MATH. SCAND. 109 (2011), 225–239

MATRICES OF UNITARY MOMENTS

KEN DYKEMA and KATE JUSCHENKO*

Abstract

We investigate certain matrices composed of mixed, second-order moments of unitaries. The unitaries are taken from C*-algebras with moments taken with respect to traces, or, alternatively, from matrix algebras with the usual trace. These sets are of interest in light of a theorem of E. Kirchberg about Connes' embedding problem.

1. Introduction

One fundamental question about operator algebras is Connes' embedding problem, which in its original formulation asks whether every II_1-factor $\mathcal{M}$ embeds in the ultrapower R^ω of the hyperfinite II_1-factor R. This is well known to be equivalent to the question of whether all elements of II_1-factors possess matricial microstates, (which were introduced by Voiculescu [16] for free entropy), namely, whether such elements are approximable in $*$-moments by matrices. Connes' embedding problem is known to be equivalent to a number of different problems, in large part due to a remarkable paper [6] of Kirchberg. (See also the survey [10], and the papers [11], [12], [13], [1], [14], [3], [7], [15], [5] for results with bearing on Connes' embedding problem.)

In Proposition 4.6 of [6], Kirchberg proved that, in order to show that a finite von Neumann algebra $\mathcal{M}$ with faithful tracial state τ embeds in R^ω, it would be enough to show that for all n, all unitary elements $U_1, \dots, U_n$ in $\mathcal{M}$ and all $\epsilon > 0$, there is $k \in \mathbf{N}$ and there are $k \times k$ unitary matrices $V_1, \dots, V_n$ such that $|\tau(U_i^* U_j) - \mathrm{tr}_k(V_i^* V_j)| < \epsilon$ for all $i, j \in \{1, \dots, n\}$, where tr_k is the normalized trace on $M_k(\mathbf{C})$. (He also required $|\tau(U_i) - \mathrm{tr}_k(V_i)| < \epsilon$, but this formally stronger condition is easily satisfied by taking the $n+1$ unitaries $U_1, \dots, U_n, U_{n+1} = I$ in $\mathcal{M}$ finding $k \times k$ unitaries $\widetilde{V}_1, \dots, \widetilde{V}_{n+1}$, so that $|\tau(U_i^* U_j) - \mathrm{tr}_k(\widetilde{V}_i^* \widetilde{V}_j)| < \epsilon$, and letting $V_i = \widetilde{V}_{n+1}^* \widetilde{V}_i$.) It is, therefore, of interest to consider the set of possible second-order mixed moments of unitaries in such $(\mathcal{M}, \tau)$ or, equivalently, of unitaries in C*-algebras with respect to

* Ken Dykema's research supported in part by NSF grant DMS-0600814, Kate Juschenko's research supported in part by NSF grant DMS-0503688.

Received 10 September 2010.

tracial states. (See also [12], where some similar sets were considered by F. Rădulescu.)

DEFINITION 1.1. Let $\mathcal{G}_n$ be the set of all $n \times n$ matrices X of the form

$$X = (\tau(U_i^* U_j))_{1 \le i, j \le n} \tag{1}$$

as $(U_1, \dots, U_n)$ runs over all n-tuples of unitaries in all C*-algebras A possessing a faithful tracial state τ.

REMARK 1.2. The set-theoretic difficulties in the phrasing of Definition 1.1 can be evaded by insisting that A be represented on a given separable Hilbert space. Alternatively, let $\mathfrak{A} = \mathbf{C}\langle U_1, \dots, U_n \rangle$ denote the universal, unital, complex $*$-algebra generated by unitary elements $U_1, \dots, U_n$. A linear functional ϕ on $\mathfrak{A}$ is positive if $\phi(a^* a) \ge 0$ for all $a \in \mathfrak{A}$. By the usual Gelfand-Naimark-Segal construction, any such positive functional ϕ gives rise to a Hilbert space $L^2(\mathfrak{A}, \phi)$ and a $*$-representation $\pi_\phi : \mathfrak{A} \to B(L^2(\mathfrak{A}, \phi))$. Thus, the set $\mathcal{G}_n$ equals the set of all matrices X as in (1) as τ runs over all positive, tracial, unital, linear functionals τ on $\mathfrak{A}$.

DEFINITION 1.3. Let $\mathcal{F}_n$ be the closure of the set

$$\left\{ (\mathrm{tr}_k(V_i^* V_j))_{1 \le i, j \le n} \mid k \in \mathbf{N},\, V_1, \dots, V_n \in \mathcal{U}_k \right\},$$

where $\mathcal{U}_k$ is the group of $k \times k$ unitary matrices.

A *correlation matrix* is a complex, positive semidefinite matrix having all diagonal entries equal to 1. Let Θ_n be the set of all $n \times n$ correlation matrices. Clearly, we have

$$\mathcal{F}_n \subseteq \mathcal{G}_n \subseteq \Theta_n.$$

Kirchberg's result is that Connes' embedding problem is equivalent to the problem of whether $\mathcal{F}_n = \mathcal{G}_n$ holds for all n.

