Polynomial and tensor invariants and combinatorial parameters

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1. Introduction

In a recent paper, Balázs Szegedy [8] characterized the 'edge model' of graph parameters. His proof is based on a highly original combination of methods from invariant theory and real algebraic geometry.

In this paper we widen scope of applications of Szegedy's method by using a recent theorem in [7] that characterizes those tensor subalgebras that arise as invariant ring of the action of some subgroup of the unitary group on the full tensor algebra.

Our key result is Theorem 1. It concerns a contraction-closed graded $*$-subalgebra A of the mixed tensor algebra T, and it gives necessary and sufficient conditions for an algebra $*$-homomorphism $f : A \to \mathbb{R}$ to be extendible to $T \to \mathbb{R}$. The majority of the results before are preparations to prove this theorem, and most of the results after are applications of it to combinatorial parameters.

In this paper, we use the notation

(1) $$[n] := \{1, \ldots, n\}$$

for any $n \in \mathbb{N}$. Moreover, $\mathbb{N} = \{0, 1, 2, \ldots\}$.

2. Extending algebra homomorphisms

We prove a theorem on tensors. We first recall some standard notions of tensor theory.

Let V be a (finite- or infinite-dimensional) real inner product space. Denote

(2) $$T := T(V) := \bigoplus_{k=0}^{\infty} V^{\otimes k}.$$

This is the *tensor algebra* over V (cf. [3]).

We denote, for $k \geq 0$ and $A \subseteq T$,

(3) $$A_k := A \cap V^{\otimes k}.$$

A subalgebra A of T is *graded* if $A = \bigoplus_k A_k$.

For any $k \in \mathbb{N}$ and $\pi \in S_k$, let $x \mapsto x^\pi$ be the linear function $T_k \to T_k$ determined by

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$$(x_1 \otimes \cdots \otimes x_k)^\pi = x_{\pi(1)} \otimes \cdots \otimes x_{\pi(k)} \tag{4}$$

for $x_1, \ldots, x_k \in V$. A graded subalgebra A is called *symmetric* if $x^\pi \in A$ for all $k \in \mathbb{N}$, $x \in A_k$, and $\pi \in S_k$. If A is symmetric, a function $f : A \to \mathbb{R}$ is called *symmetric* if $f(x^\pi) = f(x)$ for all such k, x, π. Note that each algebra homomorphism $f : T \to \mathbb{R}$ is symmetric.

Let $k \in \mathbb{N}$ and $1 \leq i < j \leq k$. The *contraction operator* $C_{i,j} : A_k \to A_{k-2}$ is the linear operator determined by

$$C_{i,j}(x_1 \otimes \cdots \otimes x_k) = \langle x_i, x_j \rangle x_1 \otimes \cdots \widehat{x}_i \cdots \widehat{x}_j \cdots \otimes x_k, \tag{5}$$

for $x_1, \ldots, x_k \in V$. (As usual, $\widehat{x}_i$ means that factor x_i is left out from the tensor product.)

A graded subalgebra is *contraction-closed* if it is closed under the contraction operators. A subalgebra A is *nondegenerate* if there is no proper subspace W of V such that $A \subseteq T(W)$.

It was proved in [7] that, if V is n-dimensional, then the nondegenerate contraction-closed graded subalgebras of $T(V)$ are precisely the sets that are the invariant ring of some subgroup of the orthogonal group $O(n)$. This is a basis in our proof. This result implies that each contraction-closed graded subalgebra of T is symmetric.

We define a bilinear function $(.,.) : T \times T \to T$ by

$$(y, z) := \sum_{i=1}^{k} \sum_{j=1}^{l} C_{i,k+j}(y \otimes z), \tag{6}$$

for $k, l \in \mathbb{N}$ and $y \in T_k$, $z \in T_l$.

Theorem 1. *Let V be a (finite- or infinite-dimensional) real inner product space. Let A be a contraction-closed graded subalgebra of $T := T(V)$ and let $f : A \to \mathbb{R}$ be an algebra homomorphism. Then f can be extended to an algebra homomorphism $T \to \mathbb{R}$ if and only if f is symmetric and $f((x,x)) \geq 0$ for each $x \in A$.*

Proof. Necessity follows directly from the fact that any algebra homomorphism $f : T \to \mathbb{R}$ is symmetric and satisfies $f((x,x)) \geq 0$ for each $x \in T$. We prove sufficiency.

I. We first assume that V is finite-dimensional, say $V = \mathbb{R}^n$, and that A is nondegenerate. Then, by [7], $A = T^G$ for some compact subgroup G of the orthogonal group $O(n)$.

Here, for any $U \in \mathrm{GL}(n, \mathbb{R})$, the function $x \mapsto x^U$ is the unique algebra homomorphism $T \to T$ satisfying $x^U = Ux$ for $x \in V$. Then for any subgroup G of $\mathrm{GL}(n, \mathbb{R})$:

$$T^G := \{x \in T \mid x^U = x \text{ for each } U \in G\}. \tag{7}$$

Let $\xi : T \to T$ be the linear function determined by

$$\xi(z) := k!^{-1} \sum_{\pi \in S_k} z^\pi \tag{8}$$

for $k \in \mathbb{N}$ and $z \in T_k$. Since f is symmetric, we know $f \circ \xi = f$.

Introduce variables $x_1, \ldots, x_n$. We can identify the set $\xi(T)$ of all symmetric tensors with the polynomial algebra $\mathbb{R}[x_1, \ldots, x_n]$, by identifying $e_{f(1)} \otimes \cdots \otimes e_{f(k)}$ with the monomial $x_{f(1)} \cdots x_{f(k)}$, for all k and all $f : [k] \to [n]$.

Using this identification, the product pq of polynomials $p, q \in \mathbb{R}[x_1, \ldots, x_n]$ satisfies $pq = \xi(p \otimes q)$. Then

$$\xi(T^G) = \mathbb{R}[x_1, \ldots, x_n]^G =: R. \tag{9}$$

Also, $f(pq) = f(p)f(q)$ for all $p, q \in R$, since $f(pq) = f(\xi(p \otimes q)) = f(p \otimes q) = f(p)f(q)$.

Moreover, we have that for any

$$\xi((y, z)) = \sum_{t=1}^{n} \frac{d\xi(y)}{dx_i} \frac{d\xi(z)}{dx_i}. \tag{10}$$

So by the theorem of Procesi and Schwarz [6], $f|_R$ can be extended to an algebra homomorphism $\mathbb{R}[x_1, \ldots, x_n] \to \mathbb{R}$. Then $f \circ \xi$ gives the required algebra homomorphism on T.

II. We now consider the general case where V is not necessarily finite-dimensional. The following is easy but useful (where $C_{1,2} : X \otimes X \otimes Y \to Y$ is given by $C_{1,2}(x' \otimes x'' \otimes y) = \langle x, x'' \rangle y$):

Claim 1. Let X and Y be finite-dimensional real spaces, where X is an inner product space, and let $a \in X \otimes Y$. Define

$$Z := \{C_{1,2}(x \otimes a) \mid x \in X\}. \tag{11}$$

Then $a \in X \otimes Z$.

Proof. Let $m = \dim Z$. Let $e_1, \ldots, e_n$ form a basis of Y such that $e_1, \ldots, e_m$ form a basis of Z. We can write $a = \sum_{i=1}^{n} x_i \otimes e_i$ for some $x_1, \ldots, x_n \in X$. Suppose $x_j \neq 0$ for some $j > m$. Then

$$C_{1,2}(x_j \otimes a) = \sum_{i=1}^{n} \langle x_j, x_i \rangle e_i \tag{12}$$

belongs to Z. As $\langle x_j, x_j \rangle \neq 0$, this contradicts the condition on $e_1, \ldots, e_n$. □

We have to show that there exists $h \in V^*$ such that for each $k \in \mathbb{N}$ and each $y \in A_k$:

$$f(y) = h^{\otimes k}(y), \tag{13}$$

where the linear function $h^{\otimes k} : T_k \to \mathbb{R}$ is determined by

$$h^{\otimes k}(x_1 \otimes \cdots \otimes x_k) := h(x_1) \cdots h(x_k) \tag{14}$$

for $x_1, \ldots, x_k \in V$.

