert space $\mathcal{H}$ is extreme if any decomposition, $A = A_1 + \cdots + A_r$, into a sum of CP operators $A_1, \ldots, A_r$ is irrelevant, i.e. all the operators $A_1, \ldots, A_r$ are proportional to A, $A_k = a_k A$, for some $a_k \in \mathbb{R}_+$. In particular, all operators V_i are proportional and A can be written as a single Kraus operator*

$$A\rho = V^\dagger \rho V.$$

Not to deal with the cone of CP operators but rather with a compact convex set (if the dimension of $\mathcal{H}$ is finite), one has to give certain normalization conditions. We can try to use, for instance, the trace $\mathrm{Tr}(A)$ of a CP operator (22) as a linear operator on the complex vector space $gl(\mathcal{H})$ which is the same as the trace of (22) as an operator on the real vector space $u^*(\mathcal{H})$ of Hermitian operators.

Theorem 6. *If A is a CP operator in the form (22) then*

$$\mathrm{Tr}(A) = \sum_{i=1}^{s} |\mathrm{Tr}(V_i)|^2. \tag{23}$$

Proof. It suffices to prove (23) for a single Kraus map $A = M_V$. Choose an orthonormal basis $\{e_i\}$ in $\mathcal{H}$ and write V in this basis as a complex matrix $V = (v_{ij})$. As an orthonormal basis in $gl(\mathcal{H})$ we can take $\rho_{jk} = |e_j\rangle\langle e_k|$. We have

$$\begin{aligned}\mathrm{Tr}\,(M_V) &= \sum_{j,k} \langle \rho_{jk} | V^\dagger \rho_{jk} V\rangle = \sum_{j,k} \mathrm{Tr}(\rho_{kj} V^\dagger \rho_{jk} V) \\ &= \sum_{j,k} \langle e_k | \rho_{kj} V^\dagger \rho_{jk} V e_k\rangle = \sum_{j,k} \bar{v}_{jj} v_{kk} = |\mathrm{Tr}(V)|^2. \qquad \square\end{aligned}$$

As we can see, the trace can vanish for nonzero CP operators which makes the normalization by trace impossible. There is, however, another possibility of normalizing CP operators provided by the *Jamiołkowski isomorphism* [26]

$$\mathcal{J} : gl(gl(\mathcal{H})) \to gl(gl(\mathcal{H})). \tag{24}$$

The Jamiołkowski isomorphism maps the operator $M_A^B(\rho) = A\rho B^\dagger$ into the rank-1 operator $|A\rangle\langle B|$. In particular, CP operators correspond, *via* the Jamiołkowski isomorphism $\mathcal{J}$, to positive semi-definite operators on $gl(\mathcal{H})$ (see, for instance, [20]). Any Kraus operator $M_V(\rho) = V\rho V^\dagger$ corresponds to the one-dimensional Hermitian operator $|V\rangle\langle V|$. The spectral decomposition of $\mathcal{J}(A)$ results in the decomposition (22) with V_i being mutually orthogonal with respect to the Hilbert–Schmidt product $\mathrm{Tr}(A^\dagger B)$ in $gl(\mathcal{H})$. Such a decomposition of a CP operator will be called a *spectral decomposition*. We will call a CP operator *normalized* if it corresponds, *via* the Jamiołkowski isomorphism, to a trace-one operator. If (22) is a spectral decomposition of a CP operator, then it is normalized if

$$\mathrm{Tr}\left(\sum_{i=1}^{s} V_i^\dagger V_i\right) = 1.$$

We will call $\mathrm{Tr}_s(A) = \mathrm{Tr}\big(\sum_{i=1}^s V_i^\dagger V_i\big)$ the *spectral trace* of a CP operator A. The spectral trace is greater than or equal to 0 and equals 0 only if $A = 0$. We will denote by $NCP(\mathcal{H})$ the convex set of normalized CP operators on $gl(\mathcal{H})$. It is clear that extreme points in $NCP(\mathcal{H})$ are exactly single normalized Kraus maps.

From now on, we assume the Hilbert space $\mathcal{H}$ to be of a finite dimension n.