PROPOSITION 1.4. *For each n,*

(i) *$\mathcal{F}_n$ and $\mathcal{G}_n$ are invariant under conjugation with $n \times n$ diagonal unitary matrices and permutation matrices,*

(ii) *$\mathcal{F}_n$ and $\mathcal{G}_n$ are compact, convex subsets of Θ_n,*

(iii) *$\mathcal{F}_n$ and $\mathcal{G}_n$ are closed under taking Schur products of matrices.*

PROOF. Part (i) is clear. Note that Θ_n is a norm-bounded subset of $M_n(\mathbf{C})$. That $\mathcal{F}_n$ is closed is evident. That $\mathcal{G}_n$ is closed follows from the description in Remark 1.2 and the fact that a pointwise limit of positive traces on $\mathfrak{A}$ is a positive trace. This proves compactness. Convexity of $\mathcal{F}_n$ follows from by observing that if V is a $k \times k$ unitary and V' is a $k' \times k'$ unitary, then for arbitrary $\ell, \ell' \in \mathbf{N}$,

$$\underbrace{V \oplus \cdots \oplus V}_{\ell \text{ times}} \oplus \underbrace{V' \oplus \cdots \oplus V'}_{\ell' \text{ times}}$$

can be realized as a block-diagonal $(k\ell + k'\ell') \times (k\ell + k'\ell')$ matrix whose normalized trace is

$$\frac{k\ell}{k\ell + k'\ell'} \operatorname{tr}_k(V) + \frac{k'\ell'}{k\ell + k'\ell'} \operatorname{tr}_{k'}(V').$$

Convexity of $\mathscr{G}_n$ follows because a convex combination of positive traces on $\mathfrak{A}$ is a positive trace. This proves (ii).

Closedness of $\mathscr{F}_n$ under taking Schur products follows by observing that if V and V' are unitaries as above, then $V \otimes V'$ is a $kk' \times kk'$ unitary whose normalized trace is $\operatorname{tr}_k(V)\operatorname{tr}_{k'}(V')$. For $\mathscr{G}_n$, we observe that if U and respectively, U', are unitaries in C*-algebras A and A' having tracial states τ and τ', then the spatial tensor product C*-algebra $A \otimes A'$ has tracial state $\tau \otimes \tau'$ that takes value $\tau(U)\tau'(U')$ on the unitary $U \otimes U'$. This proves (iii).

Since it is important to decide whether we have $\mathscr{F}_n = \mathscr{G}_n$ for all n, it is interesting to learn more about the sets $\mathscr{F}_n$. A first question is whether $\mathscr{F}_n = \Theta_n$ holds. In Section 2, we show that this holds for $n = 3$ but fails for $n \geq 4$. The proof relies on a characterization of extreme points of Θ_n, and it uses also the set $\mathscr{C}_n$ of matrices of moments of commuting unitaries. In Section 3 we prove $M_n(\mathbf{R}) \cap \Theta_n \subseteq \mathscr{F}_n$, and some further results concerning $\mathscr{C}_n$. In Section 4, we show that $\mathscr{F}_n$ has nonempty interior, as a subset of Θ_n.

2. Extreme points of Θ_n and some consequences

The set Θ_n of $n \times n$ correlation matrices is embedded in the affine space consisting of the self-adjoint complex matrices having all diagonal entries equal to 1; it is just the intersection of the set of positive, semidefinite matrices with this space. Every element of Θ_n is bounded in norm by n (*cf* Remark 2.9), and Θ_n is a compact, convex space. Since, in the space of self-adjoint matrices, every positive definite matrix is the center of a ball consisting of positive matrices, it is clear that the boundary of Θ_n (for $n \geq 2$) consists of singular matrices.

The extreme points of Θ_n and $\Theta_n \cap M_n(\mathbf{R})$ have been studied in [2], [9], [4] and [8]. In this section, we will use an easy characterization of the extreme points of Θ_n to draw some conclusions about matrices of unitary moments. The papers cited above contain the facts about extreme points of Θ_n found below, and have results going well beyond; the elementary techniques used here to characterize extreme points are essentially the same as used by Li and Tam [8]. In fact, we learned of these and the other results on correlation matrices only after our first version of this paper appeared. Because our presentation has a slightly different emphasis and these ideas are used later in examples, we provide the proofs, which are brief.

We also introduce the subset $\mathscr{C}_n$ of $\mathscr{F}_n$, consisting of matrices of moments of commuting unitaries. The new result in the section is Proposition 2.10, from which we can conclude that there are no rank 2 extreme points of $\mathscr{G}_n$ and, thus, $\mathscr{G}_4 \neq \mathscr{F}_4$.

This is a convenient place to recall the following standard fact. We include a proof for convenience.

LEMMA 2.1. *The set of all $X \in \Theta_n$ of rank r is the set of all frame operators $X = F^*F$ of frames $F = (f_1, \dots, f_n)$, consisting of n unit vectors $f_j \in \mathbf{C}^r$, where $r = \operatorname{rank}(X)$. If, in addition, $X \in M_n(\mathbf{R})$, then the frame $f_1, \dots, f_n$ can be chosen in $\mathbf{R}^r$.*

PROOF. Every frame operator F^*F as above clearly belongs to Θ_n and has rank r.

Recall that the support projection of a Hermitian matrix X is the projection onto the orthocomplement of the nullspace of X. Suppose $X \in \Theta_n$ has $\operatorname{rank}(X) = r$. Let P be the support projection of X and let $\lambda_1 \geq \cdots \geq \lambda_r > 0$ be the nonzero eigenvalues of X with corresponding orthonormal eigenvectors $g_1, \dots, g_r \in \mathbf{C}^n$. Let $V : \mathbf{C}^r \to P(\mathbf{C}^n)$ be the isometry defined by $e_i \mapsto g_i$, where $e_1, \dots, e_r$ are the standard basis vectors of $\mathbf{C}^r$. So $P = VV^*$. Then $X = F^*F$, where F is the $r \times n$ matrix

$$F = V^*X^{1/2} = \operatorname{diag}(\lambda_1, \dots, \lambda_r)^{1/2}V^*.$$

If $f_1, \dots, f_n \in \mathbf{C}^r$ are the columns of F, then $\|f_i\| = X_{ii} = 1$ and the linear span of $f_1 \dots, f_n$ is $\mathbf{C}^r$. Thus, $f_1, \dots, f_n$ comprise a frame.