For each $y \in T_2$, let C_y be the column space of y, considering y as matrix in $\mathrm{End}(V)$. So

$$C_y := \{yv \mid v \in V\}, \tag{15}$$

where yv denotes the product of matrix y and vector v. Now for each $y, z \in T_2$, we have $C_y = C_{yy^\mathsf{T}}$ and $C_y + C_z = C_{yy^\mathsf{T}+zz^\mathsf{T}}$. Hence the union of the C_y over $y \in A_2$ is a subspace W of V. Then

$$A \subseteq T(W). \tag{16}$$

To see this, choose $y \in A_k$ for some k. It suffices to show by symmetry that

$$y \in V^{\otimes k-1} \otimes W. \tag{17}$$

(This follows from the fact (cf. [3] Section 1.14) that $(X' \otimes Y) \cap (X \otimes Y') = X' \otimes Y'$ for any linear spaces $X' \subseteq X$ and $Y' \subseteq Y$.)

Let U be a finite-dimensional subspace of V such that $y \in U^{\otimes k}$. Now let $X := V^{\otimes k-1}$ and $Y := U$. By Claim 1, it suffices to show that $C_{1,2}(w \otimes y) \in W$ for each $w \in X$. But this follows from the fact that $C_{1,2}(w \otimes y)$ belongs to the column space of $C_{1,2}(y \otimes y) \in A_2$. This proves (16).

Since any $h \in W^*$ can be extended to $\tilde{h} \in V^*$ such that $h = \tilde{h}|_W$, (16) implies that we can assume that $W = V$.

Choose a (not necessarily orthonormal) basis B of V. Consider any $b \in B$. By definition of W, there exists a $y_b \in A_2$ and $v_b \in V$ such that $b = y_b v_b$. We can normalize b such that $f(y_b y_b^\mathsf{T}) v_b^\mathsf{T} v_b \leq 1$.

For any finite subset B' of B, define

$$H_{B'} := \{h|_B \mid h \in V^*, \oplus_k h^{\otimes k}(y) = f(y) \text{ for each } y \in A \cap T(\text{lin.hull}(B')) \text{ and } |h(b)| \leq 1 \text{ for each } b \in B\}. \tag{18}$$

Then

$$H_{B'} \neq \emptyset. \tag{19}$$

For let U be a finite-dimensional subspace of V such that $y_b \in U \otimes U$ for each $b \in B'$ (this implies $B' \subseteq U$). By part I of this proof, there exists an $h \in U^*$ such that $\oplus_n h^{\otimes k}(y) = f(y)$ for each $y \in A \cap T(U)$. Then for any $b \in B'$, by Cauchy-Schwarz:

$$|h(b)| = |h(y_b v_b)| \leq \sqrt{(h \otimes h)(y_b y_b^\mathsf{T})}\sqrt{v_b^* v_b} = \sqrt{f(y_b y_b^\mathsf{T})}\sqrt{v_b^\mathsf{T} v_b} \leq 1. \tag{20}$$

Therefore, define $\tilde{h} \in V^*$ by: $\tilde{h}(b) := h(b)$ if $b \in B'$ and $\tilde{h}(b) := 0$ if $b \in B \setminus B'$. Then $\tilde{h} \in H_{B'}$, proving (19).

Since $H_{B' \cup B''} \subseteq H_{B'} \cap H_{B''}$, the intersection of any finite number of sets $H_{B'}$ is nonempty. Hence, as $H_\emptyset$ is compact by Tychonoff's theorem, the intersection of all $H_{B'}$ is nonempty. Any h in this intersection is as required by the theorem. ∎

3. Structured hypergraphs

Let $\mathcal{S}$ be a (finite or infinite) collection of finite sets. For each $S \in \mathcal{S}$, let Γ_S be a group of permutations of S. Call functions ϕ, ψ defined on S *equivalent* if $\psi = \phi \circ \pi$ for some $\pi \in \Gamma_S$. Let $[\phi]$ denote the equivalence class of ϕ.

Let V be a finite set. A *structured subset* of V (of *type* S) is an equivalence class of functions $\phi : S \to V$ for some $S \in \mathcal{S}$.

A *structured hypergraph* is a pair $H = (VH, EH)$, where VH is a finite set and EH is a finite multiset of structured subsets of VH. The elements of VH and EH are called the *vertices* and *edges* of H respectively. The set of edges in EH of type S is denoted by $E_S H$.

Let $\mathcal{H}$ be the collection of isomorphism classes of structured hypergraphs. Then $\mathcal{H}$ is a semigroup, taking disjoint union as multiplication. A *quantum structured hypergraph* is a formal $\mathbb{R}$-linear combination of structured hypergraphs. The quantum structured hypergraphs then form the semigroup algebra $\mathcal{QH}$ of the semigroup $\mathcal{H}$.

Let H be a structured hypergraph and let Φ and Ψ be two distinct edges of H of the same type, S say. For any $\phi \in \Phi$ and $\psi \in \Psi$, let $H_{\phi,\psi}$ be the structured hypergraph obtained from H by deleting edges Φ and Ψ and identifying $\phi(s)$ and $\psi(s)$ for each $s \in S$. Define, for any $\Phi, \Psi \in EH$, the quantum structured hypergraph $H_{\Phi,|psi}$ by

$$(21) \qquad H_{\Phi,\Psi} := \begin{cases} |\Phi|^{-1}|\Psi|^{-1} \displaystyle\sum_{\phi \in \Phi, \psi \in \Psi} H_{\phi,\psi} & \text{if } \Phi \text{ and } \Psi \text{ are of the same type,} \\ 0 & \text{otherwise.} \end{cases}$$

We denote

$$(22) \qquad H_{\Phi_1,\Psi_1,\ldots,\Phi_k,\Psi_k} := (\cdots(H_{\Phi_1,\Psi_1})\cdots)_{\Phi_k,\Psi_k}.$$

For any $H, J \in \mathcal{H}$ and $k \in \mathbb{N}$, define

$$(23) \qquad \lambda_k(H,J) = \sum_{\substack{\Phi_1,\ldots,\Phi_k \in EH \\ \Psi_1,\ldots,\Psi_k \in EJ}} (HJ)_{\Phi_1,\Psi_l,\ldots,\Phi_k,\Psi_k},$$

where $\Phi_1, \ldots, \Phi_k$ range over distinct edges of H and $\Psi_1, \ldots, \Psi_k$ range over distinct edges of J. This can be extended to a bilinear form $\lambda_k : \mathcal{QH} \times \mathcal{QH} \to \mathcal{QH}$.

Let $n \in \mathbb{N}$, and let $a : \bigcup_S [n]^S \to \mathbb{R}$ be such that $a|[n]^S$ is Γ_S-invariant, for each $S \in \mathcal{S}$. Define a function $f_a : \mathcal{QH} \to \mathbb{R}$ by

$$(24)\qquad f_a(H) = \sum_{\chi:VH\to[n]} \prod_{\Phi\in EH} a_{\chi\circ\Phi}.$$

Here $a_{\chi\circ\Phi}$ is the common value of $a(\chi\circ\phi)$ for $\phi\in\Phi$. (As a is Γ-invariant, $a(\chi\circ\phi)$ is independent of the choice of $\phi\in\Phi$.)

Let K_0 and K_1 be the hypergraphs with no edges and 0 and 1 vertex, respectively. We call a collection $\mathcal{H}$ of structured hypergraphs *closed* if it contains K_0 is closed under taking disjoint unions and under the operation $H\to H_{\phi,\psi}$ for $H\in\mathcal{H}$ and $\phi\in\Phi\in E_SH$ and $\psi\in\Psi\in E_SH$, for any $S\in\mathcal{S}$.

We call a function $f:\mathcal{H}\to\mathbb{R}$ *multiplicative* if $f(K_0)=1$ and $f(HJ)=f(H)f(J)$ for all $H,J\in\mathcal{H}$. We call f *reflection positive* if $f(\lambda_k(H,H))\geq 0$ for each $k\in\mathbb{N}$ and each $H\in\mathcal{QH}$.

For each $S\in\mathcal{S}$, let D_S be the structured hypergraph with $VD_S=S$ and $ED_S:=\{\Gamma_S,\Gamma_S\}$.

Theorem 2. *Let $\mathcal{H}$ be a closed collection of structured hypergraphs containing K_1 and D_S for each $S\in\mathcal{S}$. Let $f:\mathcal{H}\to\mathbb{R}$ and $n\in\mathbb{N}$. Then $f=f_a$ for some Γ-invariant $a:\bigcup_S[n]^S\to\mathbb{R}$ if and only if $f(K_1)=n$ and f is multiplicative and reflection positive.*

Proof. Let U denote the collection of equivalence classes of functions in $\bigcup_{S\in\mathcal{S}}[n]^S$. For each $u\in U$, introduce a varable x_u. For each $H\in\mathcal{H}$, define $p_n(H)\in\mathbb{R}[x_u\mid u\in U]$ by

$$(25)\qquad p_n(H) := \sum_{\chi:VH\to[n]} \prod_{\Phi\in EH} x_{\chi\circ\Phi}.$$

So $f_a(H)=p_n(H)(a)$ (the evaluation of the polynomial $p_n(H)$ at a).

