

# Graph parameters and semigroup functions

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**Abstract.** We prove a general theorem on semigroup functions that implies characterizations of graph partition functions in terms of the positive semidefiniteness (‘reflection positivity’) and rank of certain derived matrices. The theorem applies to undirected and directed graphs and to hypergraphs.

## 1. Introduction

Let  $\mathcal{G}$  be the collection of all undirected graphs. (In this paper, (undirected or directed) graphs may have multiple edges, but no loops. *Simple* graphs have no multiple edges.) A graph parameter  $f : \mathcal{G} \rightarrow \mathbb{R}$  is called a *partition function* (or a *graph homomorphism function*) if there exists a  $k \in \mathbb{Z}_+$ , a vector  $\alpha \in \mathbb{R}_+^k$ , and a symmetric matrix  $\beta \in \mathbb{R}^{k \times k}$  such that for each  $G \in \mathcal{G}$ :

$$(1) \quad f(G) = f_{\alpha, \beta}(G) := \sum_{\phi : VG \rightarrow [k]} \left( \prod_{v \in VG} \alpha_{\phi(v)} \right) \left( \prod_{uv \in EG} \beta_{\phi(u), \phi(v)} \right).$$

Here, as usual,

$$(2) \quad [k] := \{1, \dots, k\}$$

for any integer  $k$ .

Partition functions arise in statistical mechanics. Here  $[k]$  is considered as a set of states, and any function  $\phi : VG \rightarrow [k]$  as a configuration that  $G$  may adopt. Then  $\ln \alpha_i$  can be considered as the external energy if a vertex is in state  $i$ . If  $\sum_i \alpha_i = 1$ ,  $\alpha_i$  can alternatively be seen as the probability that a vertex is in state  $i$ . Moreover,  $\ln \beta_{i,j}$  may represent the contribution of two adjacent vertices in states  $i$  and  $j$  to the energy. Then  $f_{\alpha, \beta}(G)$  is the partition function of the model.

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If  $\alpha_i = 1$  for each  $i$  and  $\beta$  is the adjacency matrix of a graph  $H$ , then  $f_{\alpha,\beta}(G)$  is equal to the number of homomorphisms  $G \rightarrow H$ . If we take for  $H$  the complete graph on  $k$  vertices,  $f_{\alpha,\beta}(G)$  is the number of proper  $k$ -colourings of the vertices of  $G$ .

Freedman, Lovász, and Schrijver [4] characterized partition functions, among all graph parameters, by the ‘reflection positivity’ and ‘rank connectivity’ of  $f$  (see Corollary 1). In that same paper examples of graph parameters are mentioned where these conditions were first observed and this lead to a representation as a partition function (an example is the number of nowhere-zero  $k$ -flows). So such a theorem may reveal a ‘hidden structure’ behind a graph parameter (or of a physical quantity in statistical mechanics).

The proof technique of [4] can be extended to include related structures like directed graphs and hypergraphs. It amounts to a general theorem on semigroup functions, which is the content of this paper. In Section 11 we describe applications to graphs and hypergraphs.

Our theorem relates to results of Lindahl and Maserick [5], Berg, Christensen, and Ressel [1], and Berg and Maserick [3] (cf. the book of Berg, Christensen, and Ressel [2]) characterizing ‘positive definite’ semigroup functions. We describe this relation in Section 2.

## 2. Positive semidefinite $*$ -semigroup functions

A natural general setting for our results is functions on  $*$ -semigroups. A  $*$ -semigroup is a semigroup  $S$  with a ‘conjugation’  $s \mapsto s^*$  such that  $(s^*)^* = s$  and  $(st)^* = t^*s^*$  for all  $s, t \in S$ . Note that each commutative semigroup  $S$  can be turned into a  $*$ -semigroup by defining  $s^* := s$  for each  $s \in S$  (we say in this case that  $*$  is *trivial*). A  $*$ -automorphism is an automorphism  $\rho : S \rightarrow S$  such that  $\rho(s^*) = \rho(s)^*$  for all  $s \in S$ .

A  $*$ -semicharacter is a function  $h : S \rightarrow \mathbb{C}$  such that  $h(s^*) = \overline{h(s)}$  and  $h(st) = h(s)h(t)$ . The set of all  $*$ -semicharacters is denoted by  $S^*$ . We can equip  $S^*$  with the topology of pointwise convergence.