Recall that on the space of Hermitian operators on $\mathcal{H}$ we have a canonical scalar product $\langle\rho, \rho'\rangle_* = \mathrm{Tr}\,\rho\rho'$ and that $\mathcal{P}(\mathcal{H})$ denotes the cone of positive semi-definite operators. We will call elements $\rho_1, \ldots, \rho_k$, $k \geqslant n$, of $\mathcal{P}(\mathcal{H})$ to be *in general position* if for any nonzero $\rho \in \mathcal{P}(\mathcal{H})$ we cannot find n of them which are orthogonal to ρ. If ρ_i are of rank 1, $\rho_i = |x_i\rangle\langle x_i|$, where $|x_i\rangle \in \mathcal{H}$, this simply means that any n vectors of $|x_1\rangle, \ldots, |x_k\rangle$ form a linear basis in $\mathcal{H}$.

Theorem 7. *The following statements are equivalent:*

(a) A is invertible and A^{-1} is a CP operator.
(b) A is invertible and extreme, i.e.

$$A\rho = V^\dagger \rho V$$

with V—invertible.
(c) For any set of pure states $\rho_1, \ldots, \rho_{n+1}$ in general position, $A\rho_1, \ldots, A\rho_{n+1}$ are operators of rank 1 in general position.
(d) In the image $A(P(\mathcal{H}))$, there are $n + 1$ rank-1 operators in general position.
(e) There exists a set of pure states $\rho_1, \ldots, \rho_{n+1}$ in general position such that $A\rho_1, \ldots, A\rho_{n+1}$ are operators of rank 1 in general position.

Proof. (a) $\Rightarrow$ (b). It was proven in [27] (theorem 7).

(b) $\Rightarrow$ (c). If $\rho = |x\rangle\langle x|$ then $V^\dagger\rho V = |V^\dagger x\rangle\langle V^\dagger x|$, hence A maps pure states into rank-1 operators, and V, being invertible, preserves all linear independencies.

(c) $\Rightarrow$ (d)—trivial.

(d) $\Rightarrow$ (e). Let $\rho_1, \ldots, \rho_{n+1} \in P(\mathcal{H})$ be positive semi-definite operators such that $\eta_j = A\rho_j$, $j = 1, \ldots, n+1$, are rank-1 operators in general position. First, let us remark that we can assume that ρ_j are density states, since proportionality plays no role here. Second, we can assume further that they are pure. Indeed, if ρ is a state with the spectral decomposition $\rho = \sum_k a_k\xi_k$ into a convex combination of pure states ξ_k and if $A\rho = \eta$ is a rank-1 positive semi-definite operator, then $\eta = A\rho = \sum_k a_k A\xi_k$ is a convex combination of rank-1 positive semi-definite operators $A\xi_k$, so η is positively proportional to $A\xi_k$ for all k, since pure states are extreme points in the convex body of all states. By a similar argument, all states $V_i^\dagger\rho_j V_i$, $i = 1, \ldots, s$, are proportional to η_j, say $V_i^\dagger\rho_j V_i = \beta_j\eta_j$, where, of course, $\sum_{i=1}^s \beta_i^j = 1$.

Let us write $\rho_j = |x_j\rangle\langle x_j|$, $\eta_j = |y_j\rangle\langle y_j|$, $j = 1, \ldots, n+1$, for some vectors $|x_j\rangle, |y_j\rangle$. We claim that the states $\rho_1, \ldots, \rho_{n+1}$ are in general position, i.e. any n among the vectors $|x_1\rangle, \ldots, |x_{n+1}\rangle$ are linearly independent.

For, assume the contrary, i.e. that, say, $|x_1\rangle, \ldots, |x_n\rangle$ are linearly dependent. Hence, one of the vectors, say $|x_n\rangle$, can be written as a linear combination $|x_n\rangle = b_1|x_1\rangle + \cdots b_{n-1}|x_{n-1}\rangle$. Since $V_i^\dagger\rho_j V_i = |V_i^\dagger x_j\rangle\langle V_i^\dagger x_j|$ is proportional to $\eta_j = |y_j\rangle\langle y_j|$, the vector $|V_i^\dagger x_j\rangle$ is proportional to $|y_j\rangle$ for $j = 1, \ldots, n+1$. In particular, all the vectors $|V_i^\dagger x_j\rangle$ with $i = 1, \ldots, s$ and $j = 1, \ldots, n-1$, belong to the linear span $\mathrm{span}\langle|y_1\rangle, \ldots, |y_{n-1}\rangle\rangle$ of the vectors $|y_1\rangle, \ldots, |y_{n-1}\rangle$. Therefore

$$V_i^\dagger|x_n\rangle = b_1 V_i^\dagger|x_1\rangle + \cdots + b_{n-1}V_i^\dagger|x_{n-1}\rangle \in \mathrm{span}\langle|y_1\rangle, \ldots, |y_{n-1}\rangle\rangle.$$

