

# 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  $S$  representing the sos polynomial  $p$ . As a consequence, the cone of (sums of) squares of polynomials is closed in the 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 17<sup>th</sup> 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 [HM04, 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  $\mathbf{g}$ . Let  $\langle x \rangle$  denote the free monoid on the  $\mathbf{g}$  letters of the alphabet  $x = \{x_1, \dots, x_{\mathbf{g}}\}$ . 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

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

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  $*$  as follows. 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  $X = (X_1, \dots, X_{\mathbf{g}})$  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  $\mathbb{F}_{\mathbf{g}}$  on the  $\mathbf{g}$  letters  $x_i$ ,  $i = 1, \dots, \mathbf{g}$ . Elements of  $\mathbb{F}_{\mathbf{g}}$  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  $r = \text{col} \begin{pmatrix} r_1 & \cdots & r_{N(d)} \end{pmatrix} \in \mathcal{A}^{N(d)} = \mathcal{B}(\mathcal{H}, \mathcal{H}^{N(d)}) \langle x \rangle$ , (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?). There are several novel results and constructions of independent interest necessitated by the consideration of operator coefficients. In the large, the proofs of Theorem 1.1 and Theorem 1.3 proceed in the by a now standard approach to establishing sum of squares (sos) representations (factorizations). Namely, Hahn-Banach separation produces a separating linear functional  $\varphi$  followed by a Gelfand-Naimark-Segal (GNS) construction based on  $\varphi$  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  $S$  that represents  $p$ . See Proposition 3.3. Via this route we obtain the key fact needed for Hahn-Banach separation. Namely that the cone of sums of squares is weak operator topology (WOT) closed. In the GNS construction, we introduce a new argument that exploits the WOT to associate to a separating linear functional a finite rank psd non-commutative representing Hankel matrix. Continuing with the GNS construction, a proof of Theorem 1.3 demands a new construction to produce a tuple of unitary operators together with a representing vector that realizes the separating linear functional as a vector state. See 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  $\mathcal{F}_{\mathbf{g}}^2$  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 4.4. 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 5.3. Then Theorem 1.1 is proved in Section 6 and Theorem 1.3 is proved in Section 7. The paper concludes with an Appendix that collects auxiliary results that may be well-known to experts.

## 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, 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  $\mathbf{g} = 2$  and  $d = 2$ , then

$$V_2 = \text{col} \begin{pmatrix} 1 & x_1 & x_2 & x_1^2 & x_1x_2 & x_2x_1 & x_2^2 \end{pmatrix}.$$

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

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

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  $V_d^*SV_d$  for a psd matrix  $S$ .

**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  $S$  such that*

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

*In fact, if  $p = V_d^* S V_d$ , then factoring  $S = \sum_{j=1}^{N(d)} R_j R_j^*$  with  $R_j : \mathcal{H} \rightarrow \oplus_{w \in \langle x \rangle_d} \mathcal{H}$  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 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  $p = V_d^* S V_d$ , where  $S = \sum_{i=1}^{N(d)} R_i R_i^*$ . In particular,  $S : \mathcal{H}^{N(d)} \rightarrow \mathcal{H}^{N(d)}$  is a psd linear map.

Conversely, suppose there is a psd linear map  $S : \oplus_{w \in \langle x \rangle_d} \mathcal{H} \rightarrow \oplus_{w \in \langle x \rangle_d} \mathcal{H}$  such that  $p = V_d^* S V_d$ . By Lemma 2.1, there exist  $R_j : \mathcal{H} \rightarrow \oplus_{w \in \langle x \rangle_d} \mathcal{H}$  such that  $S = \sum_{j=1}^{N(d)} R_j R_j^*$ . 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  $p = V^* S_p V$  and  $q = V^* S_q V$ . Now  $p + q = V_d^* (S_p + S_q) V_d$ . Since  $S_p + S_q : \mathcal{H}^{N(d)} \rightarrow \mathcal{H}^{N(d)}$  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*

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

**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 (3.2). 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*  $\Omega$ . 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  $\{e_1, \dots, e_{\mathbf{g}}\}$  be any orthonormal basis of  $\mathbb{C}^{\mathbf{g}}$ . With any  $w = x_{i_1} \dots x_{i_n} \in \langle x \rangle$ , associate a vector