We first observe that for any $H\in\mathcal{H}$ and $u_1,\ldots,u_k\in U$:

$$(26)\qquad \frac{d}{du_1}\cdots\frac{d}{du_k}p_n(H) = \sum_{\chi:VH\to[n]} \sum_{\substack{\Phi_1,\ldots,\Phi_k\in EH\\ \forall i:\chi\circ\Phi_i=u_i}} \prod_{\Phi\in EH\setminus\{\Phi_1,\ldots,\Phi_k\}} x_{\chi\circ\Phi},$$

where $\Phi_1,\ldots,\Phi_k$ range over *distinct* elements of EH. Moreover, for any $H\in\mathcal{H}$ and distinct $\Phi_1,\Psi_1,\ldots,\Phi_k,\Psi_k\in EH$:

$$(27)\qquad p_n(H_{\Phi_1,\Psi_1,\ldots,\Phi_k,\Psi_k}) = \sum_{\substack{\chi:VH\to[n]\\ \forall i:\chi\circ\Phi_i=\chi\circ\Psi_i}} \left(\prod_{i=1}^k |\chi\circ\Phi_i|^{-1}\right) \prod_{\Phi\in EH\setminus\{\Phi_1,\Psi_1,\ldots,\Phi_k,\Psi_k\}} x_{\chi\circ\Phi}.$$

Indeed, we may assume that for each i, $\Phi_i,\Psi_i:S_i\to VH$ for some $S_i\in\mathcal{S}$. Now fix some $\phi_i\in\Phi_i$ and $\psi_i\in\Psi_i$, for each i. Then

$$(28)\qquad H_{\Phi_1,\Psi_1,\ldots,\Phi_k,\Psi_k} = \left(\prod_{i=1}^k |\Gamma_{S_i}|^{-1}\right) \sum_{\pi_i\in\Gamma_S} H_{\phi'\circ\pi,\phi''}\ldots\ldots$$

Hence

$$p_n(H_{\Phi',\Phi''}) = |\Gamma_S|^{-1} \sum_{\pi\in\Gamma_S} p_n(H_{\phi'\circ\pi,\phi''}) = \tag{29}$$
$$|\Gamma_S|^{-1} \sum_{\pi\in\Gamma_S} \sum_{\substack{\chi:VH\to[n]\\ \chi\circ\phi'\circ\pi=\chi\circ\phi''}} \prod_{\Phi\in EH\setminus\{\Phi',\Phi''\}} x_{\chi\circ\Phi} =$$
$$|\Gamma_S|^{-1} \sum_{\chi:VH\to[n]} \sum_{\substack{\pi\in\Gamma_S\\ \chi\circ\phi'\circ\pi=\chi\circ\phi''}} \prod_{\Phi\in EH\setminus\{\Phi',\Phi''\}} x_{\chi\circ\Phi} =$$
$$\sum_{\substack{\chi:VH\to[n]\\ \chi\circ\Phi'=\chi\circ\Phi''}} |\chi\circ\Phi'|^{-1} \prod_{\Phi\in EH\setminus\{\Phi',\Phi''\}} x_{\chi\circ\Phi}.$$

The latter follows from the fact that for each $\chi : VH \to [n]$, the number of $\pi \in \Gamma_S$ with $\chi \circ \phi' \circ \pi = \chi \circ \phi''$ is equal to $|\Gamma_S||\chi \circ \Phi'|^{-1}$. This proves (27).

It implies for any $H, J \in \mathcal{H}$:

$$p_n(\lambda_k(H, J)) = \sum_{\substack{\Phi_1,\ldots,\Phi_k\in EH\\ \Psi_1,\ldots,\Psi_k\in EJ}} p_n((HJ)_{\Phi_1,\Psi_1,\ldots,\Phi_k,\Psi_k}) = \tag{30}$$
$$\sum_{\substack{\Phi_1,\ldots,\Phi_k\in EH\\ \Psi_1,\ldots,\Psi_k\in EJ}} \sum_{\substack{\chi:VH\to[n]\\ \eta:VJ\to[n]\\ \forall i:\chi\circ\Phi_i=\eta\circ\Psi_i}} \left(\prod_{i=1}^k |\chi\circ\Phi_i|^{-1}\right) \left(\prod_{\Phi\in EH\setminus\{\Phi_1,\ldots,\Phi_k\}} x_{\chi\circ\Phi}\right) \left(\prod_{\Psi\in EJ\setminus\{\Psi_1,\ldots,\Psi_k\}} x_{\eta\circ\Psi}\right) =$$
$$\sum_{u_1,\ldots,u_k\in U} \left(\prod_{i=1}^k |u_i|^{-1}\right) \left(\frac{d}{du_1}\cdots\frac{d}{du_k} p_n(H)\right) \left(\frac{d}{du_1}\cdots\frac{d}{du_k} p_n(J)\right).$$

Now necessity in the theorem follows directly. Trivially, f_a is multiplicative. Moreover, reflection positivity of f_a follows from (30), as $f_a(H)$ is the evaluation of the polynomial $p_n(H)$ at a.

We next show sufficiency. We can trivially extend p_n to an algebra homomorphism $\mathcal{QH} \to \mathbb{R}[x_u \mid u \in U]$. Next we can 'pull back' f:

Claim 1. There is an algebra homomorphism $\hat{f} : p_n(\mathcal{QH}) \to \mathbb{R}$ such that $f = \hat{f} \circ p_n$.

Proof. For this we must show that for any $H \in \mathcal{QH}$: if $p_n(H) = 0$ then $f(H) = 0$. By (30), we know that for any $H \in \mathcal{QH}$:

(31) if $p_n(H) = 0$ then $p_n(\lambda_k(H, J)) = 0$ for each $k \in \mathbb{N}$ and $J \in \mathcal{QH}$.

For any $H \in \mathcal{H}$, with edges of types $S_1, \ldots, S_k$ say, each monomial occurring in $p_n(H)$ is a product

$$x_{[\alpha_1]} \cdots x_{[\alpha_k]} \tag{32}$$

where $\alpha_i \in [n]^{S_i}$ for $i = 1, \ldots, k$. So in proving that $p_n(H) = 0$ implies $f(H) = 0$, we can assume that all hypergraphs occurring in H have edges of the same series of types, $S_1, \ldots, S_k$ say. Now we prove $p_n(H) = 0 \Longrightarrow f(H) = 0$ by induction on k, the case $k = 0$ being trivial, as $f(K_1) = n = p_n(1)$.

As $\lambda_k(H, H)$ has no edges, it is a linear combination of hypergraphs with no edges, i.e., of powers of K_1. Since $f(K_1) = n = p_n(K_1)$, it follows that

$$f(\lambda_k(H, H)) = p_n(\lambda_k(H, H)) = 0, \tag{33}$$

by (31), as $p_n(H) = 0$. Hence, by the reflection positivity of f, $f(\lambda_k(H, J)) = 0$ for each $J \in \mathcal{QH}$. Now define

$$J := \prod_{i=1}^{k} D_{S_i}. \tag{34}$$

Now the sum making $\lambda_k(H, J)$ can be decomposed according to the set I of factors D_{S_i} for which both edges are linked with H and the set L of factors D_{S_i} for which no edges are linked with H (necessarily $|I| = |L|$). This gives

$$\lambda_k(H, J) = \sum_{\substack{I, L \subseteq [k] \\ I \cap L = \emptyset, |I| = |L|}} \alpha_{I,L} H_I \prod_{j \in L} D_{S_j}, \tag{35}$$

where $\alpha_{I,L}$ is a natural number, with $\alpha_{I,L} \neq 0$ if $I = L = \emptyset$, and where

$$H_I := \lambda_{2|I|}(H, \prod_{i \in I} D_{S_i}). \tag{36}$$

So $\lambda_0(H, K_0)$ is a linear combination of $\lambda_k(H, J)$ and $H_I \prod_{j \in L} D_{S_j}$ with I, L nonempty disjoint subsets of $[k]$ with $|I| = |L|$. Note that $\lambda_0(H, K_0) = H$. By reflection positivity, $f(\lambda_k(H, J)) = 0$.