If X is real, then the vectors $g_1, \dots, g_r$ can be chosen in $\mathbf{R}^n$. Then V and $X^{1/2}$ are real matrices and $f_1, \dots, f_n$ are in $\mathbf{R}^r$.

LEMMA 2.2. *Let $X \in M_n(\mathbf{C})$ be a positive semidefinite matrix and let P be the support projection of X. Then a Hermitian $n \times n$ matrix Y has the property that there is $\epsilon > 0$ such that $X + tY$ is positive semidefinite for all $t \in (-\epsilon, \epsilon)$ if and only if $Y = PYP$.*

PROOF. If $X = 0$ then this is trivially true, so suppose $X \neq 0$. After conjugating with a unitary, we may without loss of generality assume $P = \operatorname{diag}(1, \dots, 1, 0, \dots, 0)$ with $\operatorname{rank}(X) = \operatorname{rank}(P) = r$. Then PXP, thought of as an $r \times r$ matrix, is positive definite. By continuity of the determinant, we see that if $Y = PYP$, then Y enjoys the property described above.

Conversely, if $Y \neq PYP$, then we may choose two standard basis vectors e_i and e_j for $i \leq r < j$, such that the compressions of X and Y to the subspace spanned by e_i and e_j are given by the matrices

$$\widehat{X} = \begin{pmatrix} x & 0 \\ 0 & 0 \end{pmatrix}, \qquad \widehat{Y} = \begin{pmatrix} a & b \\ \overline{b} & c \end{pmatrix}$$

for some $x > 0$, $a, c \in \mathbf{R}$ and $b \in \mathbf{C}$ with c and b not both zero. But

$$\det(\widehat{X} + t\widehat{Y}) = txc + t^2(ac - |b|^2).$$

If $c \neq 0$, then $\det(\widehat{X}+t\widehat{Y}) < 0$ for all nonzero t sufficiently small in magnitude and of the appropriate sign, while if $c = 0$ then $b \neq 0$ and $\det(\widehat{X} + t\widehat{Y}) < 0$ for all $t \neq 0$.

Proposition 2.3. *Let $n \in \mathbf{N}$, let $X \in \Theta_n$ and let P be the support projection of X. A necessary and sufficient condition for X to be an extreme point of Θ_n is that there be no nonzero Hermitian $n \times n$ matrix Y having zero diagonal and satisfying $Y = PYP$. Consequently, if X is an extreme point of Θ_n, then* $\operatorname{rank}(X) \leq \sqrt{n}$.

Proof. X is an extreme point of Θ_n if and only if there is no nonzero Hermitian $n \times n$ matrix Y such that $X + tY \in \Theta_n$ for all $t \in \mathbf{R}$ sufficiently small in magnitude. Now use Lemma 2.2 and the fact that Θ_n consists of the positive semidefinite matrices with all diagonal values equal to 1.

For the final statement, if $r = \operatorname{rank}(X)$ then the set of Hermitian matrices with support projection under P is a real vector space of dimension r^2, while the space of $n \times n$ Hermitian matrices with zero diagonal has dimension $n^2 - n$. If $r^2 > n$, then the intersection of these two spaces is nonzero.

Proposition 2.4. *Let $X \in \Theta_n$. Suppose $f_1, \dots, f_n$ is a frame consisting of n unit vectors in $\mathbf{C}^r$, where $r = \operatorname{rank}(X)$, so that $X = F^*F$ with $F = (f_1, \dots, f_n)$ is the corresponding frame operator. (See Lemma 2.1.) Then X is an extreme point of Θ_n if and only if the only $r \times r$ self-adjoint matrix Z satisfying $\langle Zf_j, f_j \rangle = 0$ for all $j \in \{1, \dots, n\}$ is the zero matrix.*

Proof. Since F is an $r \times n$ matrix of rank r, the map $M_r(\mathbf{C})_{\text{s.a.}} \to M_n(\mathbf{C})_{\text{s.a.}}$ given by $Z \mapsto F^*ZF$ is an injective linear map onto $PM_n(\mathbf{C})_{\text{s.a.}}P$, where P is the support projection of X. If $Y = F^*ZF$, then $Y_{jj} = \langle Zf_j, f_j \rangle$. Thus, the condition for X to be extreme now follows from the characterization found in Proposition 2.3.

PROPOSITION 2.5. *Let $n \in \mathbf{N}$ and suppose $X \in \Theta_n$ satifies* $\operatorname{rank}(X) = 1$. *Then X is an extreme point of Θ_n and $X \in \mathcal{F}_n$. Moreover, using the notation introduced in Remark 1.2, we have*

$$\text{(2)} \quad \operatorname{conv}\{X \in \Theta_n \mid \operatorname{rank}(X) = 1\} = \left\{ (\tau(U_i^* U_j))_{1 \le i,j \le n} \;\middle|\; \begin{array}{l} \tau : \mathfrak{A} \to \mathbf{C} \text{ a positive trace,} \\ \tau(1) = 1, \pi_\tau(\mathfrak{A}) \text{ commutative} \end{array} \right\}$$

and this set is closed in Θ_n.

NOTATION 2.6. We let $\mathcal{C}_n$ denote the set given in (2). Thus, we have $\mathcal{C}_n \subseteq \mathcal{F}_n$. Moreover, (*cf* Remark 1.2), $\mathcal{C}_n$ is the set of matrices as in (1) where $(U_1, \dots, U_n)$ runs over all n-tuples of commuting unitarires in C*-algebras A with faithful tracial state τ.

