

POSITIVE OPERATOR-VALUED NONCOMMUTATIVE POLYNOMIALS ARE SQUARES

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ABSTRACT. We establish operator-valued versions of the earlier foundational factorization results for noncommutative polynomials due to Helton (Ann. Math., 2002) and one of the authors (Linear Alg. Appl., 2001). Specifically, we show that every positive operator-valued noncommutative polynomial p admits a single-square factorization $p = r^*r$. An analogous statement holds for operator-valued noncommutative trigonometric polynomials (i.e., operator-valued elements of a free group algebra).

Our approach follows the now standard sum-of-squares (sos) paradigm but requires new results and constructions tailored to operator coefficients. Assuming a positive p is not sos, Hahn–Banach separation yields a linear functional that is positive on the sos cone and negative on p ; a Gelfand–Naimark–Segal (GNS) construction then produces a representing tuple Y leading to contradiction since p was assumed positive on Y .

The key technical input is a canonical tuple of self-adjoint operators A and unitaries U , respectively, constructed from the left-regular representation on Fock space. We prove that, up to a universal constant, the norms $\|p(A)\|$ and $\|p(U)\|$ bound the operator norm of any positive semidefinite Gram matrix G representing the sos polynomial p . This uniform control yields that the cone of (sums of) squares of polynomials is closed in the product ultraweak topology on the coefficients and, via an approximation argument, in the resulting product weak operator topology. Exploiting this closedness, the GNS construction associates to a separating linear functional a finite-rank positive semidefinite noncommutative Hankel matrix and, on its range, produces the desired tuple Y .

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1. INTRODUCTION

Positivity and factorization lie at the heart of real algebraic geometry and operator theory. In the commutative setting, positivity certificates via sums of squares (sos) trace back to Hilbert's 17th problem in 1900; for classical results and modern treatments see [BCR98, Mar08, Sce24].

In the 21st century, motivated by developments in linear systems theory [SIG98, dOHMP09], quantum physics [BCPSW14], and free probability [MiSp17], the free (noncommutative) counterpart has evolved into a broad program within noncommutative function theory [KVV14, MuSo11, AM15, BMV16, PTD22]. This framework encompasses noncommutative factorizations and noncommutative Positivstellensätze. Early landmarks include Helton's theorem that (scalar) positive noncommutative polynomials are sums of squares [Hel02] and McCullough's factorization theory for noncommutative polynomials [McC01]; see also [HMP04, HMP04, Pop95, JM12, JMS21] and the references therein for further developments.

This paper establishes operator-valued analogs of these factorization theorems: every positive operator-valued noncommutative polynomial p admits a single-square factorization $p = r^*r$, with an analogous result for operator-valued noncommutative trigonometric polynomials (elements of the free group algebra).

Beyond the noncommutative positivity literature, our results resonate with classical and modern operator factorization themes, including canonical/state-space factorizations of Bart–Gohberg–Kaashoek and collaborators [BGK79, BGKR10], and the operator Fejér–Riesz and

multivariable outer factorization lines [DR10, DW05, GW05]. While our focus is the free (noncommutative) polynomial and free group contexts, the methods developed, such as the WOT-closure mechanism via Fock-space evaluations and the finite-rank Hankel realization, are of independent interest and may be useful in adjacent problems within free analysis and operator theory.

Guide to the introduction. Notation is introduced in Subsection 1.1. The main results are stated and their proofs outlined in Subsection 1.2, while Subsection 1.3 provides a roadmap for the remainder of the paper.

1.1. Notation. Fix a positive integer g . Let $\langle x \rangle$ denote the free monoid on the g letters of the alphabet $x = \{x_1, \dots, x_g\}$. Its multiplicative identity is the empty word \emptyset . We endow $\langle x \rangle$ with the *graded lexicographic order*. The length of a word $w \in \langle x \rangle$ is denoted by $|w|$. The set of all elements (words) of $\langle x \rangle$ of length (or degree) at most d is denoted $\langle x \rangle_d$. The cardinality of $\langle x \rangle_d$ is

$$N(d) = \sum_{i=0}^d g^i = \frac{g^{d+1} - 1}{g - 1}.$$

Let \mathcal{H} be a fixed complex Hilbert space. Let $\mathcal{B}(\mathcal{H})$ be the space of all bounded linear operators on \mathcal{H} , and let \mathcal{A} to be the free semigroup $\mathcal{B}(\mathcal{H})$ -algebra on x , i.e., $\mathcal{A} = \mathcal{B}(\mathcal{H})\langle x \rangle$. An element p of \mathcal{A} takes the form,

$$p = \sum_{w \in \langle x \rangle}^{\text{finite}} P_w w, \quad (1.1)$$

where $P_w \in \mathcal{B}(\mathcal{H})$, and is referred to as an (operator-valued) *polynomial* in x . Let \mathcal{A}_d denote the elements from \mathcal{A} of degree at most d .

Equip \mathcal{A} with the involution $*$: on letters, $x_j^* = x_j$, on a word $w = x_{i_1} \cdots x_{i_n} \in \langle x \rangle$,

$$w^* = x_{i_n} \cdots x_{i_1};$$

and, on a polynomial p as in (1.1),

$$p^* = \sum P_w^* w^*,$$

where P_w^* is the adjoint of the operator P_w in $\mathcal{B}(\mathcal{H})$.

Let \mathcal{K} be a Hilbert space and $X = (X_1, \dots, X_g)$ be a tuple of operators from $\mathcal{B}(\mathcal{K})$. The *evaluation* of p at X is defined as

$$p(X) = \sum P_w \otimes X^w,$$

where $X^w = X_{i_1} \cdots X_{i_n}$ for $w = x_{i_1} \cdots x_{i_n}$. In general, $p(X)^*$ (the adjoint of $p(X)$) and $p^*(X)$ are not the same. They are the same if X is a tuple of self-adjoint operators.

1.1.1. Trigonometric polynomials. We will also be interested in evaluating noncommutative polynomials in tuples of unitaries on Hilbert space. An appropriate setting to consider these is the group algebra of the free group \mathbb{F}_g on the g letters x_i , $i = 1, \dots, g$. Elements of \mathbb{F}_g are (reduced) words in the alphabet x_i, x_i^{-1} .

Let \mathcal{A} be the algebra $\mathcal{B}(\mathcal{H})[\mathbb{F}_g] = \mathcal{B}(\mathcal{H}) \otimes \mathbb{C}[\mathbb{F}_g]$. Its elements are called *trigonometric polynomials*, and \mathcal{A} is endowed with the involution

$$\sum_{u \in \mathbb{F}_g}^{\text{finite}} P_u u \mapsto \sum_u P_u^* u^{-1}. \quad (1.2)$$

If X is a tuple of unitary operators, then $(X^w)^* = X^{w^{-1}}$ and so

$$p(X)^* = \left(\sum P_w \otimes X^w \right)^* = \sum P_w^* \otimes X^{w^*} = p^*(X)$$

for all $p \in \mathcal{A}$. The notions of length of a word, degree of a polynomial, etc. extend naturally to \mathcal{A} and we let

$$\mathcal{A}_d = \left\{ \sum_{\substack{u \in \mathbb{F}_g \\ |u| \leq d}} P_u u : P_u \in \mathcal{B}(\mathcal{H}) \right\}.$$

The number of words in \mathbb{F}_g of length $\leq d$, $(\mathbb{F}_g)_d$, is denoted by $N_{\text{red}}(d)$ and equals

$$N_{\text{red}}(d) = 1 + \sum_{k=1}^d 2g(2g-1)^{k-1} = \frac{g(2g-1)^d - 1}{g-1}.$$

1.2. Main results. We are now ready to state our main results. The first is an operator-valued version of the classical sum of squares theorem of Helton [Hel02] and McCullough [McC01], Theorem 1.1. The second, Theorem 1.3, is a factorization result for positive operator-valued trigonometric polynomials extending a long list of results pertaining to scalar-valued noncommutative trigonometric polynomials [McC01, HMP04, BT07, NT13, KVV17, Oza13]. For a bounded operator T , the notation $T \succeq 0$ means that the operator T is positive semidefinite (psd).

Theorem 1.1. *For $f \in \mathcal{A}_{2d}$ the following are equivalent:*

- (i) *For any Hilbert space \mathcal{K} and any tuple of self-adjoint operators $Y = (Y_1, \dots, Y_g) \in \mathcal{B}(\mathcal{K})^g$, $f(Y) \succeq 0$;*
- (ii) *For any $n \in \mathbb{N}$ and any tuple of self-adjoint matrices $Y = (Y_1, \dots, Y_g) \in M_n(\mathbb{C})^g$, $f(Y) \succeq 0$;*
- (iii) *There exist $r_1, \dots, r_{N(d)} \in \mathcal{A}_d$ s.t.*

$$f = \sum_{i=1}^{N(d)} r_i^* r_i. \quad (1.3)$$

If \mathcal{H} is infinite-dimensional, then the above statements are also equivalent to

- (iv) *There exists $r \in \mathcal{A}_d$ s.t.*

$$f = r^* r. \quad (1.4)$$

Remark 1.2. Several remarks related to Theorem 1.1 are in order.