Moreover, $f(H_I) = 0$ for each nonempty I. This follows by the induction hypothesis on k, since each structured hypergraph occuring in the quantum structured hypergraph H_I has $k - 2|I| < k$ edges, and since $p_n(H_I) = 0$, by (31), as $p_n(H) = 0$. So $f(H) = 0$. $\square$

Let V be a linear space spanned by the linearly independent vectors b_u for $u \in U$. Let $T = T(V)$. For each $H \in \mathcal{H}$ and for each linear order $\Phi_1, \ldots, \Phi_k$ of the edges of H, let $\tau_{H,\Phi_1,\ldots,\Phi_k}$ be the following tensor in $V^{\otimes k}$:

$$\tau_{H,\Phi_1,\ldots,\Phi_k} := \sum_{\chi: VH \to [n]} \bigotimes_{i=1}^{k} x_{\chi \circ \Phi_i}. \tag{37}$$

Let A be the linear space spanned by these tensors. Then A is a contraction-closed graded subalgebra of T. Let $\xi : T \to \mathbb{R}[x_u \mid u \in U]$ be the symmetrization operator. As f is reflection positive, we know that $\hat{f} \circ \xi((x,x)) \geq 0$ for each $x \in A$.

Hence by Theorem 1, $\hat{f} \circ \xi$ can be extended to an algebra homomorphism $T \to \mathbb{R}$. Define

$$a_\alpha := \hat{f}(x_{[\alpha]}) \tag{38}$$

for each $\alpha \in \bigcup_T [n]^T$. This gives the required function a. ∎

We cannot delete the condition that each D_S belongs to $\mathcal{H}$: Let $\mathcal{S} := \{[2]\}$ and let $\Gamma_{[2]} := \{\mathrm{id}_{[2]}\}$. Let $\mathcal{H}$ be the collection of structured hypergraphs H such that VH is split into two sets U and W, such that each $\phi \in \Phi \in EH$ has $\phi(1) \in U$ and such that for each $w \in W$ there is precisely one $\Phi \in EH$ such that $\phi(2) = w$ for $\phi \in \Phi$. Define $f(H) := 2^{|W|}$. Then f is multiplicative and reflection positive and $f(K_1) = 1$, but there is no $a : [1]^2 \to \mathbb{R}$ such that $f = f_a$.

Let C_k and $\vec{C}_k$ be the undirected and directed circuit, respectively, with k vertices.

Theorem 3. *Let $\mathcal{H}$ be a closed collection of structured hypergraphs containing C_k for all $k \geq 1$, or $\vec{C}_k$ for all $k \geq 1$. Let $f : \mathcal{H} \to \mathbb{R}$ be multiplicative and reflection positive. Then $K_1 \in \mathcal{H}$ and $f(K_1)$ is a nonnegative integer.*

Proof. First assume that $\mathcal{H}$ contains C_k for all k. Then $K_1 \in \mathcal{H}$, as $K_1 = (C_1)_{\phi,\psi}$ for some ϕ, ψ. We prove that $f(K_1)$ is a nonnegative integer. Suppose not. Then there exists an $m \in \mathbb{N}$ such that $\binom{f(K_1)}{m} < 0$.

For each $\pi \in S_m$, let G_π be the graph with vertex set $[m]$ and edges $\{i, \pi(i)\}$ for $i = 1, \ldots, m$. Then

$$\begin{aligned} &\sum_{\pi,\rho \in S_m} \mathrm{sgn}(\pi)\mathrm{sgn}(\rho) G_\pi G_\rho = \\ &\sum_{\pi,\rho \in S_m} \mathrm{sgn}(\pi)\mathrm{sgn}(\rho) \sum_{\substack{\Phi_1,\ldots,\Phi_m \in EG_\pi \\ \Psi_1,\ldots,\Psi_m \in EG_\rho}} \sum_{\substack{\phi_1 \in \Phi_1,\ldots,\phi_m \in \Phi_m \\ \psi_1 \in \Psi_1,\ldots,\psi_m \in \Psi_m}} (G_\pi G_\rho)_{\phi_1,\psi_1,\ldots,\phi_k,\psi_k} = \\ &\sum_{\pi,\rho \in S_m} \mathrm{sgn}(\pi)\mathrm{sgn}(\rho) \sum_{\substack{\Phi_1,\ldots,\Phi_m \in EG_\pi \\ \Psi_1,\ldots,\Psi_m \in EG_\rho}} \sum_{\substack{\phi_1 \in \Phi_1,\ldots,\phi_m \in \Phi_m \\ \psi_1 \in \Psi_1,\ldots,\psi_m \in \Psi_m}} K_1^{\tau(\phi_1,\psi_1,\ldots,\phi_k,\psi_k)} \end{aligned} \tag{39}$$

for some $\tau(\phi_1, \psi_1, \ldots, \phi_m, \psi_m) \in \mathbb{N}$. Now for each $x \in \mathbb{R}$ one has

$$\sum_{\pi,\rho \in S_m} \mathrm{sgn}(\pi)\mathrm{sgn}(\rho) \sum_{\substack{\Phi_1,\ldots,\Phi_m \in EG_\pi \\ \Psi_1,\ldots,\Psi_m \in EG_\rho}} \sum_{\substack{\phi_1 \in \Phi_1,\ldots,\phi_m \in \Phi_m \\ \psi_1 \in \Psi_1,\ldots,\psi_m \in \Psi_m}} x^{\tau(\phi_1,\psi_1,\ldots,\phi_k,\psi_k)} = c\binom{x}{m} \tag{40}$$

for some positive constant c (independent of x).

To see this we can assume $x \in \mathbb{N}$ (as both sides are polynomials). Then

$$\sum_{\pi,\rho \in S_m} \mathrm{sgn}(\pi)\mathrm{sgn}(\rho) \sum_{\substack{\Phi_1,\ldots,\Phi_m \in EG_\pi \\ \Psi_1,\ldots,\Psi_m \in EG_\rho}} \sum_{\substack{\phi_1 \in \Phi_1,\ldots,\phi_m \in \Phi_m \\ \psi_1 \in \Psi_1,\ldots,\psi_m \in \Psi_m}} x^{\tau(\phi_1,\psi_1,\ldots,\phi_k,\psi_k)} = \tag{41}$$

$$\sum_{\pi,\rho\in S_m} \mathrm{sgn}(\pi)\mathrm{sgn}(\rho) \sum_{\substack{\Phi_1,\ldots,\Phi_m\in EG_\pi\\ \Psi_1,\ldots,\Psi_m\in EG_\rho}} \sum_{\substack{\phi_1\in\Phi_1,\ldots,\phi_m\in\Phi_m\\ \psi_1\in\Psi_1,\ldots,\psi_m\in\Psi_m}} |\{\chi:[m]\to[x] \mid \forall i\in[m] \text{ and } j\in [2]:\chi(\phi_i(j))=\chi(\psi_i(j))\}| =$$
$$\sum_{\chi:[m]\to[x]} \sum_{\pi,\rho\in S_m} \mathrm{sgn}(\pi)\mathrm{sgn}(\rho) \sum_{\substack{\Phi_1,\ldots,\Phi_m\in EG_\pi\\ \Psi_1,\ldots,\Psi_m\in EG_\rho}} |\{(\phi_1,\psi_1,\ldots,\phi_m,\psi_k)\in \Phi_1\times\Psi_1\times\cdots\times\Phi_m\times\Psi_m \mid \forall i\in[m] \text{ and } j\in[2]:\chi(\phi_i(j))=\chi(\psi_i(j))\}|.$$

Consider now some $\chi:[m]\to[x]$ such that $\chi(i)=\chi(j)$ for two distinct $i,j\in[m]$. Let σ be the permutation (i,j). Then for π and $\pi\circ\sigma$, the third summations have the same value, but $\mathrm{sgn}(\pi\circ\sigma)=-\mathrm{sgn}(\pi)$. So then the sum is 0. Hence we can restrict ourselves to injective functions $\chi:[m]\to[x]$. Then the sum is $\binom{x}{m}m!$ times the value for taking $\chi:[m]\to[m]$ being the identity. Then ϕ_i and ψ_i can be restricted to those with $\phi_i=\psi_i$. Hence $G_\pi=G_\rho$. So (41) is equal to

$$(42)\qquad \binom{x}{m}m!\sum_{\substack{\pi,\rho\in S_m\\ G_\pi=G_\rho}} \mathrm{sgn}(\pi)\mathrm{sgn}(\rho)m!2^m = \binom{x}{m}m!^2 2^m\sum_G(\sum_{\substack{\pi\in S_m\\ G_\pi=G}}\mathrm{sgn}(\pi))^2 = c\binom{x}{m}.$$

This proves (40).

