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Extreme Affine Transformations*

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Abstract. We classify the extreme points of the compact convex set of affine maps of $\mathbb{R}^n$ which map into itself the closed unit ball. This work is a preliminary step towards solving the problem of finding the extreme points of the compact convex set of affine maps of the $N \times N$ density matrices (dynamical maps of an N-level system) and for $n=3$ furnishes the solution of the problem in the simplest case of a two-level system.

1. Introduction

Let $D_n(n=1,2,3,\ldots)$ denote the set of affine maps $\mathbb{R}^n \to \mathbb{R}^n$ which map into itself the closed unit ball B_n. D_n is convex, compact and finite-dimensional, hence each point of D_n can be written as a finite convex combination of extreme points of D_n. In this note we prove a theorem which classifies the extreme points of D_n. The theorem was stated and commented upon in [1] and is a first step towards solving the problem of finding the extreme points of the compact convex set F_N of the affine maps $K_N \to K_N$, where $K_N = \{\varrho | \varrho$ an $N \times N$ complex matrix, $\varrho \geqq 0, \mathrm{Tr}(\varrho) = 1\}$ is the convex set of $N \times N$ density matrices. Indeed, F_2 can be identified to D_3 through the identification of K_2 to B_3 by means of the representation of a 2×2 density matrix as $\varrho = (1/2)(1_2 + \sum_{i=1}^3 \alpha_i \sigma_i) \to \alpha = \{\alpha_1, \alpha_2, \alpha_3\}$, where $\{\sigma_1, \sigma_2, \sigma_3\}$ are the familiar Pauli matrices or, more generally, any maximal set of 2×2 self-adjoint traceless matrices satisfying $\mathrm{Tr}(\sigma_i \sigma_j) = 2\delta_{ij}$. The structure analysis of F_N is of interest in connection with the study of the dynamics of an N-level quantum mechanical open system, since the dynamical evolution of such a system is represented by a one parameter family $t \to A_t$, $t \in [0, \infty)$, $A_t \in F_N$, $A_0 = 1$, whereby the density matrix (state) ϱ_t of the system at time t is given in terms of the initial state ϱ_0 by $\varrho_t = A_t \varrho_0$ (for this reason, we refer to the elements of F_N as *dynamical maps* [2]). Familiar examples are encountered in spin magnetic resonance and relaxation [3, 4] and in quantum optics [5, 6].

After the completion of this work we became aware that, as a particular case of our theorem, a result equivalent to the classification of the extreme points of

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D_3 had been previously obtained by Størmer [7]. However, the geometrical aspect of the problem and the symmetry properties of the extreme points are not readily apparent in Størmer's treatment, since he works in a dual context. On the other hand, we feel that symmetry considerations should play an important role in the determination of the extreme points of F_N. We refer to [1] for a discussion thereof and for an explicit (though as yet unproved) conjecture in this connection.

In Section 2 we collect a few notations. In Section 3 we give two instrumental parametrizations of D_n (Theorem 1). In Section 4 we determine the extreme points of D_n (Theorem 2). In Section 5 we briefly comment upon the geometrical meaning of Theorems 1 and 2.

2. Notations

If n is a positive integer, $\mathbb{R}^n=\{x|x=\{x_i\}_{i=1,\dots,n};\, x_j\in\mathbb{R}, j=1,\dots,n\}$ is the n-dimensional euclidean space and we denote by M(n) [respectively, by AF(n)] the real algebra of linear maps (respectively of affine maps) of $\mathbb{R}^n$ into itself. An element Δ of AF(n) acts on $\mathbb{R}^n$ as $\Delta: x\to Tx+b:=(b,T)x$, $x\in\mathbb{R}^n$, $b\in\mathbb{R}^n$, $T\in$ M(n) and we can identify Δ to the pair (b, T), where T can in turn be identified to an $n\times n$ matrix with real entries $\{T_{ij}\}_{i,j=1,\dots,n}$ (we refer to b and T respectively as the translation and the linear parts of Δ). This establishes a canonical topological vector space isomorphism between AF(n) [respectively, M(n)] and $\mathbb{R}^{n(n+1)}$ (respectively $\mathbb{R}^{n^2}$). We use the standard notations for the real orthogonal group in n dimensions and for its connected component, respectively O(n)$=\{Q|Q\in \mathrm{M(n)}, QQ^T=1_n\}$ and SO(n)$=\{Q|Q\in\mathrm{O(n)}, \det Q=1\}$ (A^T denotes the transpose of a matrix A). Whenever $Q\in$ O(n), we write Q in place of $(0, Q)$ and if G is a subgroup of O(n) and $x\in\mathbb{R}^n$ we denote by G_x the stabilizer of x relative to the canonical action of G on $\mathbb{R}^n$. 1_n and 0_n denote respectively the identity and the zero map of $\mathbb{R}^n$ and $\mathrm{diag}\{\alpha_i\}_{i=1,\dots,n}$ denotes a diagonal matrix with diagonal elements $\alpha_1,\dots,\alpha_n$. If X is a convex subset of $\mathbb{R}^l$ we denote by extr X the set of the extreme points of X. $B_n=\{x|x\in\mathbb{R}^n;\, \|x\|=(\sum_{i=1}^n x_i^2)^{\frac{1}{2}}\leqq 1\}$ and $S_n=\mathrm{extr}\,B_n=\{x|x\in\mathbb{R}^n, \|x\|=1\}$ are respectively the closed unit ball and the unit sphere in $\mathbb{R}^n$. We define $D_n=\{\Delta|\Delta\in\mathrm{AF(n)}, x\in B_n\Rightarrow \Delta x\in B_n\}$. D_n is a compact convex subset of AF(n), whose boundary is given by $D_n'=\{\Delta|\Delta\in D_n, \Delta x\in S_n$ for some $x\in S_n\}$. We call an element $\Delta=(a,\Lambda)$ of AF(n) *canonical* if $a_i\geqq 0, i=1,\dots,n$, and $\Lambda=\mathrm{diag}\{\lambda_l\}_{l=1,\dots,n}$, $\lambda_1\geqq\dots\geqq\lambda_n\geqq 0$. If Y is a subset of AF(n), we define $\underline{Y}=\{\Delta|\Delta\in Y, \Delta$ canonical$\}$.