Since $V_i^\dagger|x_n\rangle$ is proportional to $|y_n\rangle$, and $|y_1\rangle, \ldots, |y_n\rangle$ are linearly independent, we have $V_i^\dagger|x_n\rangle = 0$ for all $i = 1, \ldots, s$. But this contradicts the property $A\rho_n = \eta_n$, i.e. $\sum_{i=1}^s V_i^\dagger|x_n\rangle = |y_n\rangle$.

(e) $\Rightarrow$ (a). Put $\rho_j = |x_j\rangle\langle x_j|, \eta_j = A\rho_j = |y_j\rangle\langle y_j|$ for some $|x_j\rangle, |y_j\rangle \in \mathcal{H}$, $j = 1, \ldots, n+1$. Since $\eta_j = A\rho_j$ is of rank 1, all the positive semi-definite operators $V_i^\dagger \rho_j V_i$ of its decomposition,

$$\eta_j = \sum_{i=1}^s V_i^\dagger \rho_j V_i,$$

must be proportional to η_j, $V_i^\dagger \rho_j V_i \sim \eta_j$. This, in turn, means that $V_i^\dagger|x_j\rangle$ are proportional to $|y_j\rangle$,

$$V_i^\dagger|x_j\rangle = \alpha_i^j|y_j\rangle, \qquad i = 1, \ldots, s, \qquad j = 1, \ldots, n+1.$$

As any n vectors of $|x_1\rangle, \ldots, |x_{n+1}\rangle$ are linearly independent, all the coefficients a_j of the decomposition

$$|x_{n+1}\rangle = a_1|x_1\rangle + \cdots + a_n|x_n\rangle$$

are nonzero, $a_j \neq 0$. Since

$$V_i^\dagger|x_{n+1}\rangle = a_1 V_i^\dagger|x_1\rangle + \cdots + a_n V_i^\dagger|x_n\rangle = a_1\alpha_i^1|y_1\rangle + \cdots + a_n\alpha_i^n|y_n\rangle$$

are proportional to $|y_{n+1}\rangle$ and $|y_{n+1}\rangle$ has a decomposition $|y_{n+1}\rangle = b_1|y_1\rangle + \cdots + b_n|y_n\rangle$ into a linear combination of linearly independent $|y_1\rangle, \ldots, |y_n\rangle$, the vector $\left(\alpha_i^1, \ldots, \alpha_i^n\right) \in \mathbb{C}^n$ must be proportional to $(a_1/b_1, \ldots, a_n/b_n) \in \mathbb{C}^n$. In consequence, it means that the operators $V_i^\dagger$ are proportional to the operator $V^\dagger$ uniquely defined by the conditions

$$V^\dagger|x_j\rangle = \frac{b_j}{a_j}|y_j\rangle.$$

Hence

$$A\rho = \beta V^\dagger \rho V$$

for some $\beta \in \mathbb{R}_+$ and, clearly, $\beta \neq 0$. □

Remark 2. It is not enough to take only n pure states $\rho_1, \ldots, \rho_n$. Let us take, for example, V_i diagonal, $V_i = \operatorname{diag}\left(\lambda_i^1, \ldots, \lambda_i^n\right)$, $\lambda_j^k \neq 0$, and not proportional. If now $\lambda_i^1 = \lambda_i^2$, we have an infinite set of pure states that are mapped to rank-1 operators and any n of them are not in general position, but $A = \sum_{i=1}^s V_i^\dagger \rho V_i$ is not extreme.

Corollary 2. *If a CP operator*

$$A\rho = \sum_{i=1}^s V_i^\dagger \rho V_i \tag{25}$$

is trace-preserving (resp., unity-preserving) and such that the image of density states $A(\mathcal{D})$ *contains* $n+1$ *pure states in general position, then* A *is unitary,* $A\rho = U^\dagger \rho U$.

Proof. It is enough to make use of theorem 7 and observe that trace-preserving (unity-preserving) yields $VV^\dagger = I$ (resp., $V^\dagger V = I$), so V is unitary. □

6. Extreme bistochastic CP maps

Extreme unity-preserving CP maps have been described by Man-Duen Choi [24]. We can reformulate his result as follows.