PROOF OF PROPOSITION 2.5. By Lemma 2.1, we have $X = F^* F$ where $F = (f_1, \dots, f_n)$ for complex numbers f_j with $|f_j| = 1$. Using Proposition 2.4, we see immediately that X is an extreme point of Θ_n. Thinking of each f_j as a 1×1 unitary, we have $X \in \mathcal{F}_n$ and, moreover, $X = (\tau(U_i^* U_j))_{1 \le i,j \le n}$, where $\tau : \mathfrak{A} \to \mathbf{C}$ is the character defined by $\tau(U_i) = f_i$; in fact, it is apparent that every character on $\mathfrak{A}$ yields a rank one element of Θ_n. Since the set of traces τ on $\mathfrak{A}$ having $\pi_\tau(\mathfrak{A})$ commutative is convex, this implies the inclusion $\subseteq$ in (2).

That the left-hand-side of (2) is compact follows from Caratheodory's theorem, because the rank one projections form a compact set. If $\tau : \mathfrak{A} \to \mathbf{C}$ is a positive trace with $\tau(1) = 1$ and $\pi_\tau(\mathfrak{A})$ commutative, then $\tau = \psi \circ \pi_\tau$ for a state ψ on the C*-algebra completion of $\pi_\tau(\mathfrak{A})$. Since every state on a unital, commutative C*-algebra is in the closed convex hull of the characters of that C*-algebra, τ is itself the limit in norm of a sequence of finite convex combinations of characters of $\mathfrak{A}$. Thus, $X = (\tau(U_i^* U_j))_{1 \le i,j \le n}$ is the limit of a sequence of finite convex combinations of rank one elements of Θ_n, and we have $\supseteq$ in (2).

REMARK 2.7. We see immediately from (2) that $\mathcal{C}_n$ is a closed convex set that is closed under conjugation with diagonal unitary matrices and permutation matrices; also, since the set of rank one elements of Θ_n is closed under taking Schur products, so is the set $\mathcal{C}_n$. Furthermore, since $\mathcal{C}_n$ lies in a vector space of real dimension $m := n^2 - n$, by Caratheodory's theorem every element of $\mathcal{C}_n$ is a convex combination of not more than $m + 1$ rank one elements of Θ_n.

An immediate application of Propositions 2.3 and 2.5 is the following.

COROLLARY 2.8. *The extreme points of Θ_3 are precisely the rank one elements of Θ_3. Moreover, we have*

$$\mathcal{C}_3 = \mathcal{F}_3 = \mathcal{G}_3 = \Theta_3.$$

REMARK 2.9. Let $X \in \mathcal{G}_n$ and take A, τ and $U_1, \dots, U_n$ as in Definition 1.1 so that (1) holds, and assume without loss of generality that τ is faithful on A. If we identify $M_n(A)$ with $A \otimes M_n(\mathbf{C})$, then we have $X = n(\tau \otimes \mathrm{id}_{M_n(\mathbf{C})})(P)$, where P is the projection

$$P = \frac{1}{n} \begin{pmatrix} U_1^* \\ U_2^* \\ \vdots \\ U_n^* \end{pmatrix} \begin{pmatrix} U_1 & U_2 & \dots & U_n \end{pmatrix}$$

in $M_n(A)$. If $c = (c_1, \dots, c_n)^t \in \mathbf{C}^n$ is such that $Xc = 0$, then this yields $\tau(Z^*Z) = 0$, where $Z = c_1U_1 + \dots + c_nU_n$. Since τ is a faithful, we have $Z = 0$.

PROPOSITION 2.10. *Let $n \in \mathbf{N}$. If $X \in \mathcal{G}_n$ and* $\operatorname{rank}(X) \leq 2$*, then $X \in \mathcal{C}_n$.*

PROOF. If $\operatorname{rank}(X) = 1$, then this follows from Propostion 2.5, so assume $\operatorname{rank}(X) = 2$. Let $\tau : \mathfrak{A} \to \mathbf{C}$ be a positive, unital trace such that $X = (\tau(U_i^*U_j))_{1 \leq i,j \leq n}$ and let $\pi_\tau : \mathfrak{A} \to B(L^2(\mathfrak{A}, \tau))$ be the $*$-representation as described in Remark 1.2. Let $\sigma : \mathfrak{A} \to \pi_\tau(\mathfrak{A})$ be the $*$-representation defined by $\sigma(U_i) = \pi_\tau(U_1)^*\pi_\tau(U_i)$ for each $i \in \{1, \dots, n\}$ and let $\tau' = \tau \circ \sigma$. Then τ' is a positive, unital trace on $\mathfrak{A}$ and the matrix $(\tau'(U_i^*U_j))_{1 \leq i,j \leq n}$ is equal to X. Furthermore, $\pi_{\tau'}(U_1) = I$. Consequently, we may without loss of generality assume $\pi_\tau(U_1) = I$.

Let $e_1, \dots, e_n$ denote the standard basis vectors of $\mathbf{C}^n$. Let $i, j \in \{2, \dots, n\}$, with $i \neq j$. Since $\operatorname{rank}(X) = 2$, there are $c_1, c_i, c_j \in \mathbf{C}$ with $c_1 \neq 0$ such that $X(c_1e_1 + c_ie_i + c_je_j) = 0$. By Remark 2.9, we have $\pi_\tau(c_1I + c_iU_i + c_jU_j) = 0$. We do not have $c_i = c_j = 0$, so assume $c_i \neq 0$. If $c_j = 0$, then $\pi_\tau(U_i)$ is a scalar multiple of the identity, while if $c_j \neq 0$, then $\pi_\tau(U_i)$ and $\pi_\tau(U_j)$ generate the same C*-algebra, which is commutative. In either case, we have that the $*$-algebras generated by $\pi_\tau(U_i)$ and $\pi_\tau(U_j)$ commute with each other. Therefore, $\pi_\tau(\mathfrak{A})$ is commutative, and $X \in \mathcal{C}_n$.