It follows with (39) that

$$(43)\qquad 0\le f(\sum_{\pi,\rho\in S_m}\mathrm{sgn}(\pi)\mathrm{sgn}(\rho)G_\pi G_\rho) = c\binom{f(K_1)}{m} < 0,$$

a contradiction.

The case that $\vec{C}_k\in\mathcal{H}$ for all k is proved similarly. ∎

4. Hypergraphs

We now start with deriving more specific combinatorial applications of Theorems 2 and 3. A *hypergraph* is a pair $H=(VH,EH)$, where VH is a finite set and EH is a finite multisets of submultisets of VH. Let $\mathcal{H}$ denote the collection of hypergraphs.

Consider any $n\in\mathbb{N}$ and any symmetric $c:\bigcup_{t\in\mathbb{N}}[n]^t\to\mathbb{R}$. Define a hypergraph parameter f_c by

$$(44)\qquad f_c(H) := \sum_{\phi:VH\to[n]}\prod_{e\in EH} c(\phi(e)).$$

Here we take for $\phi(e)$ the multiset $\{\phi(v)\mid v\in e\}$, ordered arbitrarily. We characterize which functions f are equal to f_c for some c.

The *disjoint union* of hypergraphs H and H' is obtained by first making VH and VH' disjoint (by renaming the vertices) and then taking $(VH\cup VH', EH\cup EH')$, where $EH\cup EH'$ is multiset union (taking multiplicities into account).

For $H_1,H_2\in\mathcal{H}$ and $k\in\mathbb{N}$, we make a multiset $\mathcal{J}^k_{H_1,H_2}$ of hypergraphs as follows.

Let H be the disjoint union of H_1 and H_2. For distinct $e_1,\ldots,e_k \in EH_1$ and distinct $f_1,\ldots,f_k \in EH_2$ such that $|e_i| = |f_i|$ for $i = 1,\ldots,k$ and for bijections $\pi_i : e_i \to f_i$, let $H(e_1, f_1, \pi_1, \ldots, e_k, f_k, \pi_k)$ be the hypergraph obtained from H by, for each $i = 1,\ldots,k$, deleting e_i and f_i and for each $u \in e_i$ identifying u and $\pi_i(u)$. (This might mean repeated identification if e or f has multiple elements.) Then

(45) $$\mathcal{J}^k_{H_1,H_2} := \{H(e_1, f_1, \pi_1, \ldots, e_k, f_k, \pi_k) \mid \text{distinct } e_1,\ldots,e_k \in EH_1, \text{distinct } f_1,\ldots,f_k \in EH_2, \text{bijections } \pi_i : e_i \to f_i\}.$$

Define the $\mathcal{H} \times \mathcal{H}$ matrix $M_{f,k}$ by

(46) $$(M_{f,k})_{H_1,H_2} := \sum_{H \in \mathcal{J}^k_{H_1,H_2}} f(H)$$

for $H_1, H_2 \in \mathcal{H}$.

We also define a matrix $N_{f,k}$. A *k-labeled hypergraph* is a pair (H, u) of a hypergraph H and an element u of VH^k. Let $\mathcal{H}_k$ be the collection of k-labeled hypergraphs. For two k-labeled hypergraphs (H, u) and (J, w), the hypergraph $(H, u)\cdot(J, w)$ is obtained by taking the disjoint union of H and J, and next identifying u_i and w_i, for $i = 1,\ldots,k$. Then $N_{f,k}$ is the $\mathcal{H}_k \times \mathcal{H}_k$ matrix defined by

(47) $$(N_{f,k})_{(H,u),(J,w)} := f((H, u) \cdot (J, w))$$

for $(H, u), (J, w) \in \mathcal{H}_k$.

Call $f : \mathcal{H} \to \mathbb{R}$ *multiplicative* if $f(K_0) = 1$ and $f(H) = f(H_1)f(H_2)$ if H is the disjoint union of H_1 and H_2.

Theorem 4. *Let $f : \mathcal{H} \to \mathbb{R}$. Then the following are equivalent:*

(48) (i) *$f = f_c$ for some $n \in \mathbb{N}$ and some symmetric function $c : \bigcup_{t\in\mathbb{N}}[n]^t \to \mathbb{R}$,*
(ii) *f is multiplicative and $M_{f,k}$ is positive semidefinite for each $k \in \mathbb{N}$,*
(iii) *f is multiplicative and $N_{f,k}$ is positive semidefinite for each $k \in \mathbb{N}$.*

Proof. The implications (i)$\Longrightarrow$(iii)$\Longrightarrow$(ii) are direct. Note that $H(e_1, f_1, \pi_1, \ldots e_k, f_k, \pi_k)$ is a special case of the K vertex identifying operation for $K = \sum_{i=1}^k |e_i|$ where $|e_i|$ denotes the cardinality of the hyperedge e_i. So $M_{f,k}$ is a sum of matrices $N_{f,K}$ which is positive semidefinite because each $N_{f,K}$ is positive semidefinite.

The implication (ii)$\Longrightarrow$(i) follows from Theorems 2 and 3, by taking

(49) $$\mathcal{S} := \{[m] \mid m \in \mathbb{N}\}$$

and setting $\Gamma_{[m]}$ to be the symmetric group on $[m]$. ∎

We next consider the uniqueness of c. We note that the algebra A is equal to $T(V)^G$

where G is the group of transformations of $\mathbb{R}[x_1, \ldots, x_d]$ permuting the variables. (So $|G| = d!$.)

For any symmetric $c : \bigcup_t [n]^t \to \mathbb{R}$ and any $\pi \in S_n$, define $c^\pi : \bigcup_t [n]^t \to \mathbb{R}$ by

$$c^\pi(\phi) := c(\pi \circ \phi) \tag{50}$$

for any $\phi \in \bigcup_t [d]^t$.

Theorem 5. *Let $c, b : \bigcup_k [d]^k \to \mathbb{R}$ be symmetric functions. Then $f_c = f_b$ if and only if $b = c^\pi$ for some $\pi \in S_d$.*

Proof. Sufficiency being direct, we show necessity. For each $t \in \mathbb{N}$, let A^t be the contraction-closed tensor subalgebra spanned by the z_P for partitions P of $X_{\boldsymbol{n}}$ for those $\boldsymbol{n}$ with $n_i \leq t$ for all i. So

$$A^t \subseteq T(V^t), \tag{51}$$

where V^t is the set of polynomials in $\mathbb{R}[x_1, \ldots, x_d]$ of total degree t. Let $m := \sum_{n \leq t} d^n$. Then $A^t = T(V^t)^{S_d}$, where S_d acts on V by permuting variables.

Since $f_c = f_d$, we know that for each $p \in \mathcal{P}[V^t]^{S_d}$ one has $p(c) = p(d)$. Hence $b|V^t = c^\pi|V^t$ for some $\pi \in S_d$. As G is finite, this implies that $b = c^\pi$ for some $\pi \in S_d$. ∎

5. Undirected graphs — vertex model

Similar results hold for graphs instead of hypergraphs. A *graph* is a pair $G = (VG, EG)$, where VG is a finite set and EG is a finite multisets of unordered pairs $\{u, v\}$ from VG, possible taken as multiset, where $u = v$ (a loop). The pair $\{u, v\}$ we sometimes denote by uv. Let $\mathcal{G}$ denote the collection of graphs. As graphs are hypergraphs, terminology and notation introduced for hypergraphs in Section 4 applies also to graphs.

Consider any $n \in \mathbb{N}$ and a symmetric function $c : [n]^2 \to \mathbb{R}$. (So c can be considered as symmetric matrix.) Define a graph parameter f_c by

$$f_c(G) := \sum_{\phi: VG \to [n]} \prod_{uv \in EG} c(\phi(u), \phi(v)). \tag{52}$$

We characterize which graph functions f are equal to f_c for some c.

For $f : \mathcal{G} \to \mathbb{R}$ and $k \in \mathbb{N}$, define the $\mathcal{G} \times \mathcal{G}$ matrix $M_{f,k}$ by

$$(M_{f,k})_{G_1,G_2} := \textstyle\sum_{G \in \mathcal{J}^k_{G_1,G_2}} f(G) \tag{53}$$

for $G_1, G_2 \in \mathcal{G}$.

We also define a matrix $N_{f,k}$. A *k-labeled graph* is a pair (G, u) of a graph G and an element u of VG^k. Let $\mathcal{G}_k$ be the collection of k-labeled graphs. For two k-labeled graphs (G, u) and (J, w), the graph $(G, u) \cdot (J, w)$ is obtained by taking the disjoint union of G and

J, and next identifying u_i and w_i, for $i = 1, \ldots, k$. Then $N_{f,k}$ is the $\mathcal{G}_k \times \mathcal{G}_k$ matrix defined by

$$(54) \qquad (N_{f,k})_{(G,u),(J,w)} := f((G,u) \cdot (J,w))$$

for $(G,u),(J,w) \in \mathcal{G}_k$.