Theorem 8. *Let $NCP_I(\mathcal{H})$ (resp., $NCP_{\mathrm{Tr}}(\mathcal{H})$) be the convex body of normalized unity-preserving (resp. trace-preserving) CP maps on $gl(\mathcal{H})$. Then $A \in NCP_I(\mathcal{H})$ (resp. $A \in NCP_{\mathrm{Tr}}(\mathcal{H})$), with the spectral decomposition*

$$A\rho = \sum_{i=1}^{s} V_i^\dagger \rho V_i \tag{26}$$

is extreme if and only if the operators $\{V_i^\dagger V_j : i, j = 1, \ldots, s\}$ (resp., $\{V_i V_j^\dagger : i, j = 1, \ldots, s\}$) are linearly independent in $gl(\mathcal{H})$.

Proof. We will sketch a proof making use of the Jamiołkowski isomorphism (24) which associates with the CP map (26) the Hermitian operator

$$\mathcal{J}(A) = \sum_{i=1}^{s} |V_i^\dagger\rangle\langle V_i^\dagger|$$

on $gl(\mathcal{H})$. Extreme normalized CP operators correspond therefore, *via* the Jamiołkowski isomorphism, to pure states on the Hilbert space $gl(\mathcal{H})$. On the space $u^*(gl(\mathcal{H}))$ of Hermitian operators acting on the Hilbert space $gl(\mathcal{H})$, in turn, we can define two canonical $\mathbb{R}$-linear maps $F_1, F_2 : u^*(gl(\mathcal{H})) \to u^*(\mathcal{H})$ which associate with rank-1 operators $|V\rangle\langle V|$ the operators $F_1(|V\rangle\langle V|) = VV^\dagger$ and $F_2(|V\rangle\langle V|) = V^\dagger V$, respectively. The unity-preserving CP operators A correspond therefore to Hermitian operators constrained by the equations $F_1(\mathcal{J}(A)) = I$. The corresponding extreme points $\mathcal{J}(A) \in u^*(gl(\mathcal{H}))$ need not be pure states. It suffices that the level sets of I of the linear constraint F_1 are transversal to the face of the point, i.e. the function F_1 has the trivial kernel on the tangent space $T_{\mathcal{J}(A)}$ of the face at $\mathcal{J}(A)$. But this tangent space is known (see, e.g., [7, 27]) to consists of all Hermitian operators with the range equal to the range of $\mathcal{J}(A)$, i.e. the operators of the form $\sum_{i,j} \lambda^{ij} |V_i^\dagger\rangle\langle V_j^\dagger|$, where (λ^{ij}) is a Hermitian matrix. Hence A is extremal in $NCP_I(\mathcal{H})$ if and only if

$$F_1\left(\sum_{i,j} \lambda^{ij} |V_i^\dagger\rangle\langle V_j^\dagger|\right) = \sum_{i,j} \lambda^{ij} V_i^\dagger V_j \neq 0 \in u^*(\mathcal{H}) \tag{27}$$

for all Hermitian $(\lambda^{ij}) \neq 0$. As we can decompose any operator into the sum of a Hermitian and an antiHermitian, we can rewrite (27) in $gl(\mathcal{H})$ instead of $u^*(\mathcal{H})$ using an arbitrary complex matrix $(\lambda^{ij}) \neq 0$. This is nothing but the complex linear independence of the operators $\{V_i^\dagger V_j : i, j = 1, \ldots, s\}$ in $gl(\mathcal{H})$. For trace-preserving CP operators, the reasoning is identical with the function F_2 replacing F_1. □

The maps from $NCP_*(\mathcal{H}) = NCP_I(\mathcal{H}) \cap NCP_{\mathrm{Tr}}(\mathcal{H})$ are sometimes called *bistochastic*. The above understanding of Choi's result gives us easily a characterization of extreme bistochastic maps.

Theorem 9. *A bistochastic map $A \in NCP_*(\mathcal{H})$ with the spectral decomposition*

$$A\rho = \sum_{i=1}^{s} V_i^\dagger \rho V_i$$

is extreme if and only if the operators $\{V_i^\dagger V_j \oplus V_i V_j^\dagger : i, j = 1, \ldots, s\}$ *are linearly independent in* $gl(\mathcal{H} \oplus \mathcal{H})$.