3. Two Parametrizations of D_n

The following theorem establishes two parametrizations of D_n which will be used in the following section.

Theorem 1.

i) $D_n=\{(b,T)|b\in\mathbb{R}^n;\, T\in \mathrm{M(n)};\, (b,T)=(Q_1a, Q_1\Lambda Q_2);\, Q_1, Q_2\in\mathrm{O(n)};$

$a_i=\beta\xi_i(1-\alpha\omega_i^2),\, i=1,\dots,n;$

$\Lambda=\mathrm{diag}\{\alpha\beta\omega_l(\sum_{j=1}^n \xi_j^2\omega_j^2)^{\frac{1}{2}}\}_{l=1,\dots,n};$

$$0 \leqq \alpha \leqq 1; 0 \leqq \beta \leqq 1; 0 \leqq \omega_n \leqq \ldots \leqq \omega_1 = 1; 0 \leqq \xi_r \leqq 1, r = 1, \ldots, n; \sum_{l=1}^n \xi_l^2 = 1\}.$$

ii) $D_n = \{(b, T) | b \in \mathbb{R}^n; T \in \mathrm{M(n)}; (b, T) = (Q_1 a, Q_1 \Lambda Q_2); Q_1, Q_2 \in \mathrm{O(n)};$
$a_i = \beta \xi_i (1 - \alpha \nu \eta_i^2), i = 1, \ldots, n;$
$\Lambda = \mathrm{diag}\{\alpha \beta \nu \eta_l\}_{l=1,\ldots,n}; 0 \leqq \alpha \leqq 1; 0 \leqq \beta \leqq 1; \nu > 0; 0 \leqq \eta_n \leqq \ldots \leqq \eta_1 = \nu^{-\frac{1}{2}};$
$0 \leqq \xi_r \leqq 1, r = 1, \ldots, n; \sum_{l=1}^n \xi_l^2 = \sum_{l=1}^n \xi_l^2 \eta_l^2 = 1\}.$

Proof. Using the polar decomposition of a matrix $A \in \mathrm{M(n)}$ as $A = QS$, $Q \in \mathrm{O(n)}$, S symmetric and positive [8], any element Δ of AF(n) can be written in the form $\Delta = (Q_1 a, Q_1 \Lambda Q_2)$, where (a, Λ) is canonical. Write

$$\begin{aligned} &\Delta(\alpha; \beta; \xi_1, \ldots, \xi_n; \omega_1, \ldots, \omega_n) \\ &= (\{\beta \xi_i (1 - \alpha \omega_i^2)\}_{i=1,\ldots,n}, \mathrm{diag}\{\alpha \beta \omega_l (\textstyle\sum_{j=1}^n \xi_j^2 \omega_j^2)^{\frac{1}{2}}\}_{l=1,\ldots,n}). \end{aligned} \tag{3.1}$$

Then, in order to prove i), it is enough to show that

$$\begin{aligned} \underline{D'_n} = \{&\Delta | \Delta \in AF(n); \Delta = \Delta(\alpha; 1; \xi_1, \ldots, \xi_n; \omega_1, \ldots, \omega_n); \\ &0 \leqq \alpha \leqq 1; 0 \leqq \omega_n \leqq \ldots \leqq \omega_1 = 1; 0 \leqq \xi_l \leqq 1, l = 1, \ldots, n; \textstyle\sum_{j=1}^n \xi_j^2 = 1\}. \end{aligned} \tag{3.2}$$

To this purpose, we first note that if x, y and z are elements of $\mathbb{R}^n$ such that $\|x\| = \|y\| = 1$ and $z_1^2 = 1$, then the following identity holds

$$\sum_{i=1}^n [(\textstyle\sum_{j=1}^n y_j^2 z_j^2)^{\frac{1}{2}} z_i x_i + y_i(1 - z_i^2)]^2 = 1 - \sum_{i=1}^n (1 - z_i^2)[(\sum_{j=1}^n y_j^2 z_j^2)^{\frac{1}{2}} x_i - y_i z_i]^2, \tag{3.3}$$

as can be readily verified by expanding the squares. Hence, under the conditions

$$0 \leqq \omega_n \leqq \ldots \leqq \omega_1 = 1; 0 \leqq \xi_l \leqq 1, l = 1, \ldots, n; \sum_{l=1}^n \xi_j^2 = 1, \tag{3.4}$$

it follows from (3.3) setting $y = \xi$ and $z = \omega$ that

$$\Delta(1; 1; \xi; \omega) = : \Delta(1; 1; \xi_1, \ldots, \xi_n; \omega_1, \ldots, \omega_n) \in \underline{D'_n}.$$

Note that $\Delta(1; 1; \xi; \omega) = 1_n$ if $\omega_n = 1$ and that $\Delta(1; 1; \xi; \omega) = (\xi, 0_n)$ if $\sum_{l=1}^n \xi_l^2 \omega_l^2 = 0$, whereas if $\omega_n < 1$ and $\sum_{l=1}^n \xi_l^2 \omega_l^2 \neq 0$ one has

$$\begin{aligned} &\{x | x \in S_n, \Delta(1; 1; \xi; \omega) x \in S_n\} \\ &\quad = \{x | x \in S_n, x_l = \xi_l \omega_l (\textstyle\sum_{i=1}^n \xi_i^2 \omega_i^2)^{-\frac{1}{2}}, l = s+1, \ldots, n, \\ &\quad \text{if} \quad \omega_s = 1, \quad \text{and} \quad \omega_{s+1} < 1\}. \end{aligned} \tag{3.5}$$