- (a) Item (iii) can also be phrased as a factorization result. Letting $r = \text{col}(r_1 \ \cdots \ r_{N(d)}) \in \mathcal{A}^{N(d)} = \mathcal{B}(\mathcal{H}, \mathcal{H}^{N(d)})\langle x \rangle$, (1.3) simply states

$$f = r^* r.$$

We refer to [BGK79, BGKR10, DW05, GW05, DR10] and the references therein for an in depth investigation of factorization.

- (b) That item (iii) implies item (i) implies item (ii) is trivial. The main content of Theorem 1.1 is that item (ii) implies item (iii). A routine argument shows the equivalence between (1.3) and (1.4) in the infinite-dimensional case, see Remark 2.4.
- (c) Our proof yields no bound on the size n of matrices needed in item (ii).
- (d) From Theorem 1.1 one can easily deduce its version for free non-self-adjoint variables z, z^* via the usual identification $z_j \mapsto \text{real } z_j = \frac{z_j + z_j^*}{2}$ and hence $z_j^* \mapsto \text{imag } z_j = \frac{z_j - z_j^*}{2i}$. \square

The following result is the unitary version of Theorem 1.1.

Theorem 1.3. *For $f \in \mathcal{A}_{2d}$ the following are equivalent:*

- (i) *For any Hilbert space \mathcal{K} and any tuple of unitary operators $U = (U_1, \dots, U_g) \in \mathcal{B}(\mathcal{K})^g$, $f(U) \succeq 0$;*
- (ii) *For any $n \in \mathbb{N}$ and any tuple of unitary matrices $U = (U_1, \dots, U_g) \in M_n(\mathbb{C})^g$, $f(U) \succeq 0$;*
- (iii) *There exist $r_1, \dots, r_{N_{\text{red}}(d)} \in \mathcal{A}_d$ s.t.*

$$f = \sum_{i=1}^{N_{\text{red}}(d)} r_i^* r_i.$$

If \mathcal{H} is infinite-dimensional, then the above statements are also equivalent to

- (iv) *There exists $r \in \mathcal{A}_d$ s.t.*

$$f = r^* r.$$

Remark 1.4 (What's new?). The passage to operator coefficients necessitates several novel results and constructions that we expect to be of independent interest. At a high level, the proofs of Theorem 1.1 and Theorem 1.3 still follow the now standard paradigm for establishing sum of squares (sos) representations (factorizations). Namely, Hahn-Banach separation produces a separating linear functional φ followed by a Gelfand-Naimark-Segal (GNS) construction based on φ that ultimately produces a tuple Y . Here we roughly follow the outline of [MP05].

A key construction is that of a tuple of self-adjoint operators A based upon the left regular representation on Fock space. See Section 3. It is then shown, that, up to a universal constant, for a sums of squares polynomial p , up to a universal constant, the norm of $p(A)$ bounds the norm of any non-commutative psd Gram matrix G that represents p . See Proposition 3.3. This uniform bound is then used in Section 4 to prove that the cone \mathcal{C}_d of sums of squares is closed in the product ultraweak topology on the coefficients, and, via an approximation argument that upgrades ultraweak continuous separating functionals to WOT-continuous ones, also closed in the resulting product WOT. This closedness is the key input for the Hahn–Banach separation step.

On the GNS side, we introduce a new argument that exploits the WOT to associate to a separating linear functional a finite-rank psd noncommutative representing Hankel matrix and, on its range, construct the desired tuple Y ; see Section 5. For the unitary result,

Theorem 1.3, we additionally modify the construction of Section 3 to produce a canonical tuple of unitary operators from the left-regular representation and adapt the GNS procedure to obtain a unitary tuple together with a representing vector that realizes the separating functional as a vector state; Subsection 7.2. \square

1.3. Reader's guide. The paper is structured as follows. The convex cone of sums of squares (making an appearance in (1.3) of Theorem 1.1) is introduced and characterized in the next Section 2. In Section 3 we define creation operators L_i on the full Fock \mathcal{F}_g^2 space and their symmetrized analogs A_i . How they pertain to the sum of squares statement at hand is explored in Subsection 3.3, where evaluations at A are used to extract coefficients of a polynomial. In Section 4 we introduce a suitable topology on \mathcal{A}_d and collect all the necessary topological properties needed in the sequel. With respect to this topology, the convex cone of sums of squares is closed, see Proposition 4.1. The fact that the cone is closed allows for an application of the Hahn–Banach Separation Theorem, which is then followed by an appropriate version of the GNS construction, carried out in Section 5; see Proposition 5.4. Then Theorem 1.1 is proved in Section 6 and Theorem 1.3 is proved in Section 7.

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2. CONVEX CONE OF (SUMS OF) SQUARES

In this section, a key player in the proof of Theorem 1.1, the convex cone of sums of squares of polynomials, is introduced and studied. The main result in this section is Proposition 2.2 (see also Remark 2.4), which gives a bound on the number of sums of squares needed to write a polynomial as a sum of squares.

Lemma 2.1. *If $T : \mathcal{H}^n \rightarrow \mathcal{H}^n$ be a psd linear map, then there exist linear maps $R_i : \mathcal{H} \rightarrow \mathcal{H}^n$, $i = 1, \dots, n$, such that $T = \sum_{i=1}^n R_i R_i^*$. Moreover, if \mathcal{H} is infinite-dimensional, then $T = RR^*$ for some $R : \mathcal{H} \rightarrow \mathcal{H}^n$.*

Proof. Since T is psd, there exists a linear map $\tilde{R} : \mathcal{H}^n \rightarrow \mathcal{H}^n$ such that $T = \tilde{R}\tilde{R}^*$. Write

$$\tilde{R} = [R_1, \dots, R_n]$$

with respect to the orthogonal decomposition $\mathcal{H}^n = \mathcal{H} \oplus \dots \oplus \mathcal{H}$. The first part of the lemma follows by noting that each R_i is a map from \mathcal{H} into \mathcal{H}^n . For the moreover part, let $U : \mathcal{H} \rightarrow \mathcal{H}^n$ be any unitary, and set $R = \tilde{R}U$. \square

Index $\mathcal{H}^{N(d)}$ and $\mathcal{A}_d^{N(d)}$ (the algebraic direct sum of \mathcal{A}_d with itself $N(d)$ times) by $\langle x \rangle_d$. Let $V_d \in \mathcal{A}_d^N$ denote the *Veronese column vector* whose $w \in \langle x \rangle_d$ entry is w (adopting the usual convention of viewing w as the the $\mathcal{B}(\mathcal{H})$ -valued polynomial $I_{\mathcal{H}}w$). For instance, if $g = 2$ and $d = 2$, then

$$V_2 = \text{col}(1 \ x_1 \ x_2 \ x_1^2 \ x_1x_2 \ x_2x_1 \ x_2^2).$$

Let \mathcal{C}_d denote the *cone of sums of squares* of polynomials of degree at most d ,

$$\mathcal{C}_d := \left\{ \sum_{i=1}^{N(d)} r_i^* r_i : r_i \in \mathcal{A}_d, i = 1, \dots, N(d) \right\} \subseteq \mathcal{A}_{2d}. \quad (2.1)$$

Given $r \in \mathcal{A}_d$, the column vector R with w entry R_w^* is called the *coefficient vector* of r since $r = R^*V_d$. In particular,

$$r^*r = V_d^*RR^*V_d$$

so that r^*r has a representation as $V_d^*GV_d$ for a psd matrix G .

Proposition 2.2. *A polynomial $p \in \mathcal{A}_{2d}$ is in \mathcal{C}_d if and only if there is a psd block matrix G such that*

$$p = V_d^*GV_d. \quad (2.2)$$

In fact, if $p = V_d^*GV_d$, then factoring $G = \sum_{j=1}^{N(d)} R_j R_j^*$ with $R_j : \mathcal{H} \rightarrow \bigoplus_{w \in \langle x \rangle_d} \mathcal{H}$ as in Lemma 2.1, setting $r_j = R_j^*V_d$ gives,

$$p = \sum_{j=1}^{N(d)} r_j^* r_j.$$

In particular, the set \mathcal{C}_d is a (convex) cone.

We call any psd block matrix G satisfying equation (2.2) a *Gram representation* for p .

Proof. Given a sum of squares $p = \sum_{i=1}^{N(d)} r_i^* r_i$, writing $r_j = R_j^*V_d$ gives $p = \sum_{i=1}^{N(d)} V_d^* R_i R_i^* V_d$, where R_i is the coefficient vector corresponding to the polynomial r_i . It follows that $p = V_d^*GV_d$, where $G = \sum_{i=1}^{N(d)} R_i R_i^*$. In particular, $G : \mathcal{H}^{N(d)} \rightarrow \mathcal{H}^{N(d)}$ is a psd linear map.

Conversely, suppose there is a psd linear map $G : \bigoplus_{w \in \langle x \rangle_d} \mathcal{H} \rightarrow \bigoplus_{w \in \langle x \rangle_d} \mathcal{H}$ such that $p = V_d^*GV_d$. By Lemma 2.1, there exist $R_j : \mathcal{H} \rightarrow \bigoplus_{w \in \langle x \rangle_d} \mathcal{H}$ such that $G = \sum_{j=1}^{N(d)} R_j R_j^*$. Setting $r_j = R_j^*V_d$, one obtains $p = \sum_{j=1}^{N(d)} r_j^* r_j$.