Proof. The proof is analogous to the above one with the difference that our constraint function is now

$$(F_1, F_2) : u^*(gl(\mathcal{H})) \to u^*(\mathcal{H}) \times u^*(\mathcal{H}) \simeq u^*(\mathcal{H}) \oplus u^*(\mathcal{H}).$$

The condition (27) is therefore replaced by the condition

$$\sum_{i,j} \lambda^{ij} V_i^\dagger V_j \neq 0 \quad \text{or} \quad \sum_{i,j} \lambda^{ij} V_i V_j^\dagger \neq 0 \quad \text{for all Hermitian } (\lambda^{ij}) \neq 0.$$

We can rewrite it as

$$\sum_{i,j} \lambda^{ij} \left(V_i^\dagger V_j \oplus V_i V_j^\dagger \right) \neq 0$$

and pass to an arbitrary complex $(\lambda^{ij}) \neq 0$ like before. □

7. Examples

Let us illustrate some of the previous reasonings and results in the simplest cases of maps on states on two- and three-dimensional spaces. In the following subsection, we show three examples of extreme maps: a generic one possessing exactly two pure states in its image, a non-generic one with only one pure state in the image and an extreme map having a continuous family of pure states in the image. The last one, according to theorem 2, is not completely positive but a merely positive extreme map. Note that these cases have also been considered in [29].

In the second subsection, we give an example of an extreme completely positive map acting on $\mathbb{C}^{3\times3}$ which does not have any pure state in its image. Such a situation is impossible for maps acting on qubits (i.e., maps on $\mathbb{C}^{2\times2}$).

7.1. *Extreme completely positive, positive, stochastic and bistochastic maps for* $n = 2$

A state on $\mathbb{C}^2$ can be parameterized by a unit vector $(x, y, z) \in \mathbb{R}^3$

$$\rho = \tfrac{1}{2}(I + x\sigma_1 + y\sigma_2 + z\sigma_3), \tag{28}$$

where

$$\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \qquad \sigma_2 = \begin{bmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{bmatrix}, \qquad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{29}$$

A positive trace-preserving map

$$\rho \mapsto \rho' = \tfrac{1}{2}(I + x'\sigma_1 + y'\sigma_2 + z'\sigma_3) \tag{30}$$

is thus determined (up to rotations which are irrelevant from the point of view of this paper) by four parameters $\lambda_1, \lambda_2, \lambda_3, t$, such that

$$x' = \lambda_1 x, \qquad y' = \lambda_2 y, \qquad z' = \lambda_3 z + t. \tag{31}$$

The parameters $\lambda_1, \lambda_2, \lambda_3, t$ must fulfill particular conditions to ensure the positivity of the map (see [28, 29] for details).

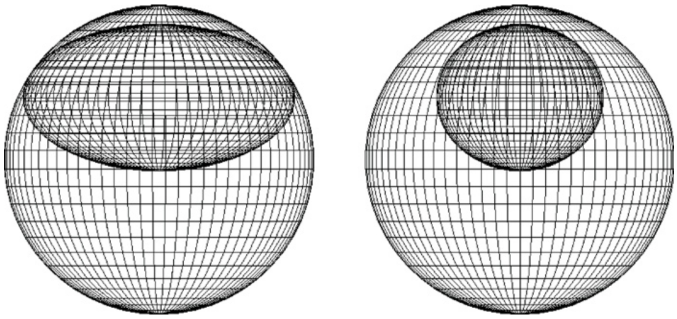

Figure 4. An extreme CP map having exactly two pure states in the image. Projections along two perpendicular axes.

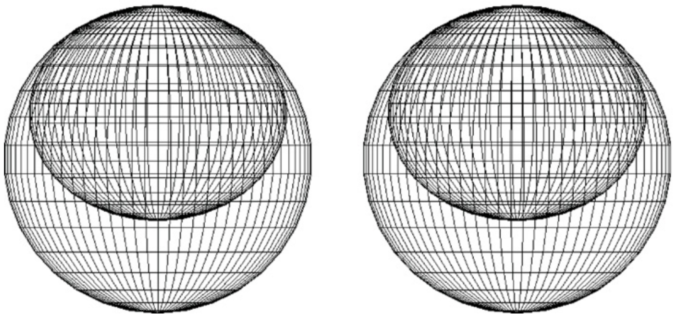

Figure 5. An extreme CP map having exactly one pure state in the image. Projections along two perpendicular axes.