Now let $\Delta = (a, \mathrm{diag}\{\lambda_l\}_{l=1,\ldots,n}) \in \underline{D'_n}$ and distinguish two cases, according to whether $\lambda_1 = 0$ or $\lambda_1 > 0$. The first case implies $\|a\| = 1$ and is obtained by setting $\alpha = 0$ in (3.2). If $\lambda_1 > 0$ define

$$\omega_j = \lambda_j / \lambda_1, \quad j = 1, \ldots, n \tag{3.6}$$

and let $\xi \in \Delta(S_n) \cap S_n$, with $\xi_i \geqq 0$, $i = 1, \ldots, n$ (since Δ is canonical it is possible to fulfill the latter requirement). Then $\sum_{l=1}^n \xi_l^2 \omega_l^2 \neq 0$. Indeed, assume the contrary and let $\xi_1 = \ldots = \xi_{s-1} = 0$ and $\xi_s > 0$, $s = 2, \ldots, n$. Then $\omega_s = \ldots = \omega_n = 0$, or $\lambda_s = \ldots = \lambda_n = 0$, so that $\xi_r = a_r$, $r = s, \ldots, n$ and hence $\sum_{r=s}^n a_r^2 = \sum_{r=s}^n \xi_r^2 = 1$. This implies $a_i=\lambda_i=0, i=1,\dots,s-1$, which contradicts the hypothesis. Then set $\alpha=\lambda_1(\sum_{l=1}^n \xi_l^2\omega_l^2)^{-\frac{1}{2}}$, whence $\lambda_i=\alpha\omega_i(\sum_{l=1}^n \xi_l^2\omega_l^2)^{\frac{1}{2}}, i=1,\dots,n$, and consider the affine map $\Delta(\alpha;1;\xi;\omega)$. One has

$$\Delta(\alpha;1;\xi;\omega)=\alpha\Delta(1;1;\xi;\omega)+(1-\alpha)\Delta(0;1;\xi;\omega) \tag{3.7}$$

and setting

$$v_l=\xi_l\omega_l(\textstyle\sum_{i=1}^n \xi_i^2\omega_i^2)^{-\frac{1}{2}}, \qquad l=1,\dots,n, \tag{3.8}$$

one gets

$$(\Delta(\alpha;1;\xi;\omega)v)_l=\xi_l, \qquad l=1,\dots,n. \tag{3.9}$$

Therefore, the two affine maps Δ and $\Delta(\alpha;1;\xi;\omega)$ have the same linear part, the point ξ belongs to $S_n\cap\Delta(S_n)\cap\Delta(\alpha;1;\xi;\omega)(S_n)$ and S_n, $\Delta(S_n)$ and $\Delta(\alpha;1;\xi;\omega)(S_n)$ all lie in one and the same, say σ, of the two closed half-spaces determined by the hyperplane π which is tangent to S_n at ξ. Let c and $d=\{\xi_i(1-\alpha\omega_i)\}_{i=1,2,\dots,n}$ denote the translation parts of Δ and, respectively, of $\Delta(\alpha;1;\xi;\omega)$ and set $e=d-c$. We have $\Delta(\alpha;1;\xi;\omega)v=\xi$ and let $x\in S_n$ such that $\Delta x=\xi$. Then $\Delta v=\xi-e\in\sigma$ and $\Delta(\alpha;1;\xi;\omega)x=\xi+e\in\sigma$. This implies $\xi-e\in\pi$ which, in turn, implies $e=0$ since, by hypothesis, $\Delta\in\underline{D}_n'$. Hence $\Delta=\Delta(\alpha;1;\xi;\omega)$. By (3.7) and since D_n is convex we have $\Delta(\alpha;1;\xi;\omega)\in\underline{D}_n'$ if $\alpha\in[0,1]$. On the other hand, it is easy to check that $\Delta(\alpha;1;\xi;\omega)x\notin B_n$ for some $x\in B_n$ if $\alpha>1$. Indeed, set

$$u_1=-\xi_1\omega_1(\textstyle\sum_{l=1}^n \xi_l^2\omega_l^2)^{-\frac{1}{2}}, \qquad u_r=\xi_r\omega_r(\sum_{l=1}^n \xi_l^2\omega_l^2)^{-\frac{1}{2}}, \qquad r=2,\dots,n$$

and $\alpha=1+\varepsilon, \varepsilon>0$. Then $\|\Delta(\alpha;1;\xi;\omega)u\|^2=1+4\varepsilon(\varepsilon+1)\xi_1^2>1$ if $\xi_1>0$. If $\xi_1=0$, let r be the smallest integer for which $\xi_r>0 (2\leqq r\leqq n)$ and note that $\omega_r>0$ since $\sum_{i=1}^n \xi_1^2\omega_1^2\neq 0$. Consider the intersections $C=S_n\cap\varrho$ and $E=\Delta(\alpha;1;\xi;\omega)(S_n)\cap\varrho$, where ϱ is the 2-plane $\{x|x\in\mathbb{R}^n; x_2=\dots=x_{r-1}=0, x_l=\xi_l, l=r+1,\dots,n\}$. C and E are respectively a circle and an ellipse whose equations are $C: x_r^2+x_1^2=\xi_r^2$ and $E:[x_r-\xi_r(1-\alpha\omega_r^2)]^2/(\alpha\xi_r\omega_r^2)^2+x_1^2/(\alpha\xi_r\omega_r)^2=1$. At their common point $(0,\xi_r)$ the second derivatives are respectively $C:(d^2x_r/dx_1^2)|_{x_1=0}=-1/\xi_r$ and $E:(d^2x_r/dx_1^2)|_{x_1=0}=-1/\alpha\xi_r$. In order that $\Delta(\alpha;1;\xi;\omega)(S_n)\subseteq S_n$ one must have $1/\xi_r\leqq 1/\alpha\xi_r$ or $\alpha\leqq 1$. This completes the proof i). In order to prove ii) take without loss of generality $\sum_{i=1}^n \xi_i^2\omega_i^2\neq 0$ in the parametrization i) and set $v=\sum_{i=1}^n \xi_i^2\omega_i^2$ and $\eta_l=\omega_l v^{-\frac{1}{2}}, l=1,2,\dots,n$. ∎

4. Extreme Points of D_n

We classify the extreme points of D_n by means of the following

Theorem 2.