By what has already been proved, if $p, q \in \mathcal{C}_d$, then there exist (psd) Gram representations $p = V^*G_p V$ and $q = V^*G_q V$. Now $p + q = V_d^*(G_p + G_q)V_d$. Since $G_p + G_q : \mathcal{H}^{N(d)} \rightarrow \mathcal{H}^{N(d)}$ is a psd linear map, what has already been proved shows $p + q \in \mathcal{C}_d$. \square

Corollary 2.3. *Letting $V_d \in \mathcal{A}_d^{N(d)}$ denote the Veronese column vector, the convex cone of sums of squares of degree at most $2d$ is*

$$\mathcal{C}_d = \{V_d^*GV_d : G = [G_{v,w}]_{v,w \in \langle x \rangle_d} \in \mathcal{B}(\mathcal{H})^{N(d) \times N(d)}, G \succeq 0\}.$$

Remark 2.4. It follows from the preceding discussion that the convex cone \mathcal{C}_d takes the form

$$\mathcal{C}_d = \{r^*r : r \in \mathcal{A}_d\}$$

when the Hilbert space \mathcal{H} is infinite-dimensional. \square

3. FULL FOCK SPACE AND GRAM MATRICES

This section recalls the well-known definition of the full Fock space [AP95, JMS21], the creation operators [Fra84], and introduces their symmetrized variants in (3.4) compressed to a suitable finite-dimensional subspace. In Subsection 3.3 we explore how these self-adjoint operators are used to extract the coefficients of a polynomial. The main result is Proposition 3.3 showing that the set of positive semidefinite Gram matrices of a polynomial is norm bounded.

The full Fock space can be defined over any Hilbert space. The *full Fock space* over \mathbb{C}^g , denoted \mathcal{F}_g^2 , is:

$$\mathcal{F}_g^2 = \bigoplus_{n=0}^{\infty} (\mathbb{C}^g)^{\otimes n},$$

where $(\mathbb{C}^g)^{\otimes 0} := \mathbb{C}$ represents the *vacuum vector* Ω . Thus elements of \mathcal{F}_g^2 are sequences $(\psi_0, \psi_1, \psi_2, \dots)$ with $\psi_n \in (\mathbb{C}^g)^{\otimes n}$ and $\|(\psi_0, \psi_1, \psi_2, \dots)\|^2 = \sum_{n=0}^{\infty} \|\psi_n\|^2 < \infty$.

3.1. Basis. Let $\{e_1, \dots, e_g\}$ be any orthonormal basis of \mathbb{C}^g . With any $w = x_{i_1} \dots x_{i_n} \in \langle x \rangle$, associate a vector

$$e_w = e_{i_1} \otimes \dots \otimes e_{i_n} \in (\mathbb{C}^g)^{\otimes n}.$$

The set $\{e_w : w \in \langle x \rangle\}$ forms an orthonormal basis for \mathcal{F}_g^2 , with e_\emptyset corresponding to the vacuum vector Ω .

3.2. Left creation operators. For each $i = 1, \dots, g$, define the *left creation operator* L_i on \mathcal{F}_g^2 by

$$L_i(e_w) = e_{x_i w} \in (\mathbb{C}^g)^{\otimes (|w|+1)}, \quad (w \in \langle x \rangle). \quad (3.1)$$

Clearly, each L_i is an isometry. Moreover $L_i^* L_j = 0$ if $i \neq j$. Thus the tuple $L = (L_1, \dots, L_g)$ is a *row isometry*. Let

$$B_i = L_i + L_i^*, \quad i = 1, \dots, g.$$

Fix a positive integer ℓ . Let $\mathcal{F}_{g,\ell}^2$ denote the subspace of \mathcal{F}_g^2 spanned by $\{e_w : w \in \langle x \rangle_\ell\}$ and $\iota = \iota_\ell : \mathcal{F}_{g,\ell}^2 \rightarrow \mathcal{F}_g^2$ the inclusion. Thus, for instance, for $|w| \leq \ell$,

$$\iota^* L_i \iota e_w = \iota^* L_i e_w = \begin{cases} e_{x_j w} & \text{if } |w| < \ell \\ 0 & \text{if } |w| = \ell. \end{cases} \quad (3.2)$$

Similarly, if $|v| \leq \ell$, then

$$\iota^* L_j^* \iota e_v = \iota^* L_j^* e_v = \begin{cases} e_u & \text{if } v = x_j u \\ 0 & \text{otherwise.} \end{cases} \quad (3.3)$$

Let

$$A_j = \iota^* B_j \iota = \iota^* (L_j + L_j^*) \iota. \quad (3.4)$$

From equations (3.2) and (3.3), $A_j w = B_j w$ for $|w| < \ell$. While A depends on ℓ , we suppress this dependence in the notation for readability; when ℓ is not clear from the context, we write $A = A^{(\ell)}$.

Lemma 3.1. *For any $w \in \langle x \rangle_\ell$,*

$$A^w \Omega = e_w + \sum_{|v| < |w|} c_{v,w} e_v$$

for some scalars $c_{v,w}$.

Proof. The proof proceeds by induction on word length. If w is the empty word, then $A^w\Omega = \Omega = e_\emptyset$. Assume $n \leq \ell$ and the claim holds for all words of length $\leq n - 1$. Let $w = x_{i_1} \dots x_{i_n} = x_{i_1}\tilde{w}$ be of length n . Then

$$A^w\Omega = L_{i_1}A^{\tilde{w}}\Omega + L_{i_1}^*A^{\tilde{w}}\Omega,$$

By the induction hypothesis,

$$\begin{aligned} A^w\Omega &= L_{i_1} \left(e_{\tilde{w}} + \sum_{|v|< n-1} c_{v,\tilde{w}}e_v \right) + L_{i_1}^* \left(e_{\tilde{w}} + \sum_{|v|< n-1} c_{v,\tilde{w}}e_v \right) \\ &= e_w + \left(\sum_{|v|< n-1} c_{v,\tilde{w}}e_{x_{i_1}v} \right) + L_{i_1}^*e_{\tilde{w}} + \left(\sum_{|v|< n-1} c_{v,\tilde{w}}L_{i_1}^*e_v \right). \end{aligned}$$

For any word u of length k , $L_{i_1}^*e_u$ is either zero or is $e_{\tilde{u}}$, for some word \tilde{u} of length $k - 1$, and the proof is complete. \square

Lemma 3.2. *The $N(\ell) \times N(\ell)$ scalar matrix*

$$\mathbb{E}_\ell = [\langle A^w\Omega, e_v \rangle]_{v,w \in \langle x \rangle_\ell}$$

is invertible.

Proof. Recall that we have endowed $\langle x \rangle$ with graded lexicographic order. If $\ell \geq |v|$ and $v > w$, then

$$\langle A^w\Omega, e_v \rangle = 0$$

by Lemma 3.1. Hence, for each k , the matrix \mathbb{E}_k is an upper triangular matrix. Moreover, each diagonal entry is 1 by Lemma 3.1. Thus, \mathbb{E}_ℓ is invertible. \square

3.3. Extraction formula for coefficients. Let $q = \sum Q_w w \in \mathcal{A}_\ell$. For $v \in \langle x \rangle_\ell$ define the linear functional $\Omega_v : \mathcal{B}(\mathcal{F}_{g,\ell}^2) \rightarrow \mathbb{C}$ by

$$\Omega_v(T) = \langle T\Omega, e_v \rangle.$$

The operator coefficients Q_v are obtained from $q(A)$ by solving the linear system

$$\begin{aligned} Z_v(q) &:= (\text{id}_{\mathcal{B}(\mathcal{H})} \otimes \Omega_v)q(A) = \sum_w Q_w \otimes \Omega_v(A^w) \\ &= \sum_w \langle A^w\Omega, e_v \rangle Q_w = \sum_w [\mathbb{E}_\ell]_{v,w} Q_w, \end{aligned}$$

where $[\mathbb{E}_\ell]_{v,w}$ is the (v, w) entry of the matrix \mathbb{E}_ℓ . In short,

$$Z(q) = \mathbb{E}_\ell Q, \tag{3.5}$$

where $Z(q)$ and Q are column vectors with $Z_v(q)$ and Q_v as the v^{th} entry of Z and Q , respectively. Since, by Lemma 3.2, \mathbb{E}_ℓ is invertible,

$$Q = \mathbb{E}_\ell^{-1}Z(q). \tag{3.6}$$

We refer to \mathbb{E} as the *extraction matrix*, and equation (3.6) as the *extraction formula* for the coefficients of q . Note that this formula depends only upon $q(A)$; that is, the coefficients of q are determined uniquely by $q(A)$.

It follows from equation (3.6) that there exists a positive constant λ_d (independent of q) such that

$$\|Q_w\| \leq \lambda_d \|q(A)\| \quad \text{for all } w \in \langle x \rangle_d. \quad (3.7)$$

Proposition 3.3. *If $p \in \mathcal{C}_d$, then the set*

$$\Gamma_p = \{G \in \mathcal{B}(\mathcal{H})^{N(d) \times N(d)} : G \succeq 0, V_d^* GV_d = p\}$$

is norm bounded (with respect to the operator norm on $\mathcal{B}(\mathcal{H}^{N(d)})$). More precisely, there exists a constant μ_d (depending only on d and \mathbf{g} and not on p) such that, for all $G \in \Gamma_p$,

$$\|G\| \leq \mu_d \|p(A)\|,$$

where the tuple $A = A^{(d)}$ is defined in (3.4) for $d \geq 2d$.