COROLLARY 2.11. $\mathcal{G}_4 \neq \Theta_4$.

PROOF. Combining Proposition 2.10 and Proposition 2.5, we see that $\mathcal{G}_4$ has no extreme points of rank 2. It will suffice to find an extreme point X of Θ_4 with $\operatorname{rank}(X) = 2$. By Proposition 2.4, it will suffice to find four unit vectors $f_1, \dots, f_4$ spanning $\mathbf{C}^2$ such that the only self-adjoint $Z \in M_2(\mathbf{C})$ satisfying $\langle Zf_i, f_i \rangle = 0$ for all $i = 1, \dots, 4$ is the zero matrix. It is easily verified that the frame

$$f_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad f_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad f_3 = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}, \quad f_4 = \begin{pmatrix} i/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}$$

does the job, and, with $F = (f_1, f_2, f_3, f_4)$, this yields the matrix

$$X = F^*F = \begin{pmatrix} 1 & 0 & \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \\ 0 & 1 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 1 & \frac{1+i}{2} \\ \frac{-i}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \frac{1-i}{2} & 1 \end{pmatrix} \in \Theta_4 \backslash \mathscr{G}_4. \tag{3}$$

REMARK 2.12. We cannot have $\mathscr{C}_n = \mathscr{F}_n$ for all n, because by an easy modification of Kirchberg's proof of Proposition 4.6 of [6], this would imply that $M_2(\mathbf{C})$ can be faithfully represented in a commutative von Neumann algebra. (This argument shows that for some n there must be two-by-two unitaries $V_1, \ldots, V_n$ such that the matrix $(\mathrm{tr}_2(V_i^* V_j))_{1 \le i, j \le n}$ does not belong to $\mathscr{C}_n$.) In fact, in Proposition 3.6 we will show $\mathscr{F}_6 \neq \mathscr{C}_6$. However, we don't know whether $\mathscr{F}_n = \mathscr{C}_n$ holds or not for $n = 4$ or $n = 5$.

3. Real matrices

The main result of this section is the following, which easily follows from the usual representation of the Clifford algebra.

THEOREM 3.1. *For every $n \in \mathbf{N}$, we have*

$$M_n(\mathbf{R}) \cap \Theta_n \subseteq \mathscr{F}_n.$$

We first recall the representation of the Clifford algebra. Let Λ be a linear map from a real Hilbert space H into the bounded, self-adjoint operators $B(\mathscr{K})_{\mathrm{s.a.}}$, for some complex Hilbert space $\mathscr{K}$, satisfying

$$\Lambda(x)\Lambda(y) + \Lambda(y)\Lambda(x) = 2\langle x, y\rangle I_H, \qquad (x, y \in H). \tag{4}$$

The real algebra generated by range of Λ is uniquely determined by H and called the real Clifford algebra.

Consider a real Hilbert space H of finite dimension r with its canonical basis $\{e_i\}$. Let

$$U = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad V = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Then the real Clifford algebra of H has the following representation by $2^r \times 2^r$ matrixes

$$\Lambda(x) = \sum \lambda_i U^{\otimes i-1} \otimes V \otimes I_2^{\otimes(n-i)},$$

where $x = \sum \lambda_i e_i$. It easy to check that the relation (4) is satisfied. Moreover if $\|x\| = 1$ then $\Lambda(x)$ is symmetry, i.e. $\Lambda(x)^* = \Lambda(x)$ and $\Lambda(x)^2 = I$.

PROOF OF THEOREM 3.1. Let r be the rank of X. By Lemma 2.1, there are unit vectors $f_1, \dots, f_n \in \mathbf{R}^r$ such that $X_{i,j} = \langle f_i, f_j \rangle$ for all i and j. Taking Λ as described above, we get $2^r \times 2^r$ unitary matrices $\Lambda(f_i)$ (in fact, they are symmetries), and from (4) we have $\mathrm{tr}(\Lambda(f_i)\Lambda(f_j)) = \langle f_i, f_j \rangle$.

Below is the result for real matrices that is entirely analogous to Proposition 2.3.

PROPOSITION 3.2. *Let $n \in \mathbf{N}$, let $X \in M_n(\mathbf{R}) \cap \Theta_n$ and let P be the support projection of X. A necessary and sufficient condition for X to be an extreme point of $M_n(\mathbf{R}) \cap \Theta_n$ is that there be no nonzero Hermitian real $n \times n$ matrix Y having zero diagonal and satisfying $Y = PYP$. Consequently, if X is an extreme point of $M_n(\mathbf{R}) \cap \Theta_n$ and $r = \mathrm{rank}(X)$, then $r(r+1)/2 \leq n$.*

PROOF. This is just like the proof of Proposition 2.3, the only difference being that the dimension of $PM_n(\mathbf{R})_{\mathrm{s.a.}}P$ for a projection P of rank r is $r(r+1)/2$.

COROLLARY 3.3. *If $n \leq 5$, then*

$$M_n(\mathbf{R}) \cap \Theta_n \subseteq \mathscr{C}_n. \tag{5}$$

PROOF. From Proposition 3.2, we see that every extreme point X of $M_n(\mathbf{R}) \cap \Theta_n$ for $n \leq 5$ has rank $r \leq 2$. But $X \in \mathscr{F}_n \subseteq \mathscr{G}_n$, by Theorem 3.1, so using Proposition 2.10, it follows that all extreme points of $M_n(\mathbf{R}) \cap \Theta_n$ lie in $\mathscr{C}_n$. Since $\mathscr{C}_n$ is closed and convex (see Proposition 2.5), the inclusion (5) follows.