Call $f : \mathcal{G} \to \mathbb{R}$ *multiplicative* if $f(K_0) = 1$ and $f(G) = f(G_1)f(G_2)$ if G is the disjoint union of G_1 and G_2.

Theorem 6. *Let $f : \mathcal{G} \to \mathbb{R}$. Then the following are equivalent:*

(55) (i) *$f = f_c$ for some $n \in \mathbb{N}$ and some symmetric function $c : [n]^2 \to \mathbb{R}$,*
(ii) *f is multiplicative and $M_{f,k}$ is positive semidefinite for each $k \in \mathbb{N}$,*
(iii) *f is multiplicative and $N_{f,k}$ is positive semidefinite for each $k \in \mathbb{N}$.*

Proof. Similar to Theorem 4, by taking $\mathcal{S} = \{\{1,2\}\}$ with $|S| = 2$ and Γ_S the symmetric group on S. ∎

An interesting question is how this theorem relates to the following theorem of Freedman, Lovász, and Schrijver [2]. For any function $a : [n] \to \mathbb{R}_+$ and any symmetric function $c : [n]^2 \to \mathbb{R}$, define a function $f_{a,c} : \mathcal{G} \to \mathbb{R}$ by

$$(56) \qquad f_{a,c}(G) := \sum_{\phi: VG \to [n]} \left(\prod_{v \in VG} a(\phi(v)) \right) \left(\prod_{uv \in EG} c(\phi(u), \phi(v)) \right)$$

for any undirected graph G. (So $f_c = f_{\mathbf{1},c}$, where $\mathbf{1}$ denotes the all-one vector.)

Consider any function $f : \mathcal{G} \to \mathbb{R}$. Let $\tilde{N}_{f,k}$ be the submatrix of $N_{f,k}$ induced by the k-labeled graphs (G,u) where the vertices in u are distinct. Then Freedman, Lovász, and Schrijver [2] proved that for each $n \in \mathbb{N}$:

(57) $f = f_{a,c}$ for some $a : [n] \to \mathbb{R}_+$ and some symmetric $c : [n]^2 \to \mathbb{R}$ if and only if $f(K_0) = 1$ and $\tilde{N}_{f,k}$ is positive semidefinite and has rank at most n^k, for each $k \in \mathbb{N}$.

The uniqueness of c in Theorem 6 can be dealt with in a way similar to Theorem 5. For any symmetric $c : [d]^2 \to \mathbb{R}$ and any $\pi \in S_d$, define $c^\pi : [d]^2 \to \mathbb{R}$ by

$$(58) \qquad c^\pi(\phi) := c(\pi \circ \phi)$$

for any k and $\phi \in [d]^2$. In other words, $c^\pi(\phi) = c(N_\pi^\mathsf{T} \phi N_\pi)$, if we consider ϕ as $d \times d$ matrix, where N_π is the permutation matrix corresponding to π.

Theorem 7. *Let $c, b : [d]^2 \to \mathbb{R}$ be symmetric functions. Then $f_c = f_b$ if and only if $b = c^\pi$ for some $\pi \in S_d$.*

Proof. Similar to the proof of Theorem 5 (in fact easier, since the underlying space V is finite-dimensional). ∎

6. Undirected graphs — edge model

We now derive the theorem of Szegedy [8]. Again, let $\mathcal{G}$ denote the collection of (undirected) graphs, where a graph may contain loops and multiple edges, and also 'pointless' loops (loops without a vertex). The 'duals' are the hypergraphs $H = (VH, EH)$ such that each vertex $v \in VH$ is in precisely two edges. This gives a reduction to the results of Section 4, but there are some complications.

Let $c : \bigcup_{k\in\mathbb{N}}[d]^k \to \mathbb{R}$ be a symmetric function, for some $d \in \mathbb{N}$. Define $f_c : \mathcal{G} \to \mathbb{R}$ by

$$(59) \qquad f_c(G) := \sum_{\phi:EG\to[d]} \prod_{v\in VG} c(\phi(\delta(v))),$$

where $\delta(v)$ takes multiplicities into account, and where $\phi(\delta(v))$ is arbitrarily ordered. We characterize which functions $f : \mathcal{G} \to \mathbb{R}$ are equal to f_c for some c.

For $G_1, G_2 \in \mathcal{G}$ and $k \in \mathbb{N}$, we make a multiset $\mathcal{K}^{(k)}_{G_1,G_2}$ of graphs as follows. Let G be the disjoint union of G_1 and G_2. Choose distinct $u_1, \ldots, u_k \in VG$ and distinct $v_1, \ldots, v_k \in VH$ and choose for each i a bijection $\pi_i : \delta_G(u_i) \to \delta_H(v_i)$ (if any). Let J be the graph obtained from GH by deleting $u_1, \ldots, u_k$ making for each i and each $e = uu_i \in \delta_G(u_i)$ a new edge connecting u and v, where $vv_i = \pi_i(e)$. Then $\mathcal{K}^{(t)}_{G,H}$ is the multiset of all graphs J obtained in this way (taking multiplicities into account). Define the $\mathcal{G} \times \mathcal{G}$ matrix $M_{f,k}$ by

$$(60) \qquad (M_{f,k})_{G,H} := \textstyle\sum_{J\in\mathcal{K}_{G,H}} f(J)$$

for $G, H \in \mathcal{G}$.

Consider some $k \in \mathbb{N}$. A *k-exit graph* is a pair (G, u) of an undirected graph G and an element $u \in VG^k$ such that the u_i are distinct vertices, each of degree 1. Let $\mathcal{G}_k$ denote the collection of k-exit graphs.

If (G, u) and (J, w) are k-exit graphs, then the undirected graph $(G, u)\cdot(J, w)$ is obtained by taking the disjoint union of G and J, and, for each $i = 1, \ldots, k$, deleting with u_i and w_i and the edges incident with them, and adding a new edge connecting the neighbours of u_i and w_i.

For $f : \mathcal{G} \to \mathbb{R}$, define the $\mathcal{G}_k \times \mathcal{G}_k$ matrix $N_{f,k}$ by

$$(61) \qquad (N_{f,k})_{(G,u),(J,w)} := f((G, u) \cdot (J, w))$$

for $(G, \boldsymbol{v}), (G', \boldsymbol{v}') \in \mathcal{G}_k$. A function $f : \mathcal{G} \to \mathbb{R}$ is called *multiplicative* if $f(K_0) = 1$ and $f(G \cup G') = f(G)f(G')$ for disjoint graphs G and G'.

The equivalence of (i) and (iii) in the following theorem is the theorem of Szegedy [8].

Theorem 8. *For any $f : \mathcal{G} \to \mathbb{R}$, the following are equivalent:*

(62) (i) *$f = f_c$ for some $n \in \mathbb{N}$ and $c : \bigcup_{t\in\mathbb{N}}[n]^t \to \mathbb{R}$,*
(ii) *f is multiplicative and $M_{f,k}$ is positive semidefinite for each $k \in \mathbb{N}$.*
(iii) *f is multiplicative and $N_{f,k}$ is positive semidefinite for each $n \in \mathbb{N}$.*

Proof. Similar to Theorem 4. We take $\mathcal{S}$ as in Theorem 4, and restrict $\mathcal{H}$ to the class of hypergraphs such that each vertex is in precisely two edges. This gives a collection of structured hypergraphs satisfying the conditions of Theorem 3. Interchanging the roles of vertices and edges gives the embedded graphs. ∎

We finally consider the uniqueness of c. We note that (by Weyl's First Fundamental Theorem) the algebra A defined in the proof of Theorem 2 is equal to $T(V)^G$, where G is the orthogonal group $O(d)$.

For any $U \in O(d)$, define $c^U : [d]^2 \to \mathbb{R}$ by

$$(63) \qquad c^U(\phi) := c(U^{\mathsf{T}}\phi U),$$

considering ϕ as symmetric matrix in $\mathbb{R}^{d\times d}$. The following theorem extends a theorem of Szegedy [8].

Theorem 9. *Let $c, b : \bigcup_k [d]^k \to \mathbb{R}$ be symmetric functions. Then $f_c = f_b$ if and only if $b = c^U$ for some $U \in O(d)$.*

Proof. Sufficiency being direct, we show necessity. Since $f_c = f_d$, we know that for each $p \in \mathcal{P}[V]^G$ one has $p(c) = p(d)$. This implies that $b = c^U$ for some $U \in O(d)$. ∎

7. Directed graphs

A *directed graph* is a pair $D = (VD, ED)$, where VD is a finite set and ED is a finite multisets of ordered pairs (u, v) from VD, possible with $u = v$ (a loop). Let $\mathcal{D}$ denote the collection of directed graphs.