Proof. Fix $p \in \mathcal{C}_d$ and $G \in \Gamma_p$. Thus $p = V_d^* GV_d$. By Proposition 2.2, there exists $Q_j : \mathcal{H} \rightarrow \bigoplus_{w \in \langle x \rangle_d} \mathcal{H}$ such that

$$p = \sum_{j=1}^{N(d)} q_j^* q_j = V_d^* \left[\sum_{j=1}^{N(d)} Q_j Q_j^* \right] V_d, \quad (3.8)$$

where

$$q_j = Q_j^* V_d = \sum_{w \in \langle x \rangle_d} Q_{j,w} w.$$

By equation (3.7), for $v \in \langle x \rangle_d$,

$$\|Q_{j,v}\| \leq \lambda_d \|q_j(A)\|.$$

From equation (3.8),

$$\|q_j(A)\|^2 = \|q_j(A)^* q_j(A)\| \leq \|p(A)\|.$$

Thus, again using equation (3.8),

$$\sum_{u,v \in \langle x \rangle_d} \|G_{u,v}\| \leq \sum_{u,v \in \langle x \rangle_d} \sum_{j=1}^{N(d)} \|Q_{j,u} Q_{j,v}^*\| \leq N(d)^3 \lambda_d^2 \|p(A)\|.$$

It follows that $\|G\| \leq \mu_d \|p(A)\|$ for $\mu_d = N(d)^3 \lambda_d^2$. \square

4. TOPOLOGY ON \mathcal{A}_d

The main purpose of this section is to define a well-behaved topology on \mathcal{A}_d in which the convex cone of sums of squares is closed.

To each polynomial in \mathcal{A}_d , we associate the vector of its coefficients as an element in $\mathcal{B}(\mathcal{H})^{\langle x \rangle_d}$. The topology on \mathcal{A}_d is then the topology induced from the product WOT on $\mathcal{B}(\mathcal{H})^{\langle x \rangle_d}$. Alternately, in this topology a net $(p_\alpha = \sum_w P_{\alpha,w} w)_\alpha$ in \mathcal{A}_d converges to $p = \sum_w P_w w \in \mathcal{A}_d$ if for each $w \in \langle x \rangle_d$, the net of operators $(P_{\alpha,w})_\alpha$ converges to P_w in WOT. Note that \mathcal{A}_d becomes a locally convex topological vector space with this topology. We refer to this topology as the WOT on \mathcal{A}_d or the *product WOT topology*. It is the default topology on \mathcal{A}_d ; that is, unless otherwise stated, it is the topology on \mathcal{A}_d .

Exclusive to this section, we will also use a product ultraweak topology on \mathcal{A}_d . The ultraweak topology on $\mathcal{B}(\mathcal{H})$ is the weak-* topology on $\mathcal{B}(\mathcal{H})$ induced by the predual $\mathcal{T}(\mathcal{H})$, the trace class operators on \mathcal{H} . It is the weakest topology such that predual elements remain continuous on $\mathcal{B}(\mathcal{H})$. As before, to each polynomial in \mathcal{A}_d , we associate a vector of its

coefficients as an element in $\mathcal{B}(\mathcal{H})^{\langle x \rangle_d}$. The ultraweak topology on \mathcal{A}_d is then the topology induced from the product ultraweak topology on $\mathcal{B}(\mathcal{H})^{\langle x \rangle_d}$. Alternately, in this topology a net $(p_\alpha = \sum_w P_{\alpha,w}w)_\alpha$ in \mathcal{A}_d converges to $p = \sum_w P_w w \in \mathcal{A}_d$ if for each $w \in \langle x \rangle_d$, the net of operators $(P_{\alpha,w})_\alpha$ converges to P_w in ultraweak topology for all $w \in \langle x \rangle_d$. Note that \mathcal{A}_d becomes a locally convex topological vector space with this topology.

4.1. Closedness of the cone \mathcal{C}_d . The main goal of this subsection is to establish the following result. In the rest of this section fix an integer $d \geq 2d$, and set $A = A^{(d)}$.

Proposition 4.1. *The convex cone \mathcal{C}_d is closed in \mathcal{A}_d .*

Firstly, since \mathcal{A}_{2d} is closed in \mathcal{A}_d , it suffices to show \mathcal{C}_d is closed in \mathcal{A}_{2d} . The proof of Proposition 4.1 proceeds in two steps. We first show that the cone \mathcal{C}_d is closed with respect to a stronger topology, the ultraweak topology, which will be used exclusively in this section. Next, we prove that if a polynomial in \mathcal{A}_{2d} can be separated from the cone \mathcal{C}_d by an ultraweak continuous linear functional, then it can also be separated by a WOT continuous linear functional. This implication will yield the desired closedness of \mathcal{C}_d .

4.1.1. Closedness of \mathcal{C}_d in the product ultraweak topology. Equip \mathcal{A}_d with a norm in the following way. For $p = \sum_{w \in \langle x \rangle_d} P_w w$,

$$\|p\| = \sum_{w \in \langle x \rangle_d} \|P_w\|,$$

where $\|T\|$ denotes the operator norm for $T \in \mathcal{B}(\mathcal{H})$.

Lemma 4.2. *For any $t > 0$, the truncated cone*

$$\mathcal{C}_{d,t} := \{p \in \mathcal{C}_d : \|p\| \leq t\}$$

is closed in the ultraweak topology on \mathcal{A}_d .

Proof. Fix $t > 0$. Let $(p_\alpha)_\alpha$ be a net in $\mathcal{C}_{d,t}$ that converges to $p \in \mathcal{A}_{2d}$. Our aim is to show that $p \in \mathcal{C}_{d,t}$. Note that for any α ,

$$\|p_\alpha(A)\| \leq \|p_\alpha\| \|A\| \leq t \|A\|.$$

Thus,

$$\sup_\alpha \|p_\alpha(A)\| < \infty.$$

By Proposition 3.3,

$$\sup_\alpha \|G_\alpha\| < \infty$$

for any $G_\alpha \in \Gamma_{p_\alpha}$. Thus, by the Banach–Alaoglu theorem, there is a subnet of operators $(G_\beta)_\beta$ that converges to some operator $G \in \mathcal{B}(\mathcal{H})^{N(d) \times N(d)}$ in the ultraweak topology. Since the convergence in the ultraweak operator topology is stronger than convergence in the weak operator topology, $G_\beta \rightarrow G$ in the WOT. Thus, $G \succeq 0$.

Let $q = V_d^* G V_d \in \mathcal{C}_d$ and observe,

$$p_\alpha(A) = V_d(A)^*(G_\alpha \otimes I_{\mathcal{F}_g^2})V_d(A),$$

where $V_d(A) : \mathcal{H} \otimes \mathcal{F}_{g,d}^2 \rightarrow \mathcal{H}^{N(d)} \otimes \mathcal{F}_{g,d}^2$, is defined by

$$V_d(A)h \otimes \xi = (h \otimes A^w \xi)_w.$$

Since $(G_\beta)_\beta$ converges to G in the WOT and the tuple A acts on a finite dimensional Hilbert space,

$$V_d(A)^*(G_\beta \otimes I_{\mathcal{F}_g^2})V_d(A) \longrightarrow V_d(A)^*(G \otimes I_{\mathcal{F}_g^2})V_d(A) = q(A)$$

in the WOT. Thus, $(p_\beta(A))_\beta$ converges to $q(A)$ in the WOT. Therefore, $p(A) = q(A)$. Since, by the extraction formula, equation (3.6), the coefficients of p and q are determined by evaluation at A , it follows that $p = q$. Hence, $p \in \mathcal{C}_d$. Since the norm is lower semicontinuous in the ultraweak topology, $\|p\| \leq t$. Hence, $p \in \mathcal{C}_{d,t}$. \square

It follows from Krein–Smulian Theorem (see, e.g., [Dav25, Theorem 3.6.2]) that the cone \mathcal{C}_d is closed in the ultraweak topology.

4.1.2. Closedness of \mathcal{C}_d in the product WOT topology.

Lemma 4.3. *Given trace-class operators $S_i \in \mathcal{T}(\mathcal{H})$, $1 \leq i \leq m$ and $\epsilon > 0$, there exists a finite-rank operator P such that*

$$\|S_i - PS_i P\|_1 < \epsilon$$

for all i . Here $\|\cdot\|_1$ denotes the trace norm.