Of course, we also have the result for real matrices (and real frames) that is analogous to Proposition 2.4, which is stated below. The proof is the same.

PROPOSITION 3.4. *Let $X \in M_n(\mathbf{R}) \cap \Theta_n$. Suppose $f_1, \dots, f_n$ is a frame consisting of n unit vectors in $\mathbf{R}^r$, where $r = \mathrm{rank}(X)$, so that $X = F^*F$ with $F = (f_1, \dots, f_n)$ is the corresponding frame operator. (See Lemma 2.1.) Then X is an extreme point of $M_n(\mathbf{R}) \cap \Theta_n$ if and only if the only real Hermitian $r \times r$ matrix Z satisfying $\langle Zf_j, f_j \rangle = 0$ for all $j \in \{1, \dots, n\}$ is the zero matrix.*

Although Corollary 3.3 shows that every element of $M_n(\mathbf{R}) \cap \Theta_n$ for $n \leq 5$ is in the closed convex hull of the rank one operators in Θ_n, it is not true that every element of $M_n(\mathbf{R}) \cap \Theta_n$ lies in the closed convex hull of rank one operators in $M_n(\mathbf{R}) \cap \Theta_n$, even for $n = 3$, as the following example shows.

EXAMPLE 3.5. Consider the frame

$$f_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad f_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad f_3 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

of three unit vectors in $\mathbf{R}^2$. It is easily verified that the only real Hermitian 2×2 matrix Z such that $\langle Z f_i, f_i \rangle = 0$ for all $i = 1, 2, 3$ is the zero matrix. Thus, by Proposition 3.4,

$$X = \begin{pmatrix} 1 & 0 & \frac{1}{\sqrt{2}} \\ 0 & 1 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 1 \end{pmatrix}$$

is a rank-two extreme point of $M_3(\mathbf{R}) \cap \Theta_3$. However, an explicit decomposition as a convex combination of rank one operators in Θ_3 is

$$X = \frac{1}{2} \begin{pmatrix} 1 & i & \frac{1+i}{\sqrt{2}} \\ -i & 1 & \frac{1-i}{\sqrt{2}} \\ \frac{1-i}{\sqrt{2}} & \frac{1+i}{\sqrt{2}} & 1 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 1 & -i & \frac{1-i}{\sqrt{2}} \\ i & 1 & \frac{1+i}{\sqrt{2}} \\ \frac{1+i}{\sqrt{2}} & \frac{1-i}{\sqrt{2}} & 1 \end{pmatrix}.$$

PROPOSITION 3.6. *We have*

$$M_6(\mathbf{R}) \cap \Theta_6 \not\subseteq \mathscr{C}_6 .$$

Thus, we have $\mathscr{F}_6 \neq \mathscr{C}_6$.

PROOF. We construct an example of $X \in (M_6(\mathbf{R}) \cap \Theta_6) \backslash \mathscr{C}_6$. In fact, it will be a rank-three extreme point of $M_6(\mathbf{R}) \cap \Theta_6$.

Consider the frame

$$f_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad f_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \qquad f_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix},$$

$$f_4 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \quad f_5 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}, \quad f_6 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

of six unit vectors in $\mathbf{R}^3$. It is easily verified that the only real Hermitian 3×3 matrix Z such that $\langle Z f_i, f_i \rangle = 0$ for all $i \in \{1, \ldots, 6\}$ is the zero matrix. Thus, by Proposition 3.4,

$$X = \begin{pmatrix} 1 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{3}} \\ 0 & 1 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \\ 0 & 0 & 1 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 1 & \frac{1}{2} & \sqrt{\frac{2}{3}} \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \frac{1}{2} & 1 & \sqrt{\frac{2}{3}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \sqrt{\frac{2}{3}} & \sqrt{\frac{2}{3}} & 1 \end{pmatrix}$$

is a rank-three extreme point of $M_6(\mathbf{R}) \cap \Theta_6$. The nullspace of X is spanned by the vectors

$$v_1 = \left(\tfrac{1}{\sqrt{2}}, \tfrac{1}{\sqrt{2}}, 0, -1, 0, 0\right)^t$$

$$v_2 = \left(0, \tfrac{1}{\sqrt{2}}, \tfrac{1}{\sqrt{2}}, 0, -1, 0\right)^t$$

$$v_3 = \left(\tfrac{1}{\sqrt{3}}, \tfrac{1}{\sqrt{3}}, \tfrac{1}{\sqrt{3}}, 0, 0, -1\right)^t.$$

Suppose, to obtain a contradiction, that we have $X \in \mathscr{C}_6$. Then there is a commutative C*-algebra $A = C(\Omega)$ with a faithful tracial state τ and there are unitaries $I = U_1, U_2, \ldots, U_6 \in A$ such that $X = \big(\tau(U_i^* U_j)\big)_{1 \le i, j \le 6}$. Taking the vectors v_1, v_2 and v_3, above, by Remark 2.9 we have

$$U_4 = \frac{1}{\sqrt{2}}(U_1 + U_2) \tag{6}$$

$$U_5 = \frac{1}{\sqrt{2}}(U_2 + U_3) \tag{7}$$

$$U_6 = \frac{1}{\sqrt{3}}(U_1 + U_2 + U_3). \tag{8}$$

Fixing any $\omega \in \Omega$, we have that $\zeta_j := U_j(\omega)$ is a point on the unit circle $\mathbf{T}$, $(1 \le j \le 6)$. From (6) and $|\zeta_4| = 1$, we get $\zeta_1 = \pm i \zeta_2$ and similarly from (7) we get $\zeta_3 = \pm i \zeta_2$. However, from (8), we then have

$$\zeta_6 \in \left\{ \frac{1-2i}{\sqrt{3}} \zeta_2, \frac{1}{\sqrt{3}} \zeta_2, \frac{1+2i}{\sqrt{3}} \zeta_2 \right\},$$

which contradicts $|\zeta_6| = |\zeta_2| = 1$.