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

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

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

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

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

$$A_i = L_i + L_i^*, \quad i = 1, \dots, \mathbf{g}. \quad (3.2)$$

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

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

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

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

$$\begin{aligned} A^w \Omega &= (L_{i_1} + L_{i_1}^*) A_{i_2} \dots A_{i_n} \Omega \\ &= L_{i_1} A_{i_2} \dots A_{i_n} \Omega + L_{i_1}^* A_{i_2} \dots A_{i_n} \Omega \\ &= L_{i_1} A^{\tilde{w}} \Omega + L_{i_1}^* A^{\tilde{w}} \Omega, \end{aligned}$$

where  $\tilde{w} = x_{i_2} \dots x_{i_n}$  is a word of length  $n-1$ . 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  $N(d) \times N(d)$  scalar matrix*

$$M_d = [\langle A^w \Omega, e_v \rangle]_{v,w \in \langle x \rangle_d}$$

*is invertible.*

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

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

by Lemma 3.1. Hence  $M_d$  is an upper triangular matrix. Moreover, each diagonal entry is 1 by Lemma 3.1. Thus,  $M_d$  is invertible.  $\square$



**3.3. Extraction formula for coefficients.** Let  $q = \sum Q_w w \in \mathcal{A}_d$ . For any basis vector  $e_v \in \mathcal{F}_g^2$ , define the linear functional

$$\Omega_v : \mathcal{B}(\mathcal{F}_g^2) \rightarrow \mathbb{C}, \quad \Omega_v(T) = \langle T\Omega, e_v \rangle.$$

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

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

where  $[M_d]_{v,w}$  is the  $(v, w)$  entry of the matrix  $M_d$ . In short,

$$Z(q) = M_d Q, \tag{3.3}$$

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

$$Q = M_d^{-1} Z(q). \tag{3.4}$$

We refer to equation (3.4) 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 (3.4) that there exists a positive constant  $\lambda_d$  (independent of  $q$ ) such that

$$\|Q_w\| \leq \lambda_d \|q(A)\| \quad \text{for all } w \in \langle x \rangle_d. \tag{3.5}$$

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

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

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

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

*where the tuple  $A$  is defined in (3.2).*

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

$$p = \sum_{j=1}^{N(d)} q_j^* q_j = V_d^* \left[ \sum_{j=1}^{N(d)} Q_j Q_j^* \right] V_d, \tag{3.6}$$

where

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

By equation (3.5), for  $v \in \langle x \rangle_d$ ,

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

From equation (3.6),

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

Thus, again using equation (3.6),

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

It follows that  $\|S\| \leq \mu_d \|p(A)\|$  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  $\mathcal{A}_{2d}$  in which the convex cone of sums of squares  $\mathcal{C}_d$  is closed. The main property of this topology is given in Proposition 4.1, and the closedness of  $\mathcal{C}_d$  is established in Proposition 4.4.

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 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  $(P_{\alpha,w})$  converges to  $P_w$  in WOT. Note that  $\mathcal{A}_d$  becomes a locally convex topological vector space with this topology.

**Proposition 4.1.** *Let  $(p_\alpha)_\alpha$  be a net in  $\mathcal{A}_d$  and  $p \in \mathcal{A}_d$ . The sequence  $(p_\alpha)_\alpha$  converges to  $p$  in the topology of  $\mathcal{A}_d$  if and only if  $(p_\alpha(A))$  converges to  $p(A)$  in the weak operator topology. Here,  $A$  is the tuple of operators defined in (3.2).*

Lemmas 4.2 and 4.3, taken together, prove Proposition 4.1.