Proof. Since finite-rank operators are dense in $\mathcal{T}(\mathcal{H})$ with respect to the trace norm, there are finite-rank operators F_i with

$$\|S_i - F_i\|_1 < \frac{\epsilon}{2}.$$

Let P be the orthogonal projection onto $\sum_i \text{ran}(F_i) + \sum_i \text{ran}(F_i^*)$. Then $PF_iP = F_i$ for all i . Hence

$$\begin{aligned} \|S_i - PS_i P\|_1 &\leq \|S_i - F_i\|_1 + \|F_i - PS_i P\|_1 \\ &= \|S_i - F_i\|_1 + \|PF_i P - PS_i P\|_1 \\ &= \|S_i - F_i\|_1 + \|P(F_i - S_i)P\|_1 \\ &\leq \frac{\epsilon}{2} + \|P\| \|F_i - S_i\|_1 \|P\| \\ &\leq \frac{\epsilon}{2} + \frac{\epsilon}{2} = \epsilon. \end{aligned} \quad \square$$

Lemma 4.4. *If $\varphi : \mathcal{A}_{2d} \rightarrow \mathbb{C}$ be an ultraweak continuous linear functional that separates the cone \mathcal{C}_d from a fixed polynomial p in \mathcal{A}_{2d} , that is,*

$$\varphi(r^*r) \geq 0 \quad \text{for all } r \in \mathcal{A}_d \quad \text{and} \quad \varphi(p + p^*) < 0,$$

then there exists a WOT continuous linear functionl $\tilde{\varphi} : \mathcal{A}_{2d} \rightarrow \mathbb{C}$ such that

$$\tilde{\varphi}(r^*r) \geq 0 \quad \text{for all } r \in \mathcal{A}_d \quad \text{and} \quad \tilde{\varphi}(p + p^*) < 0.$$

Proof. Since φ is ultraweak continuous, there exist trace class operators S_w ($w \in \langle x \rangle_{2d}$) in $\mathcal{B}(\mathcal{H})$ such that

$$\varphi(q) = \sum_{w \in \langle x \rangle_{2d}} \text{Tr}(S_w Q_w),$$

where $q = \sum_{w \in \langle x \rangle_{2d}} Q_w w$. For $r, r' \in \mathcal{A}_d$,

$$\varphi(r^*r') = \sum_{u,v \in \langle x \rangle_d} \text{Tr}(S_{u^*v} R_u^* R_v'),$$

where $r = \sum_{u \in \langle x \rangle_d} R_u u$ and $r' = \sum_{v \in \langle x \rangle_d} R'_v v$. Denote by S the $N(d) \times N(d)$ block operator matrix whose (u, v) entry is $S_{v^* u}$.

For any $r \in \mathcal{A}_d$, define the row operator $R : \bigoplus_{u \in \langle x \rangle_d} \mathcal{H} \rightarrow \mathcal{H}$ by

$$R(\bigoplus_{u \in \langle x \rangle_d} \zeta_w) = \sum_u R_u \zeta_u.$$

Thus,

$$\begin{aligned} \varphi(r^* r) &= \sum_{u, v \in \langle x \rangle_d} \text{Tr}(S_{u^* v} R_u^* R_v) \\ &= \sum_{u, v \in \langle x \rangle_d} \text{Tr}([S]_{v, u} [R^* R]_{u, v}) \\ &= \text{Tr}(SR^* R). \end{aligned}$$

We claim that

$$\text{Tr}(ST) \geq 0$$

for any positive operator $T \in \mathcal{B}(\bigoplus_{\langle x \rangle_d} \mathcal{H})$. It follows from Lemma 2.1 that $T = R^* R$ for some $R : \bigoplus_{\langle x \rangle_d} \mathcal{H} \rightarrow \mathcal{H}$. Letting $r = \sum R_u u$, where R_u is the u^{th} element of the row operator R gives

$$\text{Tr}(ST) = \text{Tr}(SR^* R) = \varphi(r^* r) \geq 0.$$

To prove that S is a positive operator, it remains to show that S is self-adjoint. For $T \succeq 0$, $\text{Tr}(ST)$ is real. Hence,

$$\text{Tr}(S^* T) = \text{Tr}(TS^*) = \text{Tr}((ST)^*) = \overline{\text{Tr}(ST)} = \text{Tr}(ST).$$

Since every bounded operator on a Hilbert space is a linear combination of four positive operators,

$$\text{Tr}(S^* T) = \text{Tr}(ST) \quad \text{for all } T \in \mathcal{B}\left(\bigoplus_{\langle x \rangle_d} \mathcal{H}\right).$$

Hence $S^* = S$ and $S \succeq 0$.

The finitely many trace class operators S_w , $w \in \langle x \rangle_{2d}$, can be approximated by finite rank operators in the trace norm as in Lemma 4.3. That is, for any $n \in \mathbb{N}$, there exists a finite-rank projection P_n of \mathcal{H} such that

$$\|S_w - P_n S_w P_n\|_1 < \frac{1}{n},$$

for all $w \in \langle x \rangle_{2d}$, where $\|\cdot\|_1$ denotes the trace norm. Letting $S^{(n)}$ the $N(d) \times N(d)$ denote the block operator matrix whose (u, v) entry is $P_n S_{v^* u} P_n$,

$$S^{(n)} = (I_{N(d)} \otimes P_n) S (I_{N(d)} \otimes P_n).$$

Whence $S^{(n)}$ is a finite-rank psd operator.

Define a linear functional $\varphi_n : \mathcal{A}_{2d} \rightarrow \mathbb{C}$ by

$$\varphi_n(Q u^* v) = \text{Tr}(P_n S_{u^* v} P_n Q)$$

for $Q \in \mathcal{B}(\mathcal{H})$ and $u, v \in \langle x \rangle_d$. For $r = \sum_{u \in \langle x \rangle_d} R_u u$ and $r' = \sum_{v \in \langle x \rangle_d} R'_v v$,

$$\begin{aligned}\varphi_n(r^* r') &= \sum_{u, v \in \langle x \rangle_d} \varphi_n(R_u^* R'_v u^* v) = \sum_{u, v \in \langle x \rangle_d} \text{Tr}(P_n S_{u^* v} P_n R_u^* R'_v) \\ &= \text{Tr}(P_n S P_n R^* R') = \text{Tr}(S^{(n)} R^* R').\end{aligned}$$

Since $S^{(n)}$ is psd,

$$\varphi_n(r^* r) = \text{Tr}(S^{(n)} R^* R) \geq 0$$

for all $r \in \mathcal{A}_d$. Further, since $S^{(n)}$ is a finite-rank operator, φ_n is WOT continuous.

Since $(P_n S_{u^* v} P_n)_n$ converges to $S_{u^* v}$ in the trace norm, $\text{Tr}(P_n S_{u^* v} P_n Q)$ converges to $\text{Tr}(SQ)$. Hence $\varphi_n(p+p^*)$ converges to $\varphi(p+p^*)$. As $\varphi(p+p^*) < 0$, there exists a natural number n such that $\varphi_n(p+p^*) < 0$. The linear functional $\tilde{\varphi} := \varphi_n$ has the desired separation properties. \square

We are finally ready to prove Proposition 4.1.

Proof of Proposition 4.1. Suppose $p \in \mathcal{A}_{2d}$ is not in \mathcal{C}_d . Since \mathcal{C}_d is ultraweak closed, there is an ultraweak continuous linear functional φ on \mathcal{A}_{2d} that separates p from \mathcal{C}_d . Now apply Lemma 4.4 to obtain a WOT continuous separating linear functional $\tilde{\varphi}$. Thus p is not in the WOT closure of \mathcal{C}_d . \square

5. GNS CONSTRUCTION

In preparation of the application of the Hahn-Banach-convex separation theorem in the proof of Theorem 1.1 in Section 6, we establish a suitable version of the GNS construction in Proposition 5.4. Before doing so, for the reader's convenience we state three well-known lemmas that will be used in the proof.

Lemma 5.1. *Let \mathcal{H} be a Hilbert space. If $f : \mathcal{B}(\mathcal{H}) \rightarrow \mathbb{C}$ is a WOT continuous linear functional, then there exist a finite index set J , vectors $h_j, k_j \in \mathcal{H}$ such that*

$$f(T) = \sum_{j \in J} \langle Th_j, k_j \rangle_{\mathcal{H}} \quad \text{for all } T \in \mathcal{B}(\mathcal{H}).$$

For a proof see [Dav25, Section 3.1 and Exercise 3.4].

Lemma 5.2. *If $\varphi : \mathcal{A}_{\ell} \rightarrow \mathbb{C}$ is a continuous linear functional, then there exist a finite index set J , vectors $h_j, k_j \in \mathcal{H}$ and scalars $c_w \in \mathbb{C}$ ($w \in \langle x \rangle_{\ell}$) such that for every $p = \sum P_w w \in \mathcal{A}_{\ell}$,*

$$\varphi(p) = \sum_{j \in J} \sum_{w \in \langle x \rangle_{\ell}} c_w \langle P_w h_j, k_j \rangle.$$

Proof. First identify \mathcal{A}_{ℓ} with $\mathcal{B}(\mathcal{H})^{N(\ell)}$ via

$$\sum P_w w \mapsto (P_w)_w.$$

This identification induces the product weak operator topology on $\mathcal{B}(\mathcal{H})^{N(\ell)}$, i.e., the topology generated by the seminorms $\|\cdot\|_{w,h,k}$ given by

$$\|P\|_{w,h,k} := |\langle P_w h, k \rangle|, \quad w \in \langle x \rangle_{\ell}, h, k \in \mathcal{H},$$

where $P = (P_w)_w$ is a tuple of $N(\ell)$ many operators in $\mathcal{B}(\mathcal{H})$. Now the statement follows from Lemma 5.1. \square

The third lemma presents a few basic properties of the vectorization map used in the proof of Proposition 5.4, Subsection 5.5. Let $HS(\mathcal{H}, \mathcal{E})$ denote the Hilbert-Schmidt operators from the Hilbert space \mathcal{H} to the Hilbert space \mathcal{E} . For a fixed orthonormal basis $(e_\delta)_\delta$ of \mathcal{H} , the *vectorization map*, $\text{vec} : HS(\mathcal{H}, \mathcal{E}) \rightarrow \mathcal{H} \otimes \mathcal{E}$ is defined, for $T \in HS(\mathcal{H}, \mathcal{E})$ by

$$\text{vec}(T) = \sum_{\delta} e_\delta \otimes Te_\delta$$

Lemma 5.3. *Let $A, B \in HS(\mathcal{H}, \mathcal{E})$ and $P, Q \in \mathcal{B}(\mathcal{H})$, $T \in \mathcal{B}(\mathcal{E})$.*

(1) *We have*

$$\langle \text{vec}(A), \text{vec}(B) \rangle_{\mathcal{H} \otimes \mathcal{E}} = \text{Tr}(A^*B).$$

In particular, $\|\text{vec}(A)\| = \|A\|_{\text{HS}}$, and the value is independent of the choice of the orthonormal basis.