Let  $f$  be any function  $f : S \rightarrow \mathbb{C}$  such that  $f(s^*) = \overline{f(s)}$  for each  $s \in S$ . We define the  $S \times S$  matrix  $M(f)$  by

$$(3) \quad M(f)_{s,t} := f(s^*t)$$

for  $s, t \in S$ . Clearly this matrix is Hermitian. The function  $f : S \rightarrow \mathbb{C}$  is called  $*$ -definite if  $M(f)$  is positive semidefinite.

It can be checked easily that each  $*$ -semicharacter is positive definite. Under certain conditions, all positive definite functions on  $S$  can be obtained from  $*$ -semicharacters as follows ([5], [1], and [3] (cf. [2])).

- (4) Let  $f : S \rightarrow \mathbb{C}$ . Then there exists a Radon measure  $\mu$  on  $S^*$  with compact support such that

$$f = \int_{S^*} \chi d\mu(\chi)$$

if and only if  $f$  is  $*$ -definite and is *exponentially bounded* — this means that there exists a function  $|\cdot| : S \rightarrow \mathbb{R}_+$  satisfying  $|1| = 1$ ,  $|st| \leq |s||t|$ ,  $|s^*| = |s|$ , and  $|f(s)| \leq |s|$  for all  $s, t \in S$ .

It is also known [1] that

- (5) (6) If  $M_f$  has finite rank  $k$ , then  $\mu$  is a sum of  $k$  Dirac measures.

Our results can be considered as refining this representation (in many cases, giving such a representation with a finite description), at the cost of introducing additional structure of the semigroup. We'll also show in Section 2 that (6) follows from our results.

### 3. Carriers

Let  $Z$  be a countable set and let  $F$  denote the  $*$ -semigroup of finite subsets of  $F$  with the operation of union and trivial  $*$ .

A commutative  $*$ -semigroup  $S$  is called a  *$*$ -semigroup with carrier* if  $F$  is a homomorphism retract of  $S$ , and every automorphism of  $F$  lifts to an automorphism of  $S$ . In this case,  $F$  is a subsemigroup of  $S$  and there is a surjective homomorphism  $C : S \rightarrow F$  such that  $C|_F = \text{id}_F$ . We call  $C$  a *carrier* for  $S$ .

In more direct terms, a carrier for  $S$  is a function  $C : S \rightarrow F$  such that

- (7) (i)  $C(s^*) = C(s)$  for each  $s \in S$ ,  
(ii)  $C(st) = C(s) \cup C(t)$  for all  $s, t \in S$ .

Furthermore,

- (8) for each  $U \in F$  there exists an element  $e_U \in S$  such that  $C(e_U) = U$  and  $e_U s = s$  for each  $s \in S$  with  $U \subseteq C(s)$ .

In particular,  $e_\emptyset$  is a unit of  $S$ . Note that  $e_U$  is unique, that  $e_U e_W = e_{U \cup W}$ , and that  $e_U^* = e_U$  for all  $U, W \in F$ . (By condition (9), it suffices to require (8) for  $U = \emptyset$  and  $U = \{1\}$  only.)

For each bijection  $\pi : Z \rightarrow Z$  there exists a  $*$ -automorphism  $\tilde{\pi} : S \rightarrow S$  such that

- (9) (i)  $C(\tilde{\pi}(s)) = \pi(C(s))$  for each  $s \in S$ ,  
(ii)  $\tilde{\pi} \circ \tilde{\pi}' = \tilde{\pi} \circ \tilde{\pi}'$  for all bijections  $\pi, \pi' : Z \rightarrow Z$ .  
(iii)  $\tilde{\text{id}}_Z = \text{id}_S$ .

We call the automorphisms  $\tilde{\pi}$  *relabelings*.

Condition (9) says that the sets  $C(s)$  by themselves are not essential, but rather serve as a ‘carrier’ carrying the ‘structure’  $s$  (like the set of vertices carrying a graph).

## 4. Examples

We give some examples that will serve as illustration and motivation for our results.