$$\begin{aligned}\operatorname{Extr} D_n=\{(b,T)|b\in\mathbb{R}^n;\, T\in \mathrm{M(n)};\, (b,T)=(Q_1a, Q_1\Lambda Q_2);\\ Q_1,Q_2\in \mathrm{O(n)};\, (a,\Lambda)=\Delta(1;1;0,\dots,0,(1-\delta^2)^{\frac{1}{2}},\delta;1,\dots,1,\varkappa);\\ 0\leqq\varkappa\leqq 1; 0<\delta\leqq 1\}.\end{aligned} \tag{4.1}$$

Proof. For $n=1$ the result is trivial, so we assume $n\geqq 2$. First note that if $(b,T)\in\operatorname{extr} D_n$ and $Q, Q'\in \mathrm{O(n)}$, then $(Qb, QTQ')\in\operatorname{extr} D_n$. Thus it is enough to look for the extreme points of D_n which are canonical, and these belong to $\underline{D}'_n$. If $\sum_{i=1}^n \xi_i^2\omega_i^2 \neq 0$, we get from (3.7) that $\Delta(\alpha;1;\xi;\omega)$ is not extreme if $0<\alpha<1$. Consider $\Delta(0;1;\xi;\omega)$. It is an extreme since it maps extreme points of B_n to extreme points of B_n and it is obtained by setting $\delta=1$, $\varkappa=0$ in (4.1) and by choosing therein Q_1 such that $Q_1 p=\xi$, where p is the "north pole",

$$p=\{0,\dots,0,1\}. \tag{4.2}$$

We now prove that $\Delta(1;1;\xi_1,\dots,\xi_n;1,\dots,1,\omega_n)$ is extreme if $0<\xi_n<1$. First we note that the statement is trivial if $\omega_n=1$ and that if $\omega_n<1$ the map

$$\Delta(1;1;\xi_1,\dots,\xi_{n-1},0;1,\dots,1,\omega_n)$$

is not extreme since it equals the convex combination $[(1+\omega_n)/2]1_n+[(1-\omega_n)/2]P_n$, where

$$P_j=:\operatorname{diag}\{\varepsilon_l\}_{l=1,\dots,n}, \quad \varepsilon_l=1 \quad \text{if} \quad l\neq j, \quad \varepsilon_j=-1. \tag{4.3}$$

Then, let

$$0<\xi_n<1, \quad 0\leqq\omega_n<1 \tag{4.4}$$

and assume $\Delta(\xi_n,\omega_n)=:\Delta(1;1;\xi_1,\dots,\xi_n;1,\dots,1,\omega_n)$ to be a convex combination

$$\Delta(\xi_n,\omega_n)=\gamma\Delta_1+(1-\gamma)\Delta_2;\ \Delta_1,\Delta_2\in D_n,\ 0<\gamma<1. \tag{4.5}$$

From (4.4) we get $0<[(1-\xi_n^2)+\xi_n^2\omega_n^2]^{\frac{1}{2}}$ and

$$0\leqq u_n=\xi_n\omega_n[(1-\xi_n^2)+\xi_n^2\omega_n^2]^{-\frac{1}{2}}<\xi_n. \tag{4.6}$$

Defining $\Sigma=\{x|x\in\mathbb{R}^n;\ \|x\|=1,\ x_n=u_n\}$ and $\hat\Sigma=\{x|x\in\mathbb{R}^n,\ \|x\|=1,\ x_n=\xi_n\}$ we have $\Delta(\xi_n,\omega_n)(\Sigma)=\hat\Sigma$ and one checks easily that if $\Delta\in\underline{D}_n$ and $\Delta(\Sigma)=\hat\Sigma$, then $\Delta=\Delta(\xi_n,\omega_n)$. Then, since $S_n=\operatorname{extr}B_n$, we have that

$$u\in\Sigma\Rightarrow\Delta(\xi_n,\omega_n)u=\Delta_1u=\Delta_2u. \tag{4.7}$$

Write $\Delta_1=Q_1\hat\Delta_1Q_2$ with $\hat\Delta_1$ canonical, $\hat\Delta_1=\Delta(\hat\alpha;1;\hat\xi_1,\dots,\hat\xi_n;\hat\omega_1,\dots,\hat\omega_n)$. From (4.7) we have $\hat\Delta_1[Q_2(\Sigma)]=Q_1^{-1}(\hat\Sigma)$. Then, since $Q_2(\Sigma)$ and $Q_1^{-1}(\hat\Sigma)$ are $(n-2)$-dimensional subspheres of S_n, from (3.5) and (3.7) we obtain $\hat\alpha=1$ and $\hat\omega_{n-1}=1$. $Q_2(\Sigma)$ and $Q_1^{-1}(\hat\Sigma)$ have radiuses respectively $(1-\hat u_n^2)^{\frac{1}{2}}$ and $(1-\xi^2)^{\frac{1}{2}}$, where $\hat u_n=\hat\xi_n\hat\omega_n[(1-\hat\xi_n^2)+\hat\xi_n^2\hat\omega_n^2]^{-\frac{1}{2}}$. Since $Q_1,Q_2\in\mathrm{O(n)}$, there follows $\hat\xi_n=\xi_n$ and $\hat u_n=u_n$, hence also $\hat\omega_n=\omega_n$. Therefore, we have $\hat\Delta_1=\Delta(\xi_n,\omega_n)$ and $Q_1p=(-1)^lp$, where $l=0$ or $l=0,1$ according to whether $\omega_n>0$ or $\omega_n=0$. Then

$$\Delta_1=Q\Delta((-1)^l\xi_n,\omega_n) \tag{4.8}$$

where $Q=Q_1Q_2$ and, by (4.6), $\Delta(\xi_n,\omega_n)u=Q\Delta((-1)^l\xi_n,\omega_n)u$, $\forall u\in\Sigma$, which implies $Q=P_n^l$. Substituting into (4.8) gives $\Delta_1=\Delta(\xi_n,\omega_n)$ which proves that under conditions (4.4) $\Delta(\xi_n,\omega_n)$ is extreme.