**Lemma 4.2.** *If  $(p_\alpha = \sum_w P_{\alpha,w} w)_\alpha \subset \mathcal{A}_d$  converges to  $p = \sum_w P_w w \in \mathcal{A}_d$ , then  $(p_\alpha(X))_\alpha$  converges to  $p(X)$  in the WOT for any  $\mathbf{g}$ -tuple of self-adjoint operators  $X = (X_1, \dots, X_{\mathbf{g}})$ .*

*Proof.* Fix a  $\mathbf{g}$ -tuple of self-adjoint operators  $X = (X_1, \dots, X_{\mathbf{g}})$ . By hypotheses, the nets  $(P_{\alpha,w})_\alpha$  converge WOT for each  $w$ . Thus, by Lemma A.1, for each fixed  $w \in \langle x \rangle_d$ , the net of operators  $(P_{\alpha,w} \otimes X^w)_\alpha$  converges to  $P_w \otimes X^w$  in the WOT, since  $X^w$  is a fixed operator. Thus,  $(p_\alpha(X) = \sum_w P_{\alpha,w} \otimes X^w)_\alpha$  is a finite sum of convergent nets.  $\square$

**Lemma 4.3.** *Let  $(p_\alpha = \sum_w P_{\alpha,w} w)_\alpha$  be a net in  $\mathcal{A}_d$  and  $A = (A_1, \dots, A_{\mathbf{g}})$  be the tuple of self-adjoint operators of (3.2). If  $(p_\alpha(A))_\alpha$  converges in the WOT, then  $(p_\alpha)_\alpha$  converges. Moreover, if  $p = \sum_w P_w w \in \mathcal{A}_d$  is the limit of  $(p_\alpha)$ , then  $p(A)$  is the limit of the convergent net  $(p_\alpha(A))_\alpha$ .*

*Proof.* Let  $Z(p_\alpha)$  be the column vector corresponding to  $p_\alpha$  as in (3.3). Since  $(p_\alpha(A))_\alpha$  converges in the WOT,  $(Z(p_\alpha))_\alpha$  converges in the WOT. Now by (3.4), it follows that  $(P_{\alpha,w})_\alpha$  converges in the WOT. Let  $P_w$  be the WOT-limit of  $(P_{\alpha,w})_\alpha$ . Then  $p = \sum_w P_w w$  is the limit of  $(p_\alpha)_\alpha$ .  $\square$

**Proposition 4.4.** *The convex cone  $\mathcal{C}_d$  is closed.*

*Proof.* Let  $(p_\alpha)_\alpha$  be a net in  $\mathcal{C}_d$  that converges to  $p \in \mathcal{A}_{2d}$ . Our aim is to show that  $p \in \mathcal{C}_d$ . By Proposition 2.2, for each  $\alpha$ , there exists an  $S_\alpha \in \mathcal{B}(\mathcal{H})^{N(d) \times N(d)}$  such that  $S_\alpha \succeq 0$  and  $V_d^* S_\alpha V_d = p_\alpha$ . Since the net of operators  $(p_\alpha(A))_\alpha$  converges in the WOT, it follows from the Uniform Boundedness Principle that

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

By Proposition 3.3,

$$\sup_{\alpha} \|S_{\alpha}\| < \infty.$$

Thus, by the Banach–Alaoglu theorem, there is a sequence of operators  $(S_{\alpha_i})_{i \in \mathbb{N}} \subset (S_{\alpha})_{\alpha}$  that converges to some operator  $S \in \mathcal{B}(\mathcal{H})^{N(d) \times N(d)}$  in the ultraweak operator topology. The ultraweak operator topology 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  $\mathcal{B}(\mathcal{H})$ . Since the convergence in the ultraweak operator topology is stronger than convergence in the weak operator topology,  $S_{\alpha_i} \rightarrow S$  in the WOT. Thus,  $S \succeq 0$ .

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

$$p_{\alpha}(A) = V_d(A)^*(S_{\alpha} \otimes I_{\mathcal{F}_{\mathbf{g}}^2})V_d(A),$$

where

$$V_d(A) : \mathcal{H} \otimes \mathcal{F}_{\mathbf{g}}^2 \rightarrow \mathcal{H}^{N(d)} \otimes \mathcal{F}_{\mathbf{g}}^2, \quad h \otimes \xi \mapsto (h \otimes A^w \xi)_w.$$