**Example 1.** Let  $\mathcal{G}$  be the collection of all finite undirected graphs  $G$  with  $VG \subseteq Z$ . For  $G, G' \in \mathcal{G}$ , define  $GG' := (VG \cup VG', EG \cup EG')$ , where  $EG \cup EG'$  takes multiplicities into account. Let  $G^* := G$  and  $C(G) := VG$  for each  $G \in \mathcal{G}$ . Then  $\mathcal{G}$  is a  $*$ -semigroup with carrier. We obtain another example if we restrict  $\mathcal{G}$  to simple graphs, and we do not take multiplicities into account when forming the union of  $EG$  and  $EG'$ .

**Example 2.** Let  $\mathcal{G}$  be the collection of all finite directed graphs  $G$  with  $VG \subseteq Z$ . For  $G, G' \in \mathcal{G}$ , define  $GG' := (VG \cup VG', EG \cup EG')$ , where  $EG \cup EG'$  takes multiplicities into account. Let  $G^* := G$  and  $C(G) := VG$  for each  $G \in \mathcal{G}$ . With these operations,  $\mathcal{G}$  is a  $*$ -semigroup with carrier as above.

**Example 3.** Let  $\mathcal{G}$  be the collection of all finite directed graphs  $G$  with  $VG \subseteq Z$ . For  $G, G' \in \mathcal{G}$ , define  $GG' := (VG \cup VG', EG \cup EG')$ , where  $EG \cup EG'$  takes multiplicities into account. Let  $G^* := G^{-1}$  (the directed graph obtained by reversing all arc directions) and  $C(G) := VG$  for each

$G \in \mathcal{G}$ . With these operations,  $\mathcal{G}$  is a  $*$ -semigroup with carrier, and with a nontrivial  $*$ -operation.

**Example 4.** Let  $\mathcal{H}$  be the collection of all finite  $m$ -uniform hypergraphs  $H$  with  $VH \subseteq Z$  (for some fixed natural number  $m$ ). For  $H, H' \in \mathcal{H}$ , define  $HH' := (VH \cup VH', EH \cup EH')$ , where  $EH \cup EH'$  takes multiplicities into account. Let  $H^* := H$  and  $C(H) := VH$  for each  $H \in \mathcal{H}$ . Then  $\mathcal{H}$  is a  $*$ -semigroup with carrier.

**Example 5.** Let  $\mathcal{H}$  be the collection of all finite hypergraphs  $H$  with  $VH \subseteq Z$ . For  $H, H' \in \mathcal{H}$ , define  $HH' := (VH \cup VH', EH \cup EH')$ , where  $EH \cup EH'$  takes multiplicities into account. Let  $H^* := H$  and  $C(H) := VH$  for each  $H \in \mathcal{H}$ . Then  $\mathcal{H}$  is a  $*$ -semigroup with carrier.

**Example 6.** In the previous examples, the carrier  $C$  meant the “underlying set” of the structures; let us describe an example where it does not. In [4] *partially labeled graphs* were considered: graphs where a subset of the nodes are labeled by distinct integers, while the rest of the nodes were left unlabeled. The product of two partially labeled graphs is obtained by taking the disjoint union and then identifying nodes with the same label. Let  $C(G)$  denote the set of labels occurring in the partially labeled graph  $G$ . Then partially labeled graphs form a  $*$ -semigroup with carrier.

## 5. Unlabeling

Example 6 above motivates the following additional structure. Consider a  $*$ -semigroup  $S$  with a carrier function  $C$ . For each  $U \in F$ , the elements  $s \in S$  with  $C(s) = U$  form a subsemigroup with identity, which we denote by  $S_U$ ; similarly, the elements  $s$  with  $C(s) \subseteq U$  and  $C(s) \supseteq U$  form subsemigroups  $S_U^-$  and  $S_U^+$ , respectively.

An *unlabeling operator* is a family of maps  $\lambda_U : S \rightarrow S$  ( $U \in F$ ), such that for all  $s \in S$  the following relations hold:

- (10) (i)  $C(\lambda_U(s)) = U \cap C(s)$ ;  
(ii)  $\lambda_U(s^*) = (\lambda_U(s))^*$ ;  
(iii)  $\lambda_{C(s)}(s) = s$ .  
(iv)  $\lambda_U(\lambda_V(s)) = \lambda_{U \cap V}(s)$ .  
(v) If  $C(s) \cap C(t) \subseteq U$ , then  $\lambda_U(st) = \lambda_U(s)\lambda_U(t)$ .  
(vi) If  $\pi$  is any permutation of  $Z$ , then  $\tilde{\pi}(\lambda_U(s)) = \lambda_{\pi(U)}(\tilde{\pi}(s))$ .