Next we show that if $n\geqq3$ and $\sum_{i=1}^n\xi_i^2\omega_i^2\neq0$, the map $\Delta(1;1;\xi_1,\dots,\xi_n;\omega_1,\dots,\omega_n$, is not extreme if $\omega_{n-1}<1$. To this purpose, we use parametrization ii) established in Theorem 1. Then, writing

$$\Gamma(v;\xi;\eta)=(\{\xi_i(1-v\eta_i^2)\}_{i=1,\dots,n},\operatorname{diag}\{v\eta_l\}_{l=1,\dots,n}), \tag{4.9}$$

we must prove that $\Gamma(v;\xi;\eta)$ is not extreme if $\eta_{n-1}<v^{-\frac{1}{2}}$. First remark that the map (4.9) satisfies the following composition law

$$\Gamma(v';\xi;\eta')\Gamma(v'';\eta'\xi;\eta'')=\Gamma(v'v'';\xi;\eta'\eta''), \tag{4.10}$$

where we have used the notation $xy=\{x_iy_i\}_{i=1,\ldots,n}$. Now, let r be the smallest integer for which $\eta_r<v^{-\frac{1}{2}}$ (by hypothesis, $2\leqq r\leqq n-1$). If $\eta_r=0$, we have

$$\Gamma(v;\xi;\eta)=(1/2)Q^{-1}\Gamma(v;\hat{\xi};\hat{\eta})Q+(1/2)Q^{-1}P_r\Gamma(v;\hat{\xi};\hat{\eta})Q$$

where,

$$\hat{\xi}=\{\xi_1,\ldots,\xi_{r-1},0,(\xi_r^2+\xi_{r+1}^2)^{\frac{1}{2}},\xi_{r+2},\ldots,\xi_n\},\hat{\eta}_r=v^{-\frac{1}{2}},\hat{\eta}_{r+1}=0$$

and

$$Q\xi=\hat{\xi},\ Q\in\mathrm{SO(n)},\ Q^{-1}\operatorname{diag}\{\eta_s\}Q=\operatorname{diag}\{\eta_s\}.$$

If $\eta_r>0$, set $\zeta=\sum_{j=1}^{r-1}\xi_j^2+v\eta_r^2\sum_{l=r}^{n}\xi_l^2$ and note that

$$\zeta\geqq\sum_{j=1}^{r-1}\xi_j^2+v\sum_{l=r}^{n}\eta_l^2\xi_l^2,\ v\sum_{i=1}^{n}\eta_i^2\xi_i^2=v>0.$$

Setting $\lambda=\zeta^{-\frac{1}{2}}$ and $\tau=\lambda v^{\frac{1}{2}}\eta_r$ we have thus by hypothesis $\lambda>\tau>0$ and we define the vectors η' and η'' as $\eta_1'=\ldots=\eta_{r-1}'=\lambda$, $\eta_r'=\ldots=\eta_n'=\tau$, $\eta_j''=\lambda^{-1}\eta_j$, $j=1,\ldots,r-1$ and $\eta_l''=\tau^{-1}\eta_l$, $l=r,\ldots,n$. Then, since $\Gamma(v;\xi;\eta)\in\underline{D_n'}$ by hypothesis, setting $v'=\lambda^{-2}$ and $v''=\lambda^2v$, it is a straightforward matter to check that the maps $\Gamma(v';\xi;\eta')$ and $\Gamma(v'';\eta'\xi;\eta'')$ belong to $\underline{D_n'}$ and by (4.10) one gets $\Gamma(v;\xi;\eta)=\Gamma(v';\xi;\eta')\Gamma(v'';\eta'\xi;\eta'')$. From this we obtain

$$\Gamma(v;\xi;\eta)=[(1+v^{\frac{1}{2}}\eta_r)/2]\Delta_1+[(1-v^{\frac{1}{2}}\eta_r)/2]\Delta_2, \tag{4.11}$$

where

$$\Delta_1=Q^{-1}\Gamma(v';\hat{\xi};\hat{\eta}')Q\Gamma(v'';\eta'\xi;\eta''), \tag{4.12}$$

$$\Delta_2=Q^{-1}P_r\Gamma(v';\hat{\xi};\hat{\eta}')Q\Gamma(v'';\eta'\xi;\eta'') \tag{4.13}$$

$$\hat{\xi}=\{\xi_1,\ldots,\xi_{r-1},0,(\xi_r^2+\xi_{r+1}^2)^{\frac{1}{2}},\xi_{r+2},\ldots,\xi_n\},\hat{\eta}_r'=\lambda,\hat{\eta}_{r+1}'=\tau,$$

$$Q\xi=\hat{\xi},\ Q\in\mathrm{SO(n)},\ Q^{-1}\operatorname{diag}\{\hat{\eta}_s'\}Q=\operatorname{diag}\{\hat{\eta}_s'\}$$

and, since $0<\eta_r<v^{-\frac{1}{2}}$, $0<(1/2)(1-v^{\frac{1}{2}}\eta_r)<1/2$. Let M and N denote the linear parts of $Q\Delta_1$ and, respectively, of $Q\Delta_2$. If $\xi_r=0$ we can take $Q=1_n$, hence $M_{rr}=v^{\frac{1}{2}}=-N_{rr}$ implying $\Delta_1\neq\Delta_2$. If $\xi_r\neq0$, we get $M_{rr}=v^{\frac{1}{2}}\xi_{r+1}(\xi_r^2+\xi_{r+1}^2)^{-\frac{1}{2}}=-N_{rr}$ and $M_{r,r+1}=-v^{\frac{1}{2}}\eta_{r+1}\eta_r^{-1}\xi_r(\xi_r^2+\xi_{r+1}^2)^{-\frac{1}{2}}=-N_{r,r+1}$, whence again $\Delta_1\neq\Delta_2$ provided that ξ_{r+1} and η_{r+1} are not both zero. On the other hand, if $\xi_r\neq0$ and $\xi_{r+1}=\eta_{r+1}=0$, set $\tilde{\xi}=(\xi_1,\ldots,\xi_{r-1},0,\xi_r,\xi_{r+2},\ldots,\xi_n)$, $\tilde{\eta}_1=\ldots=\tilde{\eta}_r=v^{-\frac{1}{2}}$, $\tilde{\eta}_{r+1}=\eta_r$, $\tilde{\eta}_{r+2}=\ldots=\tilde{\eta}_n=0$ and let Q be the rotation of $\pi/2$ in the (x_r,x_{r+1})-plane. Then $\Gamma(v;\xi;\eta)$ can be expressed as the following non trivial convex combination

$$\Gamma(v;\xi;\eta)=(1/2)Q\Gamma(v;\tilde{\xi};\tilde{\eta})Q^{-1}+(1/2)QP_r\Gamma(v;\tilde{\xi};\tilde{\eta})Q^{-1}. \tag{4.14}$$