(2) *The following compatibility with left/right actions holds:*

$$(P \otimes I_{\mathcal{E}}) \text{vec}(A) = \text{vec}(AP^*), \quad (I_{\mathcal{H}} \otimes T) \text{vec}(A) = \text{vec}(TA),$$

hence, more generally,

$$(P \otimes T) \text{vec}(A) = \text{vec}(TA P^*).$$

(3) *(Inner-product identity used in Proposition 5.4)*

$$\langle (P \otimes I_{\mathcal{E}}) \text{vec}(A), (Q \otimes I_{\mathcal{E}}) \text{vec}(B) \rangle = \text{Tr}(PA^*BQ^*).$$

Proof. Fix an orthonormal basis $(e_\delta)_\delta$ of \mathcal{H} .

Using the definition,

$$\langle \text{vec}(A), \text{vec}(B) \rangle = \sum_{\delta} \langle Ae_\delta, Be_\delta \rangle_{\mathcal{E}} = \sum_{\delta} \langle e_\delta, A^*Be_\delta \rangle_{\mathcal{H}} = \text{Tr}(A^*B).$$

The right-hand side is independent of the choice of orthonormal basis, hence so is the left-hand side, proving item (1).

To prove the first identity of item (2), observe

$$(P \otimes I_{\mathcal{E}}) \text{vec}(A) = \sum_{\delta} Pe_\delta \otimes Ae_\delta = \sum_{\delta, \delta'} \langle e'_\delta, Pe_\delta \rangle e'_\delta \otimes Ae_\delta = \sum_{\delta} e_\delta \otimes AP^*e_\delta = \text{vec}(AP^*).$$

The second identity is immediate: $(I_{\mathcal{H}} \otimes T) \sum_{\delta} e_\delta \otimes Ae_\delta = \sum_{\delta} e_\delta \otimes T(Ae_\delta) = \text{vec}(TA)$. Combine both identities to get $(P \otimes T) \text{vec}(A) = \text{vec}(TAP^*)$.

Turning to item (3), Using

(2) twice and then item (1),

$$\begin{aligned} \langle (P \otimes I) \text{vec}(A), (Q \otimes I) \text{vec}(B) \rangle &= \langle \text{vec}(AP^*), \text{vec}(BQ^*) \rangle \\ &= \text{Tr}((AP^*)^*BQ^*) \\ &= \text{Tr}(PA^*BQ^*). \end{aligned}$$

□

We have now reached the main result of this section.

Proposition 5.4. *If $\varphi : \mathcal{A}_{2d+2} \rightarrow \mathbb{C}$ is a continuous linear functional such that*

$$\varphi(p^*p) \geq 0$$

for all $p \in \mathcal{A}_{d+1}$, then there exist a finite-dimensional Hilbert space \mathcal{E} , a self-adjoint g -tuple $Y = (Y_1, \dots, Y_g)$ on \mathcal{E} , and a vector $\gamma \in \mathcal{H} \otimes \mathcal{E}$ such that

$$\varphi(q^*p) = \langle p(Y)\gamma, q(Y)\gamma \rangle_{\mathcal{H} \otimes \mathcal{E}} \quad \text{for all } p \in \mathcal{A}_{d+1}, q \in \mathcal{A}_d.$$

Therefore, for all $p \in \mathcal{A}_{2d+1}$,

$$\varphi(p) = \langle p(Y)\gamma, \gamma \rangle.$$

The proof proceeds in five steps.

5.1. The positive block matrix S . We construct a finite-rank psd block operator matrix S that determines the linear functional φ .

By Lemma 5.2, there exist a finite index set J , vectors $h_j, k_j \in \mathcal{H}$, and scalars $c_u \in \mathbb{C}$ ($u \in \langle x \rangle_{2d+2}$) such that for every $p = \sum_{u \in \langle x \rangle_{2d+2}} P_u u$,

$$\varphi(p) = \sum_{j \in J} \sum_{u \in \langle x \rangle_{2d+2}} c_u \langle P_u h_j, k_j \rangle.$$

For $v, w \in \langle x \rangle_{d+1}$ define the finite rank operators

$$S_{v^*w} := c_{v^*w} \sum_{j \in J} |h_j\rangle\langle k_j|.$$

Denote by S the $N(d+1) \times N(d+1)$ block operator matrix whose (v, w) entry is S_{w^*v} . If $p = \sum_{w \in \langle x \rangle_{d+1}} P_w w$ and $q = \sum_{v \in \langle x \rangle_{d+1}} Q_v v$, a direct computation gives the block-trace identity

$$\begin{aligned} \varphi(q^*p) &= \sum_{j \in J} \sum_{v, w \in \langle x \rangle_{d+1}} c_{v^*w} \langle Q_v^* P_w h_j, k_j \rangle \\ &= \sum_{v, w \in \langle x \rangle_{d+1}} c_{v^*w} \sum_{j \in J} \langle Q_v^* P_w h_j, k_j \rangle \\ &= \sum_{v, w \in \langle x \rangle_{d+1}} \text{Tr}_{\mathcal{H}}(S_{v^*w} Q_v^* P_w). \end{aligned} \tag{5.1}$$

Define a row operator $P : \bigoplus_{\langle x \rangle_{d+1}} \mathcal{H} \rightarrow \mathcal{H}$ by

$$P(\bigoplus_{w \in \langle x \rangle_{d+1}} \zeta_w) = \sum_w P_w \zeta_w.$$

The adjoint $P^* : \mathcal{H} \rightarrow \mathcal{H}^{N(d+1)}$ of P is given by

$$P^* \eta = \bigoplus_{w \in \langle x \rangle_{d+1}} P_w^* \eta.$$

Now

$$\begin{aligned} \varphi(p^*p) &= \sum_{v, w \in \langle x \rangle_{d+1}} \text{Tr}_{\mathcal{H}}(S_{v^*w} P_v^* P_w) \\ &= \sum_{v, w \in \langle x \rangle_{d+1}} \text{Tr}_{\mathcal{H}}([S]_{w,v} [P^* P]_{v,w}) \end{aligned}$$

$$= \text{Tr}(SP^*P).$$

We claim that

$$\text{Tr}(ST) \geq 0 \quad (5.2)$$

for any positive operator $T \in \mathcal{B}(\mathcal{H}^{N(d+1)})$. It follows from Lemma 2.1 that $T = P^*P$ (when \mathcal{H} is infinite-dimensional) for some $P : \mathcal{H}^{N(d+1)} \rightarrow \mathcal{H}$. Letting $p = \sum P_w w$, where P_w is the w^{th} element of the row operator P gives,

$$\text{Tr}(ST) = \varphi(p^*p) \geq 0.$$

In case of finite dimensional \mathcal{H} , a similar argument gives (5.2). The only difference is that instead of one polynomial, $N(d+1)$ many polynomials as per Lemma 2.1 are required. In either case it follows that $\text{Tr}(ST) \geq 0$ for all positive operators T .

The positivity of S can be concluded exactly as in the proof of Lemma 4.4. Because J and $\langle x \rangle_{d+1}$ are finite, S is finite rank.

5.2. An Auxiliary Hilbert space \mathcal{M} . We construct a finite-dimensional Hilbert space \mathcal{M} from the psd sesquilinear form induced by the psd operator S . The Hilbert space \mathcal{E} is constructed as a subspace of \mathcal{M} in Subsection 5.4.

Consider the vector space

$$V := \bigoplus_{w \in \langle x \rangle_{d+1}} \mathcal{H}.$$

Equip V with the sesquilinear form

$$\begin{aligned} \langle (\xi_w)_w, (\eta_v)_v \rangle_V &:= \langle S(\xi_w)_w, (\eta_v)_v \rangle_{\mathcal{H}^{N(d+1)}} = \sum_{v \in \langle x \rangle_{d+1}} \left\langle \sum_{w \in \langle x \rangle_{d+1}} [S]_{v,w} \xi_w, \eta_v \right\rangle_{\mathcal{H}} \\ &= \sum_{v,w \in \langle x \rangle_{d+1}} \langle S_{w^*v} \xi_w, \eta_v \rangle_{\mathcal{H}} = \sum_{v,w \in \langle x \rangle_{d+1}} \langle \xi_w, S_{v^*w} \eta_v \rangle_{\mathcal{H}}. \end{aligned}$$

This form is psd by the positivity of S . Let

$$\mathcal{N} := \{z \in V : \langle z, z \rangle_V = 0\}$$

denote its subspace of null vectors and set

$$\mathcal{M} := V/\mathcal{N}.$$

Since S has finite rank, \mathcal{M} is finite dimensional.

5.3. The coordinate maps $\Phi(w)$. The coordinate maps are important for defining the Hilbert space \mathcal{E} , the operator tuple Y , and the representing vector γ .