(All these properties are trivial if  $S$  is the  $*$ -semigroup of partially labeled

graphs (digraphs, hypergraphs etc.), and  $\lambda_U$  is the operation of deleting the labels outside  $U$ .)

## 6. State models

Let  $S$  be a  $*$ -semigroup with carrier  $C : S \rightarrow F$ . Let  $k \in \mathbb{Z}_+$ . A *state model with  $k$  states* is a pair  $(\alpha, \beta)$ , where  $\alpha : [k] \rightarrow \mathbb{R}_+$  and  $\beta : S \times [k]^Z \rightarrow \mathbb{C}$  such that

- (11) (i)  $\beta(\cdot, \phi)$  is a  $*$ -semicharacter for every  $\phi \in [k]^Z$ ,  
(ii) if  $\phi|_{C(s)} = \psi|_{C(s)}$ , then  $\beta(s, \phi) = \beta(s, \psi)$  (in other words,  $\beta(s, \phi)$  is determined by the restriction of  $\phi$  to  $C(s)$ ),  
(iii)  $\beta(\tilde{\pi}(s), \phi) = \beta(s, \phi \circ \pi)$  for each  $s \in S$ , bijection  $\pi : Z \rightarrow Z$ , and  $\phi : Z \rightarrow [k]$  (in other words,  $\beta(s, \phi)$  only depends on the states of the elements in  $C(s)$ , not on their names).

We occasionally write  $\beta_s(\phi)$  for  $\beta(s, \phi)$ .

The conditions (11) imply that a state model is fully determined by  $\alpha$  and by the  $\beta_s$  for any set of semigroup elements  $s$  that generate  $S$ , taking relabeling and conjugation into account. Furthermore, for every  $s$  we only need to specify a finite number of values to specify the function  $\beta_s$ ; therefore, we may also denote  $\beta(s, \phi)$  by  $\beta(s, \psi)$ , where  $\psi = \phi|_{C(s)}$ .

With any state model  $(\alpha, \beta)$  we associate the following function  $f_{\alpha, \beta} : S \rightarrow \mathbb{C}$ , which we call the *value* of the state model  $(\alpha, \beta)$ :

$$(12) \quad f_{\alpha, \beta}(s) = \sum_{\phi: C(s) \rightarrow [k]} \left( \prod_{v \in C(s)} \alpha_{\phi(v)} \right) \beta(s, \phi)$$

for  $s \in S$ . We could rewrite this as

$$(13) \quad f_{\alpha, \beta}(s) = \int_{\phi: Z \rightarrow [k]} \beta(s, \phi) d\alpha^Z,$$

where  $\alpha^Z$  is the measure on the Borel sets in  $[k]^Z$  defined by  $\alpha$ .

For instance, in Examples 1–3 above, any state model is determined by  $\alpha$  and by  $\beta(K_2, \cdot)$  for the two-vertex graph  $K_2$  with one edge. Note that in that case  $\beta(K_2, \cdot)$  is essentially a matrix. (All other graphs can be obtained from  $K_2$  by relabeling and multiplication in the semigroup.)

Similarly, in Example 4, any state model is determined by  $\alpha$  and by  $\beta_H$  for the  $m$ -vertex hypergraph  $H_m$  with one edge of size  $m$ . In Example 5, we need to specify  $\beta_{H_m}$  for each  $m$ .

Example 6 is much worse: since to generate  $S$  we need to use all connected partially labeled graphs in which the labeled nodes do not form a cutset, we need to specify the values  $\beta(s, \phi)$  for all these graphs. But we can use the unlabeled to make the definition more restrictive.

Suppose that our  $*$ -semigroup with carrier admits unlabeled too. Let  $s \in S$ ,  $x \in C(s)$ , and  $\phi : C(s) \setminus x \rightarrow [k]$ . Let  $\phi_i$  denote the extension of  $\phi$  to  $C(s)$  that maps  $x$  to  $i \in [k]$ . Then we require

$$(14) \quad \beta(\lambda_{C(s) \setminus x}(s), \phi) = \sum_{i \in [k]} \alpha(i) \beta(s, \phi_i).$$

For such a state model, the value of the model can be computed easily, using (14), by

$$(15) \quad f(s) = \beta(\lambda_{\emptyset}(s), \emptyset)$$

(where  $\emptyset$  is considered as the unique map of  $\emptyset$  into  $[k]$ ). So in this case,  $\beta$  can be considered as an extension of  $f$ .