It remains to show that $\Delta(\varkappa)=:\Delta(1;1;0,\ldots,0,1;1,\ldots,1,\varkappa)$ is extreme if

$$0<\varkappa<1. \tag{4.15}$$

To this purpose, for a given $\varkappa$ satisfying (4.15) we express $\Delta(\varkappa)$ as a convex combination of extreme points of D_n,

$$\Delta(\varkappa)=\sum_{i=1}^{s}\gamma_i\Delta_i,\ 0<\gamma_l<1,\ \Delta_l\in\operatorname{extr}D_n,\ l=1,\dots,s,\ \sum_{i=1}^{s}\gamma_i=1\,. \tag{4.16}$$

and we show that this implies $\Delta_i=\Delta(\varkappa)$, $i=1,\dots,s$. If μ denotes the normalized Haar measure on $\mathrm{SO(n)}_p$, we get from (4.16)

$$\Delta(\varkappa)=\sum_{i=1}^{s}(\gamma_i/2)(\bar{\Delta}_i+P\bar{\Delta}_iP)=\sum_{i=1}^{s}\gamma_i\hat{\Delta}_i\,, \tag{4.17}$$

where $P=P_{n-1}$,

$$\bar{\Delta}_i=\int Q\Delta_iQ^{-1}d\mu(Q)\,,\qquad i=1,\dots,s\,, \tag{4.18}$$

the integration being extended over $\mathrm{SO(n)}_p$, and

$$\hat{\Delta}_i=(1/2)(\bar{\Delta}_i+P\bar{\Delta}_iP)\,,\qquad i=1,\dots,s\,. \tag{4.19}$$

The $\hat{\Delta}_i$'s are invariant under $\mathrm{O(n)}_p$, hence they have the form $\hat{\Delta}_i=(\{0,\dots,0,d_i\},\ \operatorname{diag}\{b_i,\dots,b_i,c_i\})$ and since $\Delta(\varkappa)p=p$ and $p\in\operatorname{extr}B_n$ we have $\Delta_ip=p=\hat{\Delta}_ip$, $i=1,\dots,s$. Therefore $d_i=1-c_i$ and since $\hat{\Delta}_i\in D_n$, $i=1,\dots,s$, the c_i's and the b_i's satisfy the inequalities $0\leqq c_i\leqq 1$ and $c_i\geqq b_i^2$, $i=1,\dots,s$. The first inequality follows from $\hat{\Delta}_i(-p)\in B_n$. On the other hand, if it were $c_i<b_i^2$ one would get $\hat{\Delta}_ix\notin B_n$ for some points x of B_n in the neighbourhood of p. Then, from (4.17) we have $\varkappa^2=\sum_{i=1}^{s}\gamma_ic_i\geqq\sum_{i=1}^{s}\gamma_ib_i^2\geqq(\sum_{i=1}^{s}\gamma_ib_i)^2=\varkappa^2$ which implies $c_i=b_i^2=\varkappa^2$, $i=1,\dots,s$ and hence, since $\sum_{i=1}^{s}\gamma_ib_i=\varkappa$,

$$\hat{\Delta}_i=\Delta(\varkappa)\,,\qquad i=1,\dots,s\,. \tag{4.20}$$

Denoting by Δ any given Δ_i, since by hypothesis $\Delta\in\operatorname{extr}D_n$ it follows from the hitherto obtained results that it must be of the form

$$\Delta=Q_2\Delta(\xi,\omega)Q_1\,;\ Q_1,Q_2\in\mathrm{O(n)};\ 0\leqq\omega\leqq 1;\ 0<\xi\leqq 1\,, \tag{4.21}$$

where $\Delta(\xi,\omega)=\Delta(1;1;0,\dots,0,(1-\xi^2)^{\frac{1}{2}},\xi;1,\dots,1,\omega)$. If $\omega=1$ we have $\Delta(\xi,\omega)=1_n$, hence $\Delta=Q_2Q_1=\bar{Q}$ and, from (4.18)–(4.20),

$$\Delta(\varkappa)=(1/2)\int Q\bar{Q}Q^{-1}d\mu(Q)+(1/2)\int PQ\bar{Q}Q^{-1}Pd\mu(Q)\,.$$

Applying both sides to the zero vector we get $1-\varkappa^2=0$ which contradicts (4.15). If $\xi=1$ we have $\Delta=\bar{Q}\Delta(\omega)$, where $\bar{Q}\in\mathrm{O}(n)_p$. Then $\Delta(\varkappa)=(1/2)\int d\mu(Q)(Q\bar{Q}\Delta(\omega)Q^{-1}+PQ\bar{Q}\Delta(\omega)Q^{-1}P)$ and applying to the zero vector gives $\omega=\varkappa$ so that, since $\Delta(\varkappa)$ is non singular, we get $1_n=(1/2)\int d\mu(Q)(Q\bar{Q}Q^{-1}+PQ\bar{Q}Q^{-1}P)$.

Taking the trace gives $n=\mathrm{Tr}(\bar{Q})$ which implies $\bar{Q}=1_n$ and therefore $\Delta=\Delta(\varkappa)$.