Since  $(S_{\alpha_i})$  converges  $S$  in the WOT,

$$V_d(A)^*(S_{\alpha_i} \otimes I_{\mathcal{F}_{\mathbf{g}}^2})V_d(A) \rightarrow V_d(A)^*(S \otimes I_{\mathcal{F}_{\mathbf{g}}^2})V_d(A) = q(A)$$

in the WOT by Lemma A.1. Thus,  $(p_{\alpha_i}(A))$  converges to  $q(A)$  in the WOT. Therefore,  $p(A) = q(A)$ . Since, by the extraction formula, equation (3.4), the coefficients of  $p$  and  $q$  are determined by evaluation at  $A$ , it follows that  $p = q$ . Hence,  $p \in \mathcal{C}_d$ .  $\square$

## 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 5.3. The following result is well-known. We refer the reader to [Dav25, Section 3.1] and Exercise 3.4 in that book.

**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*

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

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

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

*Proof.* First identify  $\mathcal{A}_d$  with  $\mathcal{B}(\mathcal{H})^{N(d)}$  via

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

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

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

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

**Proposition 5.3.** *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  $\varphi$ .

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

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

Let  $\mathcal{H}^{N(d+1)} := \bigoplus_{w \in \langle x \rangle_{d+1}} \mathcal{H}$ . Define the row operator  $P : \mathcal{H}^{N(d+1)} \rightarrow \mathcal{H}$  by

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

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

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

Now

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

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

We claim that

$$\operatorname{Tr}(ST) \geq 0 \tag{5.2}$$

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  $w^{\text{th}}$  element of the row operator  $P$  gives,

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

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  $\operatorname{Tr}(ST) \geq 0$  for all positive operators  $T$ .

To prove that  $S$  is a positive operator, it remains to show that  $S$  is self-adjoint. For  $T \succeq 0$ , equation (5.2) says  $\operatorname{Tr}(ST)$  is real. Hence,

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

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

$$\operatorname{Tr}(S^*T) = \operatorname{Tr}(ST) \quad \text{for all } T \in \mathcal{B}(\mathcal{H}^{N(d+1)}).$$

Hence  $S^* = S$  and  $S \succeq 0$ . 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 Step 4, 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 (hence complete).

**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  $\gamma$ .

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  $\gamma$  and complete the proof.

Let  $\text{vec} : HS(\mathcal{H}, \mathcal{E}) = B(\mathcal{H}, \mathcal{E}) \rightarrow \mathcal{H} \otimes \mathcal{E}$  denote the vectorization map defined on the space of Hilbert-Schmidt operators  $HS(\mathcal{H}, \mathcal{E})$ ,

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

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

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

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 A.2)

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

we obtain

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

$$\begin{aligned}
&= \sum_{w \in \langle x \rangle_{d+1}} \sum_{v \in \langle x \rangle_d} \sum_{\delta} \langle \Phi(v) Q_v^* e_{\delta}, \Phi(w) P_w^* e_{\delta} \rangle \\
&= \sum_{w \in \langle x \rangle_{d+1}} \sum_{v \in \langle x \rangle_d} \sum_{\delta} \langle Q_v^* e_{\delta}, S_{w^*v} P_w^* e_{\delta} \rangle \quad (\text{using (5.3)}) \\
&= \sum_{w \in \langle x \rangle_{d+1}} \sum_{v \in \langle x \rangle_d} \sum_{\delta} \langle P_w S_{v^*w} Q_v^* e_{\delta}, e_{\delta} \rangle \\
&= \sum_{w \in \langle x \rangle_{d+1}} \sum_{v \in \langle x \rangle_d} \text{Tr} (P_w S_{v^*w} Q_v^*) \\
&= \sum_{w \in \langle x \rangle_{d+1}} \sum_{v \in \langle x \rangle_d} \text{Tr} (S_{v^*w} Q_v^* P_w).
\end{aligned}$$