We may interpret state models and their values as follows. We can consider the elements of  $S$  as ‘systems’, where  $C(s)$  is the set of ‘particles’. The set  $[k]$  is a set of possible states of a particle, and any function  $\phi : C(s) \rightarrow [k]$  is a configuration that the system  $s$  may adopt. The value  $\ln \beta(s, \phi)$  might represent the energy when system  $s$  is in configuration  $\phi$ . The logarithms of the  $\alpha_i$  may represent the external energy of a particle when it is in state  $i$ . Then  $f(s)$  is the partition function. If the  $\alpha_i$  add up to 1, they can alternatively be considered as probabilities, and then  $\prod_{v \in C(s)} \alpha_{\phi(v)}$  gives the probability that the system is in configuration  $\phi$ .

## 7. Characterization of functions with a state model

Let  $S$  be a  $*$ -semigroup with carrier  $C$ . We want to characterize which functions  $f$  are values of a state model with  $k$  states, in terms of the positive semidefiniteness and rank of certain submatrices  $M_n$  of  $M(f)$ .

We say that a function  $f : S \rightarrow \mathbb{C}$  is *invariant under relabeling* if it satisfies

$$(16) \quad f(\tilde{\pi}(s)) = f(s)$$

for each bijection  $\pi : Z \rightarrow Z$  and each  $s \in S$ . We say that it is *\*-covariant*, if

$$(17) \quad f(s^*) = \overline{f(s)}$$

for each  $s \in S$ .

Suppose that  $f$  is invariant under relabeling. For  $n \in \mathbb{N}$ , fix an  $n$ -element subset  $Z_n$ . For notational convenience, set  $S_n := S_{Z_n}^+$ . Let  $M_n$  be the  $S_n \times S_n$  matrix defined as follows. For  $s, t \in S_n$ , consider a bijection  $\pi : Z \rightarrow Z$  such that

$$(18) \quad \begin{aligned} \text{(i)} \quad & \pi(i) = i \text{ for } i \in Z_n, \\ \text{(ii)} \quad & \pi(C(s)) \cap C(t) = Z_n. \end{aligned}$$

Then define

$$(19) \quad M_n(s, t) := f(\tilde{\pi}(s)^*t).$$

Note that since  $f$  is invariant under relabeling,  $M_n(s, t)$  is independent of the choice of  $\pi$ .

**Theorem 1.** *Let  $S$  be a \*-semigroup with carrier  $C$ , let  $f : S \rightarrow \mathbb{C}$ , and  $k \in \mathbb{Z}_+$ . Then  $f = f_{\alpha, \beta}$  for some state model  $(\alpha, \beta)$  with  $k$  states if and only if  $f \equiv 0$  or  $f(e_\emptyset) = 1$ ,  $f$  is \*-covariant, invariant under relabeling, and for each  $n$ ,  $M_n$  is positive semidefinite and has rank at most  $k^n$ .*

We'll derive Theorem 1 from the following, which characterizes state models in the presence of unlabeling. This is best formulated for *normalized* state models, which are state models  $(\alpha, \beta)$  with  $\sum_i \alpha_i = 1$ . If  $S$  is a \*-semigroup with carrier  $C$  and unlabeling operator  $\lambda$ , we say that a function  $f : S \rightarrow \mathbb{C}$  is *invariant under unlabeling* if  $f(\lambda_U s) = f(s)$  for each  $s \in S$  and  $U \in F$ .

**Theorem 2.** *Let  $S$  be a \*-semigroup with carrier  $C$  and unlabeling operator  $\lambda$ , let  $f : S \rightarrow \mathbb{C}$ , and let  $k \in \mathbb{Z}_+$ . Then  $f = f_{\alpha, \beta}$  for some normalized state model  $(\alpha, \beta)$  with  $k$  states satisfying (14) if and only if either  $f \equiv 0$ , or  $f(e_U) = 1$  ( $U \in F$ ),  $f$  is \*-covariant and invariant under relabeling and under unlabeling,  $M(f)$  is positive semidefinite, and the rank of  $M(f|_{S_U})$  is at most  $k^{|U|}$  for every  $U \in F$ .*