The image of the unit sphere $x^2 + y^2 + z^2 = 1$ under (30) is the ellipsoid

$$\left(\frac{x}{\lambda_1}\right)^2 + \left(\frac{y}{\lambda_2}\right)^2 + \left(\frac{z-t}{\lambda_3}\right)^2 = 1. \tag{32}$$

Obviously, for a positive map (30) the ellipsoid is inside the unit sphere. For extreme maps it has to have points on its surface common with the surface of the unit sphere (i.e., some pure states are mapped into pure states). For extreme CP maps, two possibilities occur [29]:

(1) $\lambda_1 = \cos(u), \lambda_2 = \cos(v), \lambda_3 = \cos(u)\cos(v), t = \sin(u)\sin(v), < 0 < u < v$. In this case the ellipsoid (32) has three different axes and it touches the unit sphere at two points (see figure 4).

(2) $\lambda_1 = \lambda_2 = \cos(u), \lambda_3 = \cos^2(u), t = \sin^2(u)$, in which case the ellipsoid (32) touches the unit sphere at a single point $x = y = 0, z = 1$ (see figure 5).

(3) Geometrically it is obvious that without upsetting the extremality of the map we can make the ellipsoid (32) touch the unit sphere along a full circle (see figure 6). In this case

$$\lambda_1 = \lambda_2 = \sqrt{1 - \cos^2(u)\cos^2(v)},$$
$$\lambda_3 = \sin(u)\sqrt{1 - \cos^2(u)\cos^2(v)},$$
$$t = \sin(u)\sin^2(v).$$

For $u \neq 0 \neq v$, the map is definitely not a unitary one (its image is a proper subset of the unit sphere) and in its image there are more than three pure states (in fact the whole

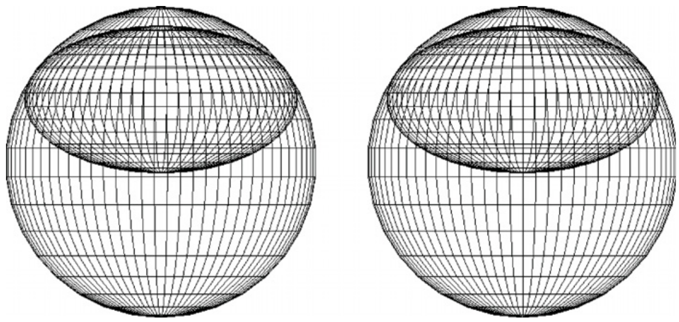

Figure 6. An extreme positive map having a continuous family of pure states in its image. Projections along two perpendicular axes.

circle of states at which the ellipsoid touches the unit sphere). From theorem 2, it thus follows that the map cannot be a completely positive one. Indeed, for the chosen values of $\lambda_1, \lambda_2, \lambda_3$ and t, the map is an extreme positive [23]. The fact that it is not completely positive can be checked independently by finding that its image under the Jamiołkowski isomorphism [26] is not positive semi-definite.

7.2. An extreme completely positive map having no pure states in its image

Let us consider a CP map on $\mathbb{C}^{3\times 3}$ defined by the following Kraus operators:

$$V_1 = \begin{bmatrix} 1/\sqrt{3} & 0 & 0 \\ 0 & 1/\sqrt{2} & 0 \\ 0 & 0 & \frac{1}{\sqrt{1+\alpha^2}} \end{bmatrix}, \qquad V_2 = \begin{bmatrix} 0 & 1/\sqrt{3} & 0 \\ 0 & 0 & 1/\sqrt{2} \\ \frac{\alpha}{\sqrt{1+\alpha^2}} & 0 & 0 \end{bmatrix},$$
$$V_3 = \begin{bmatrix} 0 & 0 & 1/\sqrt{3} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{33}$$

A straightforward calculation gives $V_1 V_1^\dagger + V_2 V_2^\dagger + V_3 V_3^\dagger = I$.

For $\alpha = 0$ the matrices $V_i V_j^\dagger$ form a basis in the space of 3×3 matrices, hence it is also true for small α. The map $A\rho = \sum_{i=1}^{3} V_i^\dagger \rho V_i$ is thus an extreme CP map (theorem 8). For $\alpha \neq 0$ there is no $|y\rangle$ such that $V_i^\dagger |x\rangle \sim |y\rangle$ for some $|x\rangle$ and $i = 1, 2, 3$, hence A does not send any pure state into a pure one.