For each $w \in \langle x \rangle_{d+1}$ define

$$\Phi(w) : \mathcal{H} \rightarrow \mathcal{M}, \quad \Phi(w)\xi = [(\delta_{u,w}\xi)_{u \in \langle x \rangle_{d+1}}],$$

where $\delta_{u,w}$ denotes the Kronecker delta. Thus, for all $v, w \in \langle x \rangle_{d+1}$ and $\xi, \eta \in \mathcal{H}$,

$$\langle \Phi(w)\xi, \Phi(v)\eta \rangle_{\mathcal{M}} = \langle \xi, S_{v^*w} \eta \rangle_{\mathcal{H}}. \quad (5.3)$$

5.4. The Hilbert space \mathcal{E} and the operator tuple Y . We define a Hilbert space \mathcal{E} and a self-adjoint tuple of operators Y on \mathcal{E} .

Let

$$\mathcal{E} := \text{span}\{\Phi(w)\xi : w \in \langle x \rangle_d, \xi \in \mathcal{H}\} \subset \mathcal{M}.$$

For $i = 1, \dots, g$, define $L_{x_i} : \mathcal{E} \rightarrow \mathcal{M}$ by

$$L_{x_i}(\Phi(w)\xi) = \Phi(x_i w)\xi \quad (w \in \langle x \rangle_d, \xi \in \mathcal{H}). \quad (5.4)$$

5.4.1. The L_{x_j} are well-defined. If $z = \sum_{w \in \langle x \rangle_d} \Phi(w)\xi_w \in \mathcal{E}$ represents 0 in \mathcal{M} (i.e., $z \in \mathcal{N}$), then for any $v \in \langle x \rangle_{d+1}$ and $\eta \in \mathcal{H}$, using (5.3) and $(x_i v)^* = v^* x_i$,

$$\begin{aligned} \langle L_{x_i} z, \Phi(v)\eta \rangle_{\mathcal{M}} &= \sum_{w \in \langle x \rangle_d} \langle \xi_w, S_{v^* x_i w} \eta \rangle_{\mathcal{H}} = \sum_{w \in \langle x \rangle_d} \langle \xi_w, S_{(x_i v)^* w} \eta \rangle_{\mathcal{H}} \\ &= \langle z, \Phi(x_i v)\eta \rangle_{\mathcal{M}} = 0. \end{aligned}$$

Since the vectors $\Phi(v)\eta$ span \mathcal{M} , we have $L_{x_i} z \in \mathcal{N}$, proving that L_{x_i} is well-defined. Let $P_{\mathcal{E}}$ be the orthogonal projection of \mathcal{M} onto \mathcal{E} . For $i = 1, \dots, g$, define $Y_i : \mathcal{E} \rightarrow \mathcal{E}$ by

$$Y_i = P_{\mathcal{E}} L_{x_i}.$$

5.4.2. The Y_j are self-adjoint. For $v, w \in \langle x \rangle_d$ and $\xi, \eta \in \mathcal{H}$,

$$\begin{aligned} \langle Y_i \Phi(w)\xi, \Phi(v)\eta \rangle_{\mathcal{E}} &= \langle L_{x_i} \Phi(w)\xi, P_{\mathcal{E}} \Phi(v)\eta \rangle_{\mathcal{M}} \\ &= \langle L_{x_i} \Phi(w)\xi, \Phi(v)\eta \rangle_{\mathcal{M}} \\ &= \langle \xi, S_{v^* x_i w} \eta \rangle_{\mathcal{H}} \\ &= \langle \xi, S_{(x_i v)^* w} \eta \rangle_{\mathcal{H}} \\ &= \langle \Phi(w)\xi, L_{x_i} \Phi(v)\eta \rangle_{\mathcal{M}} \\ &= \langle Y_i^* \Phi(w)\xi, \Phi(v)\eta \rangle_{\mathcal{E}}. \end{aligned}$$

5.5. The representing vector and evaluation. We construct the representing vector γ and complete the proof. It is here that the vectorization map of Lemma 5.3 appears.

Define

$$\gamma := \text{vec}(P_{\mathcal{E}} \Phi(\emptyset)) \in \mathcal{H} \otimes \mathcal{E},$$

where, as usual, \emptyset is the empty word. Consider a word $w = x_{i_1} \cdots x_{i_k}$ with $k \leq d + 1$. We claim that

$$Y^w P_{\mathcal{E}} \Phi(\emptyset) = P_{\mathcal{E}} \Phi(w).$$

Indeed, for $\xi \in \mathcal{H}$, a word $|w| \leq d$, and $1 \leq j \leq g$,

$$Y_j P_{\mathcal{E}} \Phi(w)\xi = P_{\mathcal{E}} L_{x_j} \Phi(w)\xi = P_{\mathcal{E}} \Phi(x_j w)\xi,$$

since $\Phi(w)\xi \in \mathcal{E}$. Hence, a finite induction argument gives,

$$\begin{aligned} Y^w P_{\mathcal{E}} \Phi(\emptyset)\xi &= Y^w \Phi(\emptyset)\xi \\ &= Y_{i_1} \cdots Y_{i_k} \Phi(\emptyset)\xi \\ &= Y_{i_1} \cdots Y_{i_{k-1}} P_{\mathcal{E}} L_{x_k} \Phi(\emptyset)\xi \\ &= Y_{i_1} \cdots Y_{i_{k-1}} \Phi(x_k)\xi \\ &= Y_{i_1} \Phi(x_{i_2} \cdots x_{i_k})\xi \end{aligned}$$

$$= P_{\mathcal{E}} \Phi(w) \xi.$$

Thus for $w \in \langle x \rangle_{d+1}$,

$$\begin{aligned} (I_{\mathcal{H}} \otimes Y^w) \gamma &= (I_{\mathcal{H}} \otimes Y^w) \left(\sum_{\delta} e_{\delta} \otimes P_{\mathcal{E}} \Phi(\emptyset) e_{\delta} \right) \\ &= \sum_{\delta} e_{\delta} \otimes P_{\mathcal{E}} \Phi(w) e_{\delta} \\ &= \text{vec}(P_{\mathcal{E}} \Phi(w)). \end{aligned} \tag{5.5}$$

Let $p = \sum_{w \in \langle x \rangle_{d+1}} P_w w$ and $q = \sum_{v \in \langle x \rangle_d} Q_v v$. Using (5.5) and the standard vectorization identity (see Lemma 5.3)

$$\langle (T \otimes I) \text{vec}(A), (R \otimes I) \text{vec}(B) \rangle = \text{Tr}(TA^*BR^*),$$

we obtain

$$\begin{aligned} \langle p(Y) \gamma, q(Y) \gamma \rangle &= \sum_{w \in \langle x \rangle_{d+1}} \sum_{v \in \langle x \rangle_d} \langle (P_w \otimes I) \text{vec}(P_{\mathcal{E}} \Phi(w)), (Q_v \otimes I) \text{vec}(P_{\mathcal{E}} \Phi(v)) \rangle \\ &= \sum_{w \in \langle x \rangle_{d+1}} \sum_{v \in \langle x \rangle_d} \text{Tr}(P_w \Phi(w)^* P_{\mathcal{E}} \Phi(v) Q_v^*) \\ &= \sum_{w \in \langle x \rangle_{d+1}} \sum_{v \in \langle x \rangle_d} \sum_{\delta} \langle P_{\mathcal{E}} \Phi(v) Q_v^* e_{\delta}, \Phi(w) P_w^* e_{\delta} \rangle \\ &= \sum_{w \in \langle x \rangle_{d+1}} \sum_{v \in \langle x \rangle_d} \sum_{\delta} \langle \Phi(v) Q_v^* e_{\delta}, \Phi(w) P_w^* e_{\delta} \rangle \\ &= \sum_{w \in \langle x \rangle_{d+1}} \sum_{v \in \langle x \rangle_d} \sum_{\delta} \langle Q_v^* e_{\delta}, S_{w^* w} P_w^* e_{\delta} \rangle \quad (\text{using (5.3)}) \\ &= \sum_{w \in \langle x \rangle_{d+1}} \sum_{v \in \langle x \rangle_d} \sum_{\delta} \langle P_w S_{v^* w} Q_v^* e_{\delta}, e_{\delta} \rangle \\ &= \sum_{w \in \langle x \rangle_{d+1}} \sum_{v \in \langle x \rangle_d} \text{Tr}(P_w S_{v^* w} Q_v^*) \\ &= \sum_{w \in \langle x \rangle_{d+1}} \sum_{v \in \langle x \rangle_d} \text{Tr}(S_{v^* w} Q_v^* P_w). \end{aligned}$$

By (5.1), the right-hand side equals $\varphi(q^* p)$, proving

$$\varphi(q^* p) = \langle p(Y) \gamma, q(Y) \gamma \rangle,$$

for all $p \in \mathcal{A}_{d+1}$, $q \in \mathcal{A}_d$. □

6. PROOF OF THEOREM 1.1

Suppose $f \in \mathcal{A}_{2d}$ satisfies item (ii) of Theorem 1.1. That is, $f(X) \succeq 0$ for all \mathbf{g} -tuples of self-adjoint matrices $X = (X_1, \dots, X_g)$. Our aim is to show that $f \in \mathcal{C}_d$. We will prove this statement via the contrapositive. Accordingly, assume that $f \notin \mathcal{C}_d$. Since the top degree terms cannot cancel, $f \notin \mathcal{C}_{d+1}$.