## 8. Proof of necessity in Theorems 1 and 2

Let  $f$  be the value function of a state model  $(\alpha, \beta)$  on a  $*$ -semigroup with carrier. Assume  $f \neq 0$ . So  $\beta(s, \cdot) \neq 0$  for some  $s$ . Hence  $\beta(se_\emptyset, \cdot) \neq 0$ , and therefore  $\beta(e_\emptyset, \cdot) \neq 0$ . That is (as  $C(e_\emptyset) = \emptyset$ ),  $\beta(e_\emptyset, \phi) \neq 0$ , where  $\phi$  is the (unique) function on the empty set. By (11)(i),  $\beta(e_\emptyset, \phi) = \beta(e_\emptyset, \phi)^2$ , so  $\beta(e_\emptyset, \phi) = 1$ . Hence  $f(e_\emptyset) = 1$ .

Consider any  $V \in F$ . Choose  $s, t \in S_n$ , and choose a bijection  $\pi : Z \rightarrow Z$  satisfying (18). Let  $s' := \tilde{\pi}(s^*)$ . Then

$$\begin{aligned}
M_n(s, t) &= f(s't) = \sum_{\phi: C(s't) \rightarrow [k]} \left( \prod_{v \in C(s't)} \alpha_{\phi(v)} \right) \beta(s't, \phi) \\
&= \sum_{\phi: C(s't) \rightarrow [k]} \left( \prod_{v \in C(s't)} \alpha_{\phi(v)} \right) \beta(s', \phi|C(s')) \beta(t, \phi|C(t)) \\
&= \sum_{\psi: V \rightarrow [k]} \left( \prod_{v \in V} \alpha_{\psi(v)} \right) \sum_{\substack{\phi': C(s') \rightarrow [k] \\ \phi'|V=\psi}} \left( \prod_{v \in C(s') \setminus V} \alpha_{\phi'(v)} \right) \beta(s', \phi') \cdot \\
&\quad \cdot \sum_{\substack{\phi'': C(t) \rightarrow [k] \\ \phi''|V=\psi}} \left( \prod_{v \in C(t) \setminus V} \alpha_{\phi''(v)} \right) \beta(t, \phi'') \\
&= \sum_{\psi: V \rightarrow [k]} \left( \prod_{v \in V} \alpha_{\psi(v)} \right) \sum_{\substack{\phi': C(s') \rightarrow [k] \\ \phi'|V=\psi}} \left( \prod_{v \in C(s') \setminus V} \alpha_{\phi'(v)} \right) \beta(s', \phi') \\
&\quad \cdot \sum_{\substack{\phi'': C(t) \rightarrow [k] \\ \phi''|V=\psi}} \left( \prod_{v \in C(t) \setminus V} \alpha_{\phi''(v)} \right) \beta(t, \phi'') \\
&= \sum_{\psi: V \rightarrow [k]} \left( \prod_{v \in V} \alpha_{\psi(v)} \right) \sum_{\substack{\phi': C(s) \rightarrow [k] \\ \phi'|V=\psi}} \left( \prod_{v \in C(s) \setminus V} \alpha_{\phi'(v)} \right) \beta(s^*, \phi') \\
&\quad \cdot \sum_{\substack{\phi'': C(t) \rightarrow [k] \\ \phi''|V=\psi}} \left( \prod_{v \in C(t) \setminus V} \alpha_{\phi''(v)} \right) \beta(t, \phi'') \\
&= \sum_{\psi: V \rightarrow [k]} \left( \prod_{v \in V} \alpha_{\psi(v)} \right) \sum_{\substack{\phi': C(s) \rightarrow [k] \\ \phi'|V=\psi}} \left( \prod_{v \in C(s) \setminus V} \alpha_{\phi'(v)} \right) \overline{\beta(s, \phi')} \\
&\quad \cdot \sum_{\substack{\phi'': C(t) \rightarrow [k] \\ \phi''|V=\psi}} \left( \prod_{v \in C(t) \setminus V} \alpha_{\phi''(v)} \right) \beta(t, \phi'').
\end{aligned}$$

Since the third sum is the complex conjugate of the second, this proves that  $M_n$  is positive semidefinite and has rank at most  $k^{|V|}$ .

The necessity part of Theorem 2 follows similarly; the only argument to add is that  $f$  is invariant under unlabeled, which is straightforward.