Finally, consider the case

$$0<\xi<1\,,\qquad 0\leqq\omega<1\,. \tag{4.22}$$

Let $p^{(1)}=(1/[(1-\xi^2)+\xi^2\omega^2]^{\frac{1}{2}})(0,\dots,0,(1-\xi^2)^{\frac{1}{2}},\xi\omega)$ and $p^{(2)}=(0,\dots,0,(1-\xi^2)^{\frac{1}{2}},\xi)$. Since $\Delta(\xi,\omega)$ maps $p^{(1)}$ to $p^{(2)}$ [compare (3.9)] whereas $\Delta p=p$, we have from (4.21)

$$\Delta=\bar{Q}_2D(\xi;\omega;m_1,m_2)\bar{Q}_1\,, \tag{4.23}$$

where

$$\bar{Q}_2, \bar{Q}_1 \in \mathrm{SO(n)}_p, \quad m_1 = 0 \quad \text{or} \quad 1, \quad m_2 = 0 \quad \text{or} \quad 1$$

and

$$D(\xi; \omega; m_1, m_2) = (c, S),$$

where

$$\begin{aligned} & c_1 = \ldots = c_{n-2} = 0, \\ & c_{n-1} = (-1)^{m_2+1} \xi (1-\xi^2)^{\frac{1}{2}} (1-\omega^2), \\ & c_n = \xi^2(1-\omega^2), S_n = \ldots = S_{n-2,n-2} = [(1-\xi^2) + \xi^2\omega^2]^{\frac{1}{2}}, \\ & S_{n-1,n-1} = (-1)^{m_1+m_2}\omega, S_{nn} = (1-\xi^2) + \xi^2\omega^2, \\ & S_{n-1,n} = (-1)^{m_2} \xi (1-\xi^2)^{\frac{1}{2}} (1-\omega^2) \end{aligned}$$

and $S_{ij} = 0$ if $i \neq j$ and $(i, j) \neq (n-1, n)$. Hence

$$\begin{aligned} \Delta(\varkappa) = {} & (1/2) \int Q\bar{Q} D(\xi; \omega; m_1, m_2) Q^{-1} d\mu(Q) \\ & + (1/2) \int PQ\bar{Q} D(\xi; \omega; m_1, m_2) Q^{-1} P d\mu(Q), \end{aligned} \tag{4.24}$$

where $\bar{Q} = \bar{Q}_1 \bar{Q}_2$. Equating the (n, n) matrix elements of the linear parts of the two sides of (4.24) gives

$$\varkappa^2 = (1-\xi^2) + \xi^2\omega^2. \tag{4.25}$$

Introducing the $(n-1) \times (n-1)$ matrix

$$E(\xi; \omega; m_1 + m_2) = \mathrm{diag}\{[(1-\xi^2) + \xi^2\omega^2]^{\frac{1}{2}}, \ldots, [(1-\xi^2) + \xi^2\omega^2]^{\frac{1}{2}}, (-1)^{m_1+m_2}\omega\}$$

we get from (4.24)

$$\begin{aligned} & (1/2) \int_{\mathrm{SO(n-1)}} Q\bar{Q} E(\xi; \omega; m_1 + m_2) Q^{-1} d\mu(Q) \\ & \quad + (1/2) \int_{\mathrm{SO(n-1)}} PQ\bar{Q} E(\xi; \omega; m_1 + m_2) Q^{-1} P d\mu(Q) = \varkappa 1_{n-1}, \end{aligned} \tag{4.26}$$

where we have used the same symbols for the restrictions of P, Q and $\bar{Q}$ to $\mathbb{R}^{n-1}$. Taking the squares of the traces of both sides of (4.26) and using Schwartz's inequality gives

$$\begin{aligned} (n-1)^2\varkappa^2 = {} & [\mathrm{Tr}(\bar{Q} E(\xi; \omega; m_1 + m_2))]^2 \leqq [\mathrm{Tr}(\bar{Q}^T Q)] \\ & \times [\mathrm{Tr}(E(\xi; \omega; m_1 + m_2)^2] = (n-1)\{(n-2)[(1-\xi^2) + \xi^2\omega^2] + \omega^2\} \end{aligned}$$

whereby, using (4.25), we get $(1-\xi^2) + \xi^2\omega^2 \leqq \omega^2$ which contradicts (4.22). ∎

5. Geometrical Considerations

Among the extreme points of D_n are those which map S_n into itself (in the physical case $n = 3$ they correspond to the transformations which map pure states to pure states). There are two types of such maps: those of the form $(0, Q)$, $Q \in \mathrm{O(n)}$, and those which map B_n onto a point of S_n. They are obtained by setting $\varkappa = 1$ and, respectively, $\varkappa = 0$ and $\delta = 1$ in (4.1). In the physical case $n = 3$, $(0, Q)$ corresponds to a unitary transformation on the density matrices $\varrho \to u\varrho u^*$, $uu^* = 1_2$, if $Q \in \mathrm{SO(3)}$.

It corresponds to a transformation of the form $\varrho \to u\varrho^T u^*$, $uu^* = 1_2$, if $Q \in O(3)$, $\det Q = -1$. Transposition on the density matrices corresponds to the antiunitary transformation $\{x_i\} \to \{\bar{x}_i\}$ on $\mathbb{C}^2$. (consider the pure states $\varrho = \{\varrho_{ij} = x_i \bar{x}_j\}$, then $\varrho_{ij} \to \bar{x}_i x_j = \varrho_{ji}$ and extend by linearity).