For any function $c : [d]^2 \to \mathbb{R}$ (for some d), define $f_c : \mathcal{D} \to \mathbb{R}$ by

$$(64) \qquad f_c(D) := \sum_{\phi:VD\to[d]} \prod_{e=(u,v)\in ED} c(\phi(u), \phi(v))$$

for $D \in \mathcal{D}$. We characterize the functions $f : \mathcal{D} \to \mathbb{R}$ for which $f = f_c$ for some real-valued c.

For $D_1, D_2 \in \mathcal{D}$ and $k \in \mathbb{N}$, we make a multiset $\mathcal{J}^k_{D_1,D_2}$ of hypergraphs as follows. Let D be the disjoint union of D_1 and D_2. For distinct $e_1, \ldots, e_k \in ED_1$ and distinct $f_1, \ldots, f_k \in ED_2$, let $D(e_1, f_1, \ldots, e_k, f_k)$ be the hypergraph obtained from D by, for each $i = 1, \ldots, k$, deleting e_i and f_i and identifying the tails of e_i and f_i, and identifying the heads of e_i and f_i. Then

(65) $\mathcal{J}^k_{D_1,D_2} := \{D(e_1, f_1, \ldots, e_k, f_k) \mid$ for distinct $e_1, \ldots, e_k \in ED_1$ and distinct

$f_1, \ldots, f_k \in ED_2\}$.

For $f : \mathcal{D} \to \mathbb{R}$ and $k \in \mathbb{N}$, define the $\mathcal{D} \times \mathcal{D}$ matrix $M_{f,k}$ by

$$(66) \qquad (M_{f,k})_{D_1,D_2} := \textstyle\sum_{D \in \mathcal{J}^k_{D_1,D_2}} f(D)$$

for $G_1, G_2 \in \mathcal{G}$.

We also define a matrix $N_{f,k}$. A *k-labeled directed graph* is a pair (D, u) of a graph D and an element u of VD^k. Let $\mathcal{D}_k$ be the collection of k-labeled directed graphs. For two k-labeled directed graphs (D, u) and (J, w), the directed graph $(D, u) \cdot (J, w)$ is obtained by taking the disjoint union of D and J, and next identifying u_i and w_i, for $i = 1, \ldots, k$. Then $N_{f,k}$ is the $\mathcal{D}_k \times \mathcal{D}_k$ matrix defined by

$$(67) \qquad (N_{f,k})_{(D,u),(J,w)} := f((D, u) \cdot (J, w))$$

for $(D, u), (J, w) \in \mathcal{D}_k$.

Call $f : \mathcal{D} \to \mathbb{R}$ *multiplicative* if $f(K_0) = 1$ and $f(D) = f(D_1)f(D_2)$ if D is the disjoint union of D_1 and D_2.

Theorem 10. *Let $f : \mathcal{D} \to \mathbb{R}$. Then the following are equivalent:*

(68) (i) *$f = f_c$ for some $d \in \mathbb{N}$ and some function $c : [n]^2 \to \mathbb{R}$,*
(ii) *f is multiplicative and $M_{f,k}$ is positive semidefinite for each $k \in \mathbb{N}$,*
(iii) *f is multiplicative and $N_{f,k}$ is positive semidefinite for each $k \in \mathbb{N}$.*

Proof. The proof is similar to that of Theorem 4. In this case, $\mathcal{S} := \{\{1, 2\}\}$ and $\Gamma_{\{1,2\}}$ consists only of the identity permutation on $\{1, 2\}$. ∎

The uniqueness of c in Theorem 10 can be dealt with in a way similar to Theorem 5. For any $c : [d]^2 \to \mathbb{R}$ and any $\pi \in S_d$, define $c^\pi : [d]^2 \to \mathbb{R}$ by

$$(69) \qquad c^\pi(\phi) := c(\pi \circ \phi)$$

for any k and $\phi \in [d]^2$. In other words, $c^\pi(\phi) = c(M_\pi^{\mathsf{T}} \phi M_\pi)$, if we consider ϕ as $d \times d$ matrix, where M_π is the permutation matrix corresponding to π.

Theorem 11. *Let $c, b : [d]^2 \to \mathbb{R}$. Then $f_c = f_b$ if and only if $b = c^\pi$ for some $\pi \in S_d$.*

Proof. Similar to the proof of Theorem 5 (in fact easier, since the underlying space V is finite-dimensional). ∎

Theorem 10 relate to a result of Lovász and Schrijver [5], although the precise relation is unclear. For any function $a : [d] \to \mathbb{R}_+$ and any function $c : [d]^2 \to \mathbb{R}$, let $f_{a,c} : D \to \mathbb{R}$ be defined by

(70) $$f_{a,c}(D) := \sum_{\phi:VD\to[d]} \left(\prod_{v\in VD} a(\phi(v))\right)\left(\prod_{uv\in ED} c(\phi(u),\phi(v))\right)$$

for any directed graph D. (So $f_c = f_{\mathbf{1},c}$.)

Consider any function $f : \mathcal{D} \to \mathbb{R}$. For any n, let $\widetilde{M}_{f,n}$ be the submatrix of $M_{f,n}$ induced by the rows and columns indexed by n-vertex-labeled directed graphs $(G, \boldsymbol{v})$ where all vertices in $\boldsymbol{v}$ are distinct. Then Lovász and Schrijver [5] proved that for each $d \in \mathbb{N}$:

(71) Let $f : \mathcal{D} \to \mathbb{R}$. Then $f = f_{a,c}$ for some $a : [d] \to \mathbb{R}_+$ and some $c : [d]^2 \to \mathbb{R}$ if and only if $f(K_0) = 1$ and $\widetilde{M}_{f,n}$ is positive semidefinite and has rank at most d^n, for each $n \in \mathbb{N}$.

8. Graphs embedded on surfaces

We next derive a characterization for parameters of graphs embedded on an oriented surface. Consider pairs (G, ψ), where G is an undirected graph and ψ is an embedding of G onto an oriented surface. (Here a surface may be a disjoint union of connected surfaces.)

Call two embeddings *equivalent* if for each vertex v, the edges incident with v leave v in the same clockwise cyclic order in the two embeddings. So an equivalence class is determined by the clockwise cyclic orders of the edges leaving the vertices. Each equivalence class contains a unique cellularly embedded graph — unique op to homeomorphisms.

Therefore, we define an *cellularly embedded graph* as a pair (G, γ), where γ assigns to each vertex v of G a cyclic order of the edges incident with v. Let $\mathcal{G}^{\mathrm{emb}}$ denote the collection of cellularly embedded graphs.

Choose $d \in \mathbb{N}$. Call $c : \bigcup_{k\in\mathbb{N}}[d]^k \to \mathbb{R}$ *cyclic*, if for each k, one has $c(\phi \circ (1,2,\ldots,k)) = c(\phi)$ for each k and each $\phi \in [d]^k$. Here $(1,2,\ldots,k)$ denotes, as usual, the cyclic permutation of $[k]$ bringing i to $i+1$ mod k, for each i.

Define $f_c : \mathcal{G}^{\mathrm{emb}} \to \mathbb{R}$ by

(72) $$f_c(G,\gamma) := \sum_{\phi:EG\to[d]} \prod_{v\in VG} c(\phi(\delta(v))),$$

where we take any linear order on $\delta(v)$ which induces the cyclic order γ_v. We characterize which functions $f : \mathcal{G}^{\mathrm{emb}} \to \mathbb{R}$ are equal to f_c for some real-valued cyclic c.

For $G_1, G_2 \in \mathcal{G}^{\mathrm{emb}}$ and $t \in \mathbb{N}$, we make a multiset $\mathcal{K}^k_{G_1,G_2}$ of cellularly embedded graphs as follows. Let G be the disjoint union of G_1 and G_2. For any distinct $u_1,\ldots,u_k \in VG_1$ and $w_1,\ldots,w_k \in VG_2$ and bijections $\pi_i : \delta(u_i) \to \delta(w_i)$ for $i = 1,\ldots,k$, each maintaining the cyclic order, let $G(u_1,w_1,\pi_1,\ldots,u_k,w_k,\pi_k)$ be the graph obtained by for each $i = 1,\ldots,k$ and each $e \in \delta(u_i)$, making a new edge connecting the vertex incident with e unequal to u_i and the vertex incident with $\pi(e)$ unequal to w_i. Then

(73) $\mathcal{K}_{G_1,G_2} := \{G(u_1,w_1,\pi_1,\ldots,u_k,w_k,\pi_k) \mid$ distinct $u_1,\ldots,u_k \in VG_1$, distinct $w_1,\ldots,w_k \in VG_2$, bijections $\pi_i : \delta(u_i) \to \delta(w_i)$ maintaining the cyclic order$\}$.