## 9. Reduction of Theorem 1 to Theorem 2

We may assume that  $f \not\equiv 0$ . Consider the matrix  $M_0$ . By assumption  $M_0$  has rank at most  $k^0 = 1$ . Since  $f(e_\emptyset) = 1$ , we know that  $(M_0)_{1,1} = 1$ . So  $M_0$  has rank 1. As  $f(s) := (M_0)_{1,s}$  for each  $s \in S_0$ , we know (by the symmetry) that, for all  $s, t \in S$ ,

$$(20) \quad f(st) = f(s)f(t) \text{ if } C(s) \cap C(t) = \emptyset$$

(since  $f(st) = f((s^*)^*t) = (M_0)_{s^*,t} = (M_0)_{s^*,1}(M_0)_{1,t} = \overline{(M_0)_{1,s^*}}(M_0)_{1,t} = \overline{f(s^*)}f(t) = f(s)f(t)$ ).

Since  $M_1$  is positive semidefinite, we know that for any  $z \in Z$ ,  $f(e_{\{z\}}) = f(e_{\{z\}}^2) \geq 0$ . Suppose  $f(e_{\{z\}}) = 0$ . Then  $f(s) = 0$  for each  $s$  with  $C(s) \neq \emptyset$ . Indeed, we can assume that  $z \in C(s)$ , by relabeling. By the positive semidefiniteness of  $M_1$ , we know that  $f(e_{\{z\}}^2) = 0$  implies  $f(se_{\{z\}}) = 0$ , hence  $f(s) = 0$ . Taking  $\alpha_i = 0$  for all  $i \in [k]$ , and  $\beta_s(\phi) = f(s)$  for each  $s \in S$  and each  $\phi : C(s) \rightarrow [k]$  gives the required state model. So we can assume that  $f(e_{\{z\}}) = c > 0$  for each  $z \in Z$  (this value is independent of  $z$  by relabeling invariance). Then we can reset each  $f(s)$  to

$$(21) \quad f(s) := f(s)/c^{|C(s)|}.$$

(This affects neither the condition nor the conclusion of the theorem.) In particular, we may assume that

$$(22) \quad f(e_{\{z\}}) = 1$$

for each  $z \in Z$ , and this implies by (20) that for each  $U \in F$ :

$$(23) \quad f(e_U) = 1.$$

Moreover, for each  $s \in S$  and  $U \in F$ :

$$(24) \quad f(e_U s) = f(s),$$

since, setting  $U' := U \setminus C(s)$  and  $U'' := U \cap C(s)$ , we have  $f(e_U s) = f(e_{U'} e_{U''} s) = f(e_{U'} s) = f(e_{U'}) f(s) = f(s)$ , using (20).

Next we show that

$$(25) \quad M(f) \text{ is positive semidefinite.}$$

Indeed, choose  $p \in \mathbb{C}^S$  with finite support. Choose a  $U \in F$  such that  $U \supseteq C(s)$  for each  $s \in S$  with  $p_s \neq 0$ . Then

$$(26) \quad (p^*)^\top M p = \sum_{s,t \in S} \bar{p}_s p_t f(s^* t) = \sum_{s,t \in S} \bar{p}_s p_t f((e_U s)^* (e_U t)) \geq 0,$$

since the matrix  $M|_{|U|}$  is positive semidefinite.

After these preparations, we can extend the semigroup with new elements so that the unlabeled operator can be defined on the new semigroup.

Let  $\mathcal{S}$  be the collection of all pairs  $(s, X)$  with  $s \in S$  and  $X \subseteq C(s)$ . Define an equivalence relation  $\sim$  on  $\mathcal{S}$  by

$$(27) \quad (s, X) \sim (s', X') \iff X = X' \text{ and there is a bijection } \pi : Z \rightarrow Z \text{ stabilizing all elements of } X \text{ such that } s' = \tilde{\pi}(s).$$

Let  $\mathcal{S}_0$  be the set of equivalence classes, and  $[(s, X)]$  denote the equivalence class containing  $(s, X)$ . Define multiplication and conjugation on  $\mathcal{S}_0$  by

$$(28) \quad [(s, X)][(r, Y)] := [(sr, X \cup Y)], [s, X]^* := [s^*, X],$$

where we have chosen  $(s, X)$  and  $(r, Y)$  in their class in such a way that  $C(s) \cap C(r) = X \cap Y$ . This turns  $\mathcal{S}_0$  into a  $*$ -semigroup, which still contains the  $*$ -semigroup  $F$  in the obvious way. Defining  $C([(s, X)]) = X$  we get a carrier. Identifying any  $s \in S$  with the class  $[(s, C(s))]$  (which only consists of  $(s, C(s))$ ) embeds  $S$  into  $\mathcal{S}_0$ . Defining  $\lambda_U([(s, X)]) = [(s, U \cap X)]$  gives an unlabeled operator.