4. Nonempty interior

In this section, we show that the interior of $\mathscr{F}_n$ and, in fact, of $\mathscr{C}_n$, is nonempty, when considered as a subset of Θ_n. (Since $\mathscr{C}_n = \Theta_n$ for $n = 1, 2, 3$, this needs proving only for $n \geq 4$.)

Given $X \in \Theta_n$, let

$$a_X = \sup\{t \in [0, 1] \mid tX + (1-t)I \in \mathscr{F}_n\}$$
$$c_X = \sup\{t \in [0, 1] \mid tX + (1-t)I \in \mathscr{C}_n\}.$$

Of course, $c_X \leq a_X$. We now show that c_X is bounded below by a nonzero constant that depends only on n. In particular, we have that the identity element lies in the interior of $\mathscr{C}_n$, when this is taken as a subset of the affine space of self-adjoint matrices having all diagonal entries equal to 1.

PROPOSITION 4.1. *Let $n \in \mathbf{N}$, $n \geq 3$, and let $X \in \Theta_n$. Then*

$$c_X \geq \frac{6}{n^2 - n}. \tag{9}$$

Moreover, if λ_0 is the smallest eigenvalue of X, then

$$c_X \geq \min\left(\frac{6}{(n^2 - n)(1 - \lambda_0)}, 1\right). \tag{10}$$

PROOF. We have $X = (x_{ij})_{i,j=1}^n$ with $x_{ii} = 1$ for all $i = 1, \ldots, n$. Denote $G = \{\sigma \in S_n \mid \sigma(1) < \sigma(2) < \sigma(3)\}$. Then

$$\#G = \binom{n}{3}(n-3)!.$$

Let $U_\sigma = (u_{ij})$ be the permutation unitary matrix where $u_{ij} = \delta_{i,\sigma(i)}$. Then $U^*XU = (x_{\sigma^{-1}(i)\sigma^{-1}(j)})_{i,j}$. Define the block-diagonal matrix

$$B_\sigma = \begin{pmatrix} 1 & x_{\sigma(1)\sigma(2)} & x_{\sigma(1)\sigma(3)} \\ x_{\sigma(2)\sigma(1)} & 1 & x_{\sigma(2)\sigma(3)} \\ x_{\sigma(3)\sigma(1)} & x_{\sigma(3)\sigma(2)} & 1 \end{pmatrix} \oplus I_{n-3}.$$

Using Corollary 2.8 (and Remark 2.7), we easily see $B_\sigma \in \mathscr{C}_n$.

Let $J_\sigma = \{(\sigma(1), \sigma(2)), (\sigma(1), \sigma(3)), (\sigma(2), \sigma(3))\}$. Put $X_\sigma = U^*B_\sigma U$. Then

$$(X_\sigma)_{k\ell} = \begin{cases} 0, & \text{if } (k, \ell) \notin \{(1, 1), \ldots, (n, n)\} \cup J_\sigma, \\ 1, & \text{if } k = \ell, \\ x_{k\ell}, & \text{if } (k, \ell) \in J_\sigma. \end{cases}$$

Since for any $k < \ell$ we have

$$\#\{\sigma \in G \mid \sigma(1) = k, \sigma(2) = \ell \,\text{or}\, \sigma(1) = k, \sigma(3) = \ell \,\text{or}\, \sigma(2) = k, \sigma(3) = \ell\} \\ = ((n-\ell) + (\ell - k - 1) + (k-1))(n-3)! = (n-2)!$$

it follows that the matrix

$$X' = \frac{1}{\#G} \sum_{\sigma \in G} X_\sigma$$

has entries $x'_{ii} = 1$, and $x'_{k\ell} = \frac{6}{n^2-n} x_{k\ell}$ if $k \neq \ell$.

Since $\mathscr{C}_n$ is closed under conjugating with permutation matrices, we have $X_\sigma \in \mathscr{C}_n$ for all $\sigma \in G$. But then the average X' also belongs to $\mathscr{C}_n$. This implies (9).

Now (10) is an easy consequence of (9). Indeed, if $\lambda_0 = 1$, then X is the identity matrix and $c_X = 1$. If $\lambda_0 < 1$, then let $Y = \frac{1}{1-\lambda_0}(X - \lambda_0 I)$. We have $Y \in \Theta_n$, and

$$(1-t)I + tY = \left(1 - \frac{t}{1-\lambda_0}\right) I + \frac{t}{1-\lambda_0} X.$$

This implies $c_X \geq \min\left(1, \frac{c_Y}{1-\lambda_0}\right)$.

Given an $n \times n$ matrix $A = (a_{ij})_{1 \leq i,j \leq n}$, let $\overline{A}$ denote matrix whose (i, j) entry is the complex conjugate of a_{ij}. If A is self-adjoint, then so is $\overline{A}$, and these two matrices have the same eigenvalues (and multiplicities).