Since \mathcal{A}_{2d+2} is a locally convex topological vector space and \mathcal{C}_{d+1} is closed by Proposition 4.1, the Hahn–Banach separation theorem (see, e.g., [Dav25, Corollary 3.3.9]) implies that there exist a WOT continuous linear functional $\varphi : \mathcal{A}_{2d+2} \rightarrow \mathbb{C}$, and real numbers γ_1, γ_2 such that

$$\text{real}(\varphi(f)) < \gamma_1 < \gamma_2 < \text{real}(\varphi(p)) \quad \text{for all } p \in \mathcal{C}_{d+1}.$$

By (3.6), it follows that $f = f^*$ as $Z(f) = Z(f^*)$. Also $p = p^*$ for all $p \in \mathcal{C}_{d+1}$. Since \mathcal{C}_{d+1} is a cone,

$$\varphi(f) = \text{real}(\varphi(f)) < 0 \leq \text{real}(\varphi(p)) = \varphi(p) \quad \text{for all } p \in \mathcal{C}_{d+1}.$$

Now apply Proposition 5.4. There exist a finite-dimensional Hilbert space \mathcal{E} , a self-adjoint g -tuple $Y = (Y_1, \dots, Y_g)$ on \mathcal{E} , and a vector $\gamma \in \mathcal{H} \otimes \mathcal{E}$ such that

$$\varphi(p) = \langle p(Y)\gamma, \gamma \rangle_{\mathcal{H} \otimes \mathcal{E}} \quad \text{for all } p \in \mathcal{A}_{2d}.$$

In particular,

$$0 > \varphi(f) = \langle f(Y)\gamma, \gamma \rangle.$$

Thus $f(Y) \not\succeq 0$. □

7. PROOF OF THEOREM 1.3

The proof of Theorem 1.3 roughly follows the outline used in the proof of Theorem 1.1 in Section 6 above. We thus only explain the differences and adaptations needed to establish Theorem 1.3.

Most of the notation we introduced for \mathcal{A} naturally carries over to \mathcal{A} . We will use \mathcal{C} to denote the sum of squares in \mathcal{A} , and a straightforward adaptation of the results of Section 2 yields an analog of Corollary 2.3 (and Remark 2.4) describing the cone \mathcal{C}_d in \mathcal{A}_{2d} . Of course, V_d is now the Veronese column vector for (reduced) words $u \in \mathbb{F}_g$ with $|u| \leq d$.

7.1. Creation operators and a tuple of unitaries. The biggest change is in the construction of suitable operators out of the creation operators. That is, we need to replace the self-adjoint A_j of (3.4) with unitary operators U_j . Let \mathbf{F}_d denote the Hilbert space obtained as the span of (the orthonormal set) $(\mathbb{F}_g)_d$ of words of length at most d . For notational purposes, let $\{x, x^{-1}\}$ denote the set $\{x_1, \dots, x_g, x_1^{-1}, \dots, x_g^{-1}\}$. Fix $y \in \{x, x^{-1}\}$ and let

$$\mathbf{M}_y = \text{span}((\mathbb{F}_g)_{d-1} \cup y(\mathbb{F}_g)_{d-1}) \subseteq \mathbf{F}_d$$

Since if $w \in \mathbf{M}_{y^{-1}}$, then $yw \in \mathbf{M}_y$, we obtain a linear map

$$L_y : \mathbf{M}_{y^{-1}} \rightarrow \mathbf{M}_y, \quad L_y w = yw.$$

Given a reduced word $u \in (\mathbb{F}_g)_{d-1}$, $y^{-1}u \in y^{-1}(\mathbb{F}_g)_{d-1}$ (or $y^{-1}u \in (\mathbb{F}_g)_{d-2}$) and $L_y y^{-1}u = u$. Thus u is in the range of L_y . Similarly, $yu \in y(\mathbb{F}_g)_{d-1}$, is in the range of L_y since $u \in \mathbf{M}_{y^{-1}}$. Hence L_y is onto. Since $\mathbf{M}_{y^{-1}}$ and \mathbf{M}_y have the same dimension (by symmetry), L_y is bijective. Now let $w, v \in (\mathbb{F}_g)_{d-1} \cup y(\mathbb{F}_g)_{d-1}$ be given. Since L_y is bijective $L_y w = L_y v$ if and only if $w = v$ and thus,

$$\langle L_y w, L_y v \rangle = \langle w, v \rangle,$$

for all $w, v \in (\mathbb{F}_g)_{d-1} \cup y(\mathbb{F}_g)_{d-1}$. Since $(\mathbb{F}_g)_{d-1} \cup y(\mathbb{F}_g)_{d-1}$ is an orthonormal basis for $\mathbf{M}_{y^{-1}}$, it follows that L_y is a unitary map. Because $\mathbf{M}_{y^{-1}}$ and \mathbf{M}_y have the same dimension, they have the same codimension in \mathbf{F}_d and hence L_y extends to a unitary operator on \mathbf{F}_d , called

U_y . Note that if $w \in (\mathbb{F}_g)_{d-1}$ and $z \in \{x, x^{-1}\}$, then $L_z L_y w = zyw$. In particular, if $z = y^{-1}$, then $L_z L_y w = w$. Finally, if $w \in (\mathbb{F}_g)_d$, then

$$L^w \emptyset = w.$$

To prove this claim, given $w \in (\mathbb{F}_g)_d$, write $w = yu$ where $u \in (\mathbb{F}_g)_{d-1}$ and $y \in \{x, x^{-1}\}$. Thus $L^w \emptyset = L_y L^u \emptyset = L_y u = yu$.

Next, the analog of Proposition 3.3 in the unitary case is the following: If $p \in \mathcal{C}_d$, then Γ_p is norm bounded. More precisely, with the U_y just constructed and

$$U = (U_{x_1}, \dots, U_{x_g}, U_{x_1^{-1}}, \dots, U_{x_g^{-1}}),$$

there exists a τ_d such that if $S \in \Gamma_p$, then

$$\|S\| \leq \tau_d \|p(U)\|.$$

To prove this claim, observe, for a word $w \in (\mathbb{F}_g)_d$ and vectors $\zeta, \eta \in \mathcal{H}$,

$$\langle p(U)\zeta \otimes \emptyset, \eta \otimes w \rangle = \langle P_w \zeta, \eta \rangle.$$

Hence, $\|P_w\| \leq \|p(U)\|$. Now follow the rest of the proof of Proposition 3.3 with the conclusion $\|S_{v,w}\| \leq N_{\text{red}}(d) \|p(U)\|$.

After the topology on \mathcal{A}_{2d} has been defined via WOT-convergence of the coefficients as in Section 4, the proof of Proposition 4.1 translates essentially verbatim to show the closedness of the cone \mathcal{C}_d .

7.2. A modified GNS construction. The only other point that needs attention is the proof of a suitable GNS construction as in Proposition 5.4. Since we cannot rely on non-cancellation of the highest order terms, we start with a continuous $\varphi : \mathcal{A}_{2d} \rightarrow \mathbb{C}$ that is positive on \mathcal{C}_d ; that is,

$$\varphi(p^* p) \geq 0$$

for all $p \in \mathcal{A}_d$. We go about obtaining S and \mathcal{E} as in the self-adjoint case - with the obvious adjustments.

For $y \in \{x, x^{-1}\}$, we now let

$$\mathcal{M}_y = \text{span}\{\Phi(w)\xi : w \in ((\mathbb{F}_g)_{d-1} \cup y^{-1}(\mathbb{F}_g)_{d-1}), \xi \in \mathcal{H}\} \subseteq \mathcal{E}.$$

It is evident that if $w \in \mathcal{M}_{y^{-1}}$, then $yw \in \mathcal{M}_y$. Hence we obtain a linear map $L_y : \mathcal{M}_{y^{-1}} \rightarrow \mathcal{M}_y$ by

$$L_y \Phi(w)\xi = \Phi(yw)\xi.$$

That L_y is well-defined works just as with the self-adjoint case. That L_y is isometric is a consequence of

$$S_{v,w} = S_{v^{-1}w} = S_{v^{-1}y^{-1}yw} = S_{(yw)^{-1}(yw)},$$

for the relevant v, w and where our involution $*$ satisfies $y^* = y^{-1}$. To see that L_y is onto, observe if $w \in \mathcal{M}_y$, then $L_y L_{y^{-1}} w = w$. Hence L_y is onto (and $L_{y^{-1}}$ is its inverse). Thus L_y is unitary.

Since \mathcal{E} is finite dimensional and L_y is bijective between them, the subspaces $\mathcal{M}_{y^{-1}}$ and \mathcal{M}_y have the same codimension and thus L_y extends to a unitary map $U_y : \mathcal{E} \rightarrow \mathcal{E}$. The novel ingredients now in place, following the, by now, beaten path of the cone separation GNS argument yields Theorem 1.3. \square

8. CONCLUDING REMARK AND A PROBLEM

The reader will have no difficulty verifying that both Theorem 1.1 and Theorem 1.3 remain true if we replace the algebra of coefficients $\mathcal{B}(\mathcal{H})$ with a von Neumann algebra. The proofs carry over to this setting in a straightforward way. On the other hand, we do not know if the results still hold if the coefficients are from a C^* -algebra.

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