We now describe the geometrical meaning of the parametrizations of D_n given in Theorem 1. Let $\Delta = (b, T)$ be an element of D_n and write $(b, T) = (Q_1 a, Q_1 \Lambda Q_2)$ with $Q_1, Q_2 \in O(n)$, (a, Λ) canonical, $\Lambda = \mathrm{diag}\{\lambda_1, \lambda_2, \ldots, \lambda_n\}$. (a, Λ) maps S_n to an ellipsoid E_n whose axes have lengths $\lambda_1, \lambda_2, \ldots, \lambda_n$ and whose center a lies in the positive cone. If $\lambda_1 = 0$, E_n degenerates to a point and Δ is extreme or not according to whether or not $a \in S_n$. Assume $\lambda_1 > 0$ and write $a_i = \beta \xi_i (1 - \alpha \omega_i^2) = \beta \xi_i (1 - \alpha v \eta_i^2)$ and $\lambda_i = \alpha \beta \omega_i (\sum_{j=1}^n \xi_j^2 \omega_j^2)^{\frac{1}{2}} = \alpha \beta v \eta_i$, $i = 1, 2, \ldots, n$, as in Theorem 1. The geometrical meaning of the parameters $\omega_1, \omega_2, \ldots, \omega_n$ is clear from the relation $\omega_i = \lambda_i / \lambda_1$. As regards the vector ξ, take $\beta = 1$ and $\alpha < 1$. Then $E_n \cap S_n = \{\xi\}$. By (3.9), the point v of S_n which is mapped to ξ by $(a, \Lambda) = \Delta(\alpha; 1; \xi; \omega)$, $\alpha < 1$, is given by (3.8) and we have $\eta_l = v_l / \xi_l$. As an illustration, in the case $n = 3$, for fixed ξ and as ω_2 and ω_3 range in their domain $0 \leqq \omega_3 \leqq \omega_2 \leqq 1$, the point v sweeps the spherical triangle whose vertices are the points ξ, $(1, 0, 0)$ and $(\xi_1/(\xi_1^2 + \xi_2^2)^{\frac{1}{2}}, \xi_2/(\xi_1^2 + \xi_2^2)^{\frac{1}{2}}, 0)$. β and α are parameters of convex combinations. Indeed we have i) $\Delta(\alpha; \beta; \xi; \omega) = \beta \Delta(\alpha; 1; \xi; \omega) + (1 - \beta) \Delta(\alpha; 0; \xi; \omega)$ [note that $\Delta(\alpha; 0; \xi; \omega) = (0, 0_n)$] and ii) $\Delta(\alpha; 1; \xi; \omega) = \alpha \Delta(1; 1; \xi; \omega) + (1 - \alpha) \Delta(0; 1; \xi; \omega)$ [see (3.7) and note that $\xi \in \Delta(1; 1; \xi; \omega)(S_n) \cap S_n$ and that $\Delta(0; 1; \xi; \omega)$ maps B_n to ξ]. Now take $\alpha = \beta = 1$ and $\xi_1 > 0$. Then, as it is seen from (3.5), if $\omega_s = 1$ and $\omega_{s+1} < 1$ the intersection $E_n \cap S_n$ is an $(s-1)$-dimensional sphere and we obtain an extreme map if $s = n - 1$ [$\delta < 1$ in (4.1)]. The remaining extreme maps are obtained as the limit of the latter as $\xi_n \to 1$ for which the $(n-2)$-dimensional sphere $E_n \cap S_n$ degenerates to the "north pole" $p = (0, \ldots, 0, 1)$ [$\delta = 1$ in (4.1)]. To be specific, divide $\underline{\mathrm{extr}\, D_n}$ into the two subsets A and B which correspond to taking $\delta = 1$ and, respectively, $0 < \delta < 1$, $\varkappa < 1$ in (4.1): $A = \{\Delta(1, \varkappa) | 0 \leqq \varkappa \leqq 1\}$ and $B = \{\Delta(\delta, \varkappa) | 0 < \delta < 1; \varkappa < 1\}$.

We have $\Delta(1, \varkappa)(S_n) \cap S_n = p$ if $\varkappa < 1$ whereas, if $\delta < 1$ and $\varkappa < 1$, $\Delta(\delta, \varkappa)(S_n) \cap S_n$ is the $(n-2)$-dimensional hypersphere $\hat{\Sigma} = \{x | x \in S_n, x_n = \delta\}$. Now assume Δ to be an element of D_n' such that $\Delta(S_n) \cap S_n$ is reduced to a point q and assume that Δ can be expressed as a non trivial convex combination $\Delta = \gamma \Delta_1 + (1 - \gamma) \Delta_2$ of elements of D_n. Then, there is at least one direction in the hyperplane which is tangent to S_n at q along which either $\Delta_1(S_n)$ or $\Delta_2(S_n)$ have at q a smaller curvature than $\Delta(S_n)$ has at q along the same direction. If $\Delta = \Delta(1, \varkappa)$ this is impossible since $\Delta(1, \varkappa)(S_n)$ has at q and along all directions the same curvature as S_n. This explains intuitively why the elements of A are extreme. As to the elements of B, if we write $\Delta(\delta, \varkappa)$ as a convex combination $\Delta(\delta, \varkappa) = \gamma \Delta_1 + (1 - \gamma) \Delta_2$, we must have that $\Delta(\delta, \varkappa)$, Δ_1 and Δ_2 agree on the $(n-2)$-dimensional hypersphere $\Sigma = \{x | x \in S_n, x_n = u_n\}$, where u_n is given by (4.6) with $\xi_n = \delta$, $\omega_n = \varkappa$. Here, the dimensionality of Σ is just large enough as to imply $\Delta_1 = \Delta_2 = \Delta(\delta, \varkappa)$. On the other hand, it is no more so if Δ_1, Δ_2 and $\Delta (= \gamma \Delta_1 + (1 - \gamma) \Delta_2)$ are to agree on an hypersphere of S_n whose dimension is less than $n - 2$ (except in the case when $\Delta = Q_1 \tilde{\Delta} Q_2$ with $Q_1, Q_2 \in O(n)$ and $\tilde{\Delta} \in A$).

Finally, we remark that the extreme elements of D_n have a high simmetry. Precisely, if $(b, T) \in D_n'$ is extreme, then there exists $C \in O(n)$ and a subgroup of $O(n)$, say Γ, isomorphic to $O(n-1)$, such that $QTC^{-1}Q^{-1}C = T$ and $Qb = b$ for every $Q \in \Gamma$. However, this condition is not sufficient for (b, T) to be extreme, as the example $\beta = \alpha = \omega_{n-1} = 1$, $\omega_n < 1$, $\xi_n = 0$ shows.

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