LEMMA 4.2. *Let $X \in \Theta_n$ and let $d > 0$ be such that*

$$I + d\left(\frac{X - \overline{X}}{2}\right) \in \mathscr{F}_n.$$

Then $a_X \geq d/(d+1)$. If $n \leq 5$ and

$$I + d\left(\frac{X - \overline{X}}{2}\right) \in \mathscr{C}_n, \tag{11}$$

then $c_X \geq d/(d+1)$.

PROOF. The matrix $(X + \overline{X})/2$ is real and lies in Θ_n. Using Theorem 3.1, we have $(X + \overline{X})/2 \in \mathscr{F}_n$. Thus, we have

$$\frac{1}{d+1} I + \frac{d}{d+1} X = \frac{1}{d+1}\left(I + d\left(\frac{X - \overline{X}}{2}\right)\right) + \frac{d}{d+1}\left(\frac{X + \overline{X}}{2}\right) \in \mathscr{F}_n.$$

If $n \leq 5$ and (11) holds, then we similarly apply Corollary 3.3.

EXAMPLE 4.3. Consider the matrix X as in (3), from Corollary 2.11. From Proposition 4.1 and closedness of $\mathscr{F}_n$, we know $\frac{1}{2} \le c_X \le a_X < 1$. It would be interesting to know the precise value of a_X, in order to have a concrete example of an element on the boundary of $\mathscr{F}_4$ in Θ_4.

Since

$$\frac{X - \overline{X}}{2} = \begin{pmatrix} 0 & 0 & 0 & \frac{i}{\sqrt{2}} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{i}{2} \\ -\frac{i}{\sqrt{2}} & 0 & -\frac{i}{2} & 0 \end{pmatrix}$$

has norm $\sqrt{3}/2$ and since it is conjugate by a permutation matrix to an element of $M_3(\mathbf{C}) \oplus \mathbf{C}$, using Corollary 2.8 we have that (11) holds with $d = 2/\sqrt{3}$. A slightly better value is obtained by letting Y be the result of conjugation of X with the diagonal unitary $\mathrm{diag}(1, 1, 1, e^{-i\pi/4})$. Then

$$\frac{Y - \overline{Y}}{2} = \begin{pmatrix} 0 & 0 & 0 & \frac{i}{2} \\ 0 & 0 & 0 & -\frac{i}{2} \\ 0 & 0 & 0 & 0 \\ -\frac{i}{2} & \frac{i}{2} & 0 & 0 \end{pmatrix}$$

which has norm $1/\sqrt{2}$ and similarly yields $d = \sqrt{2}$. Applying Lemma 4.2 gives $c_X = c_Y \ge \sqrt{2}/(1 + \sqrt{2}) \approx 0.586$.

ACKNOWLEDGMENT. The authors thank Vern Paulsen for kindly directing them to the literature on extreme correlation matrices.

REFERENCES

1. Brown, Nathanial, *Connes' embedding problem and Lance's WEP*, Int. Math. Res. Not. 2004, 501–510.
2. Christensen, J. P. R., and Vesterström, J., *A note on extreme positive definite matrices*, Math. Ann. 244 (1979), 65–68.
3. Collins, Benoît, and Dykema, Ken, *A linearlization of Connes' embedding problem*, New York J. Math. 14 (2008), 617–641.
4. Grone, R., Pierce, S., and Watkins, W., *Extremal correlation matrices*, Linear Algebra Appl. 134 (1990), 63–70.
5. Juschenko, Kate, and Popovych, S., *Algebraic reformulation of Connes embedding problem and the free group algebra*, Israel J. Math. 181 (2011), 305–315.
6. Kirchberg, Eberhard, *On nonsemisplit extensions, tensor products and exactness of group* C*-*algebras*, Invent. Math. 112 (1993), 449–489.
7. Klep, Igor, and Schweighofer, Markus, *Connes' embedding conjecture and sums of Hermitian squares*, Adv. Math. 217 (2008), 1816–1837.
8. Li, C-K., and Tam, B-S., *A note on extreme correlation matrices*, SIAM J. Matrix Anal. Appl. 15 (1994), 903–908.

9. Loewy, R., *Extreme points of a convex subset of the cone of positive semidefinite matrices*, Math. Ann. 253 (1980), 227–232.
10. Ozawa, Narutaka, *About the QWEP conjecture*, Internat. J. Math. 15 (2004), 501–530.
11. Pisier, Gilles, *A simple proof of a theorem of Kirchberg and related results on* C^**-norms*, J. Operator Theory 35 (1996), 317–335.
12. Rădulescu, Florin, *Convex sets associated with von Neumann algebras and Connes' approximate embedding problem*, Math. Res. Lett. 6 (1999), 229–236.
13. Rădulescu, Florin, *A comparison between the max and min norms on* $C^*(F_n) \otimes C^*(F_n)$, J. Operator Theory 51 (2004), 245–253.
14. Rădulescu, Florin, *Combinatorial aspects of Connes's embedding conjecture and asymptotic distribution of traces of products of unitaries*, pp. 197–205 in: Operator Theory 20 (Proc. Timişoara 2004), Theta Ser. Adv. Math. 6, Theta, Bucharest 2006.
15. Rădulescu, Florin, *A non-commutative, analytic version of Hilbert's 17-th problem in type* II_1 *von Neumann algebras*, pp. 93–101 in: Von Neumann algebras in Sibiu, Theta Ser. Adv. Math. 10, Theta, Bucharest 2008.
16. Voiculescu, Dan, *The analogues of entropy and of Fisher's information measure in free probability theory II*, Invent. Math. 118 (1994), 411–440.

DEPARTMENT OF MATHEMATICS
TEXAS A&M UNIVERSITY
COLLEGE STATION, TX 77843-3368
USA
E-mail: kdykema@math.tamu.edu, juschenko@math.tamu.edu