Define the $\mathcal{G}^{\text{emb}} \times \mathcal{G}^{\text{emb}}$ matrix M_f by

$$(M_{f,k})_{G_1,G_2} := \textstyle\sum_{G \in \mathcal{K}_{G_1,G_2}} f(G) \tag{74}$$

for $G_1, G_2 \in \mathcal{G}$.

Consider some $k \in \mathbb{N}$. A *k-exit cellularly embedded graph* is a pair (G, u) of cellularlly embedded graph G and an element $u \in VG^k$ such that the u_i are distinct vertices, each of degree 1. Let $\mathcal{G}_k^{\text{emb}}$ denote the collection of k-exit cellularly embedded graphs.

If (G, u) and (J, w) are k-exit cellularly embedded graphs, then the cellularly embedded graph $(G, u) \cdot (J, w)$ is obtained by taking the disjoint union of G and J, and, for each $i = 1, \ldots, k$, deleting u_i and w_i and the edges incident with them, and adding a new edge connecting the neighbours of u_i and w_i.

For $f : \mathcal{G} \to \mathbb{R}$, define the $\mathcal{G}_k^{\text{emb}} \times \mathcal{G}_k^{\text{emb}}$ matrix $M_{f,k}$ by

$$(M_{f,k})_{(G,u),(J,w)} := f((G, u) \cdot (J, w)) \tag{75}$$

for $(G, u), (G', w) \in \mathcal{G}_k^{\text{emb}}$.

A function $f : \mathcal{G}^{\text{emb}} \to \mathbb{R}$ is called *multiplicative* if $f(K_0) = 1$ and $f(G \cup G') = f(G)f(G')$ for disjoint cellularly embedded graphs G and G'.

Theorem 12. *For any $f : \mathcal{G}^{emb} \to \mathbb{R}$, the following are equivalent:*

(76) (i) *$f = f_c$ for some $d \in \mathbb{N}$ and some cyclic $c : \bigcup_{k \in \mathbb{N}} [d]^k \to \mathbb{R}$,*
(ii) *f is multiplicative and $M_{f,n}$ is positive semidefinite for each $n \in \mathbb{N}$,*
(iii) *f is multiplicative and $N_{f,n}$ is positive semidefinite for each $n \in \mathbb{N}$.*

Proof. Similar to Theorem 8. We take for $\mathcal{S} := \{[m] \mid m \in \mathbb{N}\}$ and for $m \in \mathbb{N}$, $\Gamma_{[m]}$ consists of all cyclic permutations of $[m]$. Moreover, $\mathcal{H}$ consists of all structured hypergraphs such that each vertex is in precisely two edges. Interchanging the roles of vertices and edges gives the embedded graphs. ∎

One may show, similar to above:

Theorem 13. *Let $c, b : \bigcup_{n \in \mathbb{N}} [d]^n \to \mathbb{R}$ be cyclic. Then $f_c(G) = f_b(G)$ for each cellularly embedded graph G if and only $b = c^U$ for some $U \in O(d)$.*

Proof. Similar to above. ∎

9. Rooted forests

Another application of the theorem is inspired by the work of Kreimer [4] and Connes and Kreimer [1] on the Hopf algebra of rooted trees as applied to renormalization in quantum field theory.

A *rooted forest* F is a directed graph with cycles such that each vertex is entered by at most one edge. The vertices not entered by any edges are called the *roots* of F. The set of vertices entered by one edge and not left by any edge are called the *tails* of F. The sets of roots and tails of F are denoted by F and TF, respectively. For any tail t, let P_t be the sequence of vertices of the unique path starting in a root and ending in t, while deleting t from P_t. (The physical interpretation is that the tails are vertices of a Feynman graph, and the nontail vertices are renormalization fragments of the Feynman graph. Then P_t gives the sequence of fragments containing t.)

Consider any $n \in \mathbb{N}$ and a symmetric function $c : \bigcup_t [n]^t \to \mathbb{R}$. Define a rooted forest parameter f_c by

$$f_c(F) := \sum_{\phi : VF \setminus TF \to [n]} \prod_{t \in TF} c(\phi(P_t)). \tag{77}$$

We characterize which graph functions f are equal to f_c for some c.

If t and u are distinct tails of a rooted forest F with $|P_t| = |P_u|$, let $F_{t,u}$ be rooted forest obtained as follows. Write $P_t = (v_1, \ldots, v_m)$ and $P_u = (w_1, \ldots, w_m)$. Identify the paths $P_t \cup \{t\}$ and $P_u \cup \{u\}$. Delete t and u, and delete all arcs that are not on any other path from root to tail than P_t $(= P_u)$. (this might mean that some vertices on this path now become roots, without outgoing edges.)

For forests F and J and $k \in \mathbb{N}$, let

$$\mathcal{J}^k_{F,J} := \{(FJ)_{t_1,u_1,\ldots,t_k,u_k} \mid \text{distinct } t_1, \ldots, t_k \in TF, \text{ distinct } u_1, \ldots, u_k \in TJ\}. \tag{78}$$

Let $\mathcal{F}$ denote the collection of rooted forests. For $f : \mathcal{F} \to \mathbb{R}$ and $k \in \mathbb{N}$, define the $\mathcal{F} \times \mathcal{F}$ matrix $M_{f,k}$ by

$$(M_{f,k})_{F,J} := \textstyle\sum_{G \in \mathcal{J}^k_{F,J}} f(G) \tag{79}$$

for $F, J \in \mathcal{F}$.

We also define a matrix $N_{f,k}$. A *k-labeled rooted forest* is a pair (F, u) of a rooted forest F and an element u of TF^k. Let $\mathcal{F}_k$ be the collection of k-labeled rooted forests. Then $N_{f,k}$ is the $\mathcal{F}_k \times \mathcal{F}_k$ matrix defined by

$$(N_{f,k})_{(F,u),(J,w)} := f((FJ)_{u_1,w_1,\ldots,u_k,w_k}) \tag{80}$$

for $(F, u), (J, w) \in \mathcal{F}_k$.

Call $f : \mathcal{F} \to \mathbb{R}$ *multiplicative* if $f(K_0) = 1$ and $f(F) = f(F_1)f(F_2)$ if F is the disjoint union of F_1 and F_2.

Theorem 14. *Let $f : \mathcal{F} \to \mathbb{R}$. Then the following are equivalent:*

(81) (i) *$f = f_c$ for some $n \in \mathbb{N}$ and some symmetric function $c : \bigcup_t [n]^t \to \mathbb{R}$,*
(ii) *f is multiplicative and $M_{f,k}$ is positive semidefinite for each $k \in \mathbb{N}$,*
(iii) *f is multiplicative and $N_{f,k}$ is positive semidefinite for each $k \in \mathbb{N}$.*

Proof. Similar to Theorem 4. We take $\mathcal{S} := \{[m] \mid m \in \mathbb{N}\}$ and let $\Gamma_{[m]}$ consist only of the identity permutation. Moreover, $\mathcal{H}$ consists of all structured hypergraphs H such that for any two edges Φ, Ψ of H and $\phi \in \Phi$, $\psi \in \Psi$, say of types $[m]$ and $[p]$ respectively, one has that if $\phi(i) = \psi(j)$ for some $i \in [m]$ and $j \in [p]$, then $i = j$ and $\phi(i') = \psi(i')$ for $i' = 1, \ldots, i$.

Any rooted forest F gives such a structured hypergraph H, as follows. Let $VH := VF \setminus TF$. For each $t \in TF$, we make an edge of H: let m be the length (= number of edges) of the (unique) path from a root to t. Define $\phi_t : [m] \to VH$ by setting, for $i = 1, \ldots, m$, $\phi_t(i)$ to be the ith vertex along this path. (So $\phi_t(1)$ is a root and $\mathrm{R}\phi_t(m)$ is the one but last vertex of the path.) Let $\Phi_t := \{\phi_t\}$. Finally define $EH := \{\Phi_t \mid t \in TF\}$.

The hypergraph constructed this way belongs to $\mathcal{H}$, and conversely, each $H \in \mathcal{H}$ comes in this way from a rooted forest. ∎

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