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References

[1] Wigner E P 1949 Invariance in physical theory *Proc. Am. Phil. Soc.* **3** 521–6

[2] Wigner E P 1964 Events, laws of nature and invariance principles *Science* **145** 995–99 (Nobel Lecture, 12 December 1963)

[3] Houtappel R M F, Van Dam H and Wigner E P 1965 The conceptual basis and use of the geometric invariance principles *Rev. Mod. Phys.* **37** 595–632
[4] Mackey G W 1963 *Mathematical Foundations of Quantum Mechanics* (New York: Benjamin)
[5] Kadison R V 1951 Isometries of operator algebras *Ann. Math.* **54** 325–38
[6] Kadison R V 1965 Transformations of states in operator theory and dynamics *Topology* **3** 177–98
[7] Grabowski J, Kuś M and Marmo G 2005 Geometry of quantum systems: density states and entanglement *J. Phys. A: Math. Gen.* **38** 10217–44
[8] Gottfried K and Yan T M 2004 *Quantum Mechanics: Fundamentals* (New York: Springer)
[9] Esposito G, Marmo G and Sudarshan G 2004 *From Classical to Quantum Mechanics: An Introduction to the Formalism, Foundations and Applications* (Cambridge: Cambridge University Press)
[10] Wigner E P 1959 *Group Theory* (New York: Academic)
[11] Hagedorn R 1959 Note on symmetry operations in quantum mechanics *Nuovo Cimento* **12** 73–86
[12] Lomont J S and Mendelson P 1963 The Wigner unitarity–antiunitarity theorem *Ann. Math.* **78** 548–59
[13] O'Raifeartaigh L and Rasche G 1963 Probability-conserving transformations and superselection rules in quantum theory *Ann. Phys., NY* **25** 155–73
[14] Bargmann V 1964 Note on Wigner's theorem on symmetry operations *J. Math. Phys.* **5** 862–8
[15] Roberts J E and Roepstorff G 1969 Some basic concepts of algebraic quantum theory *Commun. Math. Phys.* **11** 321–38
[16] Hunziker W 1972 A note on symmetry operations in quantum mechanics *Helv. Phys. Acta* **45** 233–6
[17] Bracci L, Morchio G and Strocchi F 1975 Wigner's theorem on symmetries in indefinite metric spaces *Commun. Math. Phys.* **41** 289–99
[18] Samuel J 1997 The geometric phase and ray space isometries *Pramana J. Phys.* **48** 959–67
[19] Cassinelli G, De Vito E, Lahti P J and Levrero A 1997 Symmetry groups in quantum mechanics and the theorem of Wigner on the symmetry transformations *Rev. Math. Phys.* **9** 921–42
[20] Grabowski J, Kuś M and Marmo G 2007 On the relation between states and maps in infinite dimensions *Open Sys. Inf. Dyn.* **14** 355–70
[21] Grabowska K, Grabowski J and Urbański P 2004 AV-differential geometry: Poisson and Jacobi structures *J. Geom. Phys.* **52** 398–446
[22] Grabowska K, Grabowski J and Urbański P 2007 AV-differential geometry: Euler–Lagrange equations *J. Geom. Phys.* **57** 1984–98
[23] Gorini V and Sudarshan E C G 1976 Extreme affine transformations *Commun. Math. Phys.* **46** 43–52
[24] Choi M D 1975 Completely positive linear maps on complex matrices *Linear Algebra Appl.* **10** 285–90
[25] Kraus K 1972 *States, Effects and Operations: Fundamental Notions of Quantum Theory* (Berlin: Springer)
[26] Jamiołkowski A 1972 Linear transformations which preserve trace and positive semidefinite operators *Rep. Math. Phys.* **3** 275–8
[27] Grabowski J, Kuś M and Marmo G 2006 Symmetries, group actions and entanglement *Open Sys. Inf. Dyn.* **13** 343–62
[28] Fujiwara A and Algoet P 1999 One-to-one parametrization of quantum channels *Phys. Rev.* A **59** 3290–94
[29] Ruskai M B, Szarek S and Werner E 2002 An analysis of completely positive trace-preserving maps on $\mathcal{M}_2$ *Linear Algebra Appl.* **347** 159–87