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  $X = (X_1, \dots, X_{\mathbf{g}})$ . 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, by the Hahn–Banach separation theorem (see, e.g., [Dav25, Corollary 3.3.9]), there exist a linear functional  $\varphi : \mathcal{A}_{2d+2} \rightarrow \mathbb{C}$ , and real numbers  $\gamma_1, \gamma_2$  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 (3.4), 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 5.3. There exist a finite-dimensional Hilbert space  $\mathcal{E}$ , a self-adjoint  $\mathbf{g}$ -tuple  $Y = (Y_1, \dots, Y_{\mathbf{g}})$  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  $u \in \mathbb{F}_{\mathbf{g}}$  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 (3.2) with unitary operators  $U_j$ . Let  $\mathbf{F}_d$  denote the Hilbert space obtained as the span of (the orthonormal set)  $(\mathbb{F}_{\mathbf{g}})_d$  of words of length at most  $d$ . For notational purposes, let  $\{x, x^{-1}\}$  denote the set  $\{x_1, \dots, x_{\mathbf{g}}, x_1^{-1}, \dots, x_{\mathbf{g}}^{-1}\}$ . Fix  $y \in \{x, x^{-1}\}$  and let

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

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  $u \in (\mathbb{F}_{\mathbf{g}})_{d-1}$ ,  $y^{-1}u \in y^{-1}(\mathbb{F}_{\mathbf{g}})_{d-1}$  (or  $y^{-1}u \in (\mathbb{F}_{\mathbf{g}})_{d-2}$ ) and  $L_y y^{-1}u = u$ . Thus  $u$  is in the range of  $L_y$ . Similarly,  $yu \in y(\mathbb{F}_{\mathbf{g}})_{d-1}$ , 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  $w, v \in (\mathbb{F}_{\mathbf{g}})_{d-1} \cup y(\mathbb{F}_{\mathbf{g}})_{d-1}$  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  $w, v \in (\mathbb{F}_{\mathbf{g}})_{d-1} \cup y(\mathbb{F}_{\mathbf{g}})_{d-1}$ . Since  $(\mathbb{F}_{\mathbf{g}})_{d-1} \cup y(\mathbb{F}_{\mathbf{g}})_{d-1}$  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  $w \in (\mathbb{F}_{\mathbf{g}})_{d-1}$  and  $z \in \{x, x^{-1}\}$ , then  $L_z L_y w = z y w$ . In particular, if  $z = y^{-1}$ , then  $L_z L_y w = w$ . Finally, if  $w \in (\mathbb{F}_{\mathbf{g}})_d$ , then

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

To prove this claim, given  $w \in (\mathbb{F}_{\mathbf{g}})_d$ , write  $w = yu$  where  $u \in (\mathbb{F}_{\mathbf{g}})_{d-1}$  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  $\Gamma_p$  is norm bounded. More precisely, with the  $U_y$  just constructed and

$$U = (U_{x_1}, \dots, U_{x_{\mathbf{g}}}, U_{x_1^{-1}}, \dots, U_{x_{\mathbf{g}}^{-1}}),$$

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

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

To prove this claim, observe, for a word  $w \in (\mathbb{F}_{\mathbf{g}})_d$  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 4.4 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 5.3. 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

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

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 verbatim. On the other hand, we do not know if the results still hold if the coefficients are from a  $C^*$ -algebra.

## APPENDIX A. AUXILIARY LEMMAS

For the sake of completeness, this appendix contains two well-known results used in the main body of the paper.

**Lemma A.1.** *Let  $\mathcal{H}$  and  $\mathcal{K}$  be Hilbert spaces. Let  $(T_\alpha)_\alpha$  be a net in  $\mathcal{B}(\mathcal{H})$  that converges to  $T \in \mathcal{B}(\mathcal{H})$  in the WOT. Let  $X \in \mathcal{B}(\mathcal{K})$  be fixed. Then  $(T_\alpha \otimes X)_\alpha$  converges to  $T \otimes X$  in the WOT on  $\mathcal{B}(\mathcal{H} \otimes \mathcal{K})$ .*

*Proof.* For  $h, h' \in \mathcal{H}$  and  $k, k' \in \mathcal{K}$ ,

$$\langle (T_\alpha \otimes X)(h \otimes k), h' \otimes k' \rangle = \langle T_\alpha h, h' \rangle \langle Xk, k' \rangle.$$

Since  $\langle T_\alpha h, h' \rangle \rightarrow \langle Th, h' \rangle$  and  $\langle Xk, k' \rangle$  is constant, it follows that

$$\langle (T_\alpha \otimes X)(h \otimes k), h' \otimes k' \rangle \rightarrow \langle (T \otimes X)(h \otimes k), h' \otimes k' \rangle.$$

By the Uniform Boundedness Principle, we get

$$M := \sup_{\alpha} \|T_{\alpha}\| < \infty.$$

Consequently the family  $\{T_{\alpha} \otimes X\}_{\alpha}$  is uniformly bounded in operator norm:

$$\|T_{\alpha} \otimes X\| \leq \|T_{\alpha}\| \|X\| \leq M \|X\| \quad \text{for all } \alpha.$$

Let  $\xi, \eta \in \mathcal{H} \otimes \mathcal{K}$  be arbitrary and fix  $\varepsilon > 0$ . Choose finite sums

$$\xi_0 = \sum_{i=1}^n h_i \otimes k_i, \quad \eta_0 = \sum_{j=1}^m h'_j \otimes k'_j$$

such that  $\|\xi - \xi_0\| < \delta$  and  $\|\eta - \eta_0\| < \delta$ , where  $\delta > 0$  will be chosen below. Write

$$\langle (T_{\alpha} \otimes X)\xi, \eta \rangle - \langle (T \otimes X)\xi, \eta \rangle = A_{\alpha} + B_{\alpha} + C_{\alpha},$$

where

$$\begin{aligned} A_{\alpha} &= \langle (T_{\alpha} \otimes X)\xi_0, \eta_0 \rangle - \langle (T \otimes X)\xi_0, \eta_0 \rangle, \\ B_{\alpha} &= \langle (T_{\alpha} \otimes X)(\xi - \xi_0), \eta_0 \rangle - \langle (T \otimes X)(\xi - \xi_0), \eta_0 \rangle, \\ C_{\alpha} &= \langle (T_{\alpha} \otimes X)\xi, \eta - \eta_0 \rangle - \langle (T \otimes X)\xi, \eta - \eta_0 \rangle. \end{aligned}$$

Note that  $A_{\alpha} \rightarrow 0$  as  $\alpha \rightarrow \infty$  because it is a finite linear combination of terms of the form  $\langle T_{\alpha} h_i, h'_j \rangle \langle X k_i, k'_j \rangle$ . Now

$$\begin{aligned} |B_{\alpha}| &\leq \|T_{\alpha} \otimes X\| \|\xi - \xi_0\| \|\eta_0\| + \|T \otimes X\| \|\xi - \xi_0\| \|\eta_0\| \\ &\leq 2M \|X\| \delta \|\eta_0\|, \end{aligned}$$

and

$$\begin{aligned} |C_{\alpha}| &\leq \|T_{\alpha} \otimes X\| \|\xi\| \|\eta - \eta_0\| + \|T \otimes X\| \|\xi\| \|\eta - \eta_0\| \\ &\leq 2M \|X\| \|\xi\| \delta. \end{aligned}$$

We can choose  $\delta > 0$  small enough so that

$$|B_{\alpha}| < \varepsilon/3 \quad \text{and} \quad |C_{\alpha}| < \varepsilon/3 \quad \text{for all } \alpha.$$

Thus  $\langle (T_{\alpha} \otimes X)\xi, \eta \rangle \rightarrow \langle (T \otimes X)\xi, \eta \rangle$  for all  $\xi, \eta \in \mathcal{H} \otimes \mathcal{K}$ , i.e.  $T_{\alpha} \otimes X \rightarrow T \otimes X$  in the WOT on  $B(H \otimes K)$ .  $\square$

The second lemma presents a few basic properties of the vectorization map used in the proof of Proposition 5.3, Subsection 5.5.

**Lemma A.2.** *Let  $A, B \in HS(\mathcal{H}, \mathcal{E})$  and  $P, Q \in B(\mathcal{H})$ ,  $T \in B(\mathcal{E})$ .*

(1) *We have*

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

*In particular,  $\|\text{vec}(A)\| = \|A\|_{HS}$ , 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,*

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

(3) (*Inner-product identity used in Proposition 5.3*)

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

*Proof.* Fix an orthonormal basis  $(e_r)_r$  of  $\mathcal{H}$ .

(1) 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.

(2) For the first identity,

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

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

(3) Using (2) twice and then (1),

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

□

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