Define  $f_0([(s, X)]) := f(s)$  for each  $[(s, X)] \in \mathcal{S}_0$ ; then  $f_0$  is a function on  $\mathcal{S}_0$  invariant under unlabeled and satisfies the other conditions in Theorem 2. So we can represent  $f_0$  as an unlabeled-conform state model with  $k$  states. Restricting this to  $S$ , we get a representation of  $f$ .

## 10. Sufficiency in Theorem 2

Let  $R$  be the semigroup algebra of  $S$ . That is,  $R$  is the space of formal sums

$$(29) \quad \sum_{s \in S} p_s s$$

with  $p_s \in \mathbb{C}$  for  $s \in S$  and only finitely many nonzero, and with multiplication induced by the semigroup multiplication. We can turn  $R$  into a  $*$ -algebra by defining

$$(30) \quad \left( \sum_{s \in S} p_s s \right)^* := \sum_{s \in S} \bar{p}_s s^*.$$

We will identify vectors  $(p_s \mid s \in S)$  with formal sums  $\sum_{s \in S} p_s s$ . Extend  $f$  and the  $\lambda_U$  linearly to  $R$ .

Let  $M = M(f)$ , and define

$$(31) \quad N := \{x \in R \mid Mx = 0\} = \{x \in R \mid f(xs) = 0 \text{ for each } s \in S\}.$$

Since  $M$  is positive semidefinite, we have that

$$(32) \quad N \text{ is a } *\text{-ideal in } R.$$

Indeed, if  $p \in R$  and  $q \in N$ , then  $((pq)^*)^\top M(pq) = (p^* p^* q^*)^\top Mq = 0$ , so  $pq \in N$ . Moreover, if  $q \in N$ , then  $q^* \in N$ , since

$$(33) \quad q \in N^* \implies f(qs) = 0 \text{ for each } s \in S \implies f(q^*s) = 0 \text{ for each } s \in S \implies q^* \in N.$$

So the quotient space  $A := R/N$  is a  $*$ -algebra with inner product

$$(34) \quad \langle x, y \rangle := (\bar{x})^\top My = f(x^*y).$$

We encode the elements of  $A$  just by elements of  $R$ , but write  $x \equiv y$  if and only if  $x - y \in N$ . Then

$$(35) \quad e_U \equiv e_\emptyset$$

for each  $U \in F$ , since  $f(e_U s) = f(s) = f(e_\emptyset s)$  for each  $s \in S$ .

Since  $f(x) = f(y)$  if  $x - y \in N$ , the function  $f$  is well defined on  $A$ . For each  $p \in A$  we have

$$(36) \quad f(p) = \langle p, e_\emptyset \rangle.$$

Recall that  $S_V = \{s \in S \mid C(s) = V\}$ , and let  $A_V$  be the subalgebra of  $A$  generated by the elements of  $S_V$ . Since (by assumption) the  $S_V \times S_V$  submatrix of  $M$  has rank at most  $k^{|V|}$ ,  $A_V$  has dimension at most  $k^{|V|}$ .

The unlabeled operator can also be defined in  $A$ . For this, we have to show that if  $x \equiv y$ , then  $\lambda_U x \equiv \lambda_U y$ . Since the operator  $\lambda_U$  is linear, it suffices to prove that if  $x \equiv 0$ , then  $\lambda_U x \equiv 0$ . Indeed, for every  $t \in S$ , using (10)(v),

$$\begin{aligned} \langle \lambda_U(x), t \rangle &= f(\lambda_U(x)t) = f(\lambda_U(\lambda_U(x)t)) \\ &= f(\lambda_U(x)\lambda_U(t)) = f(\lambda_U(x\lambda_U(t))) = f(x\lambda_U(t)) = 0. \end{aligned}$$

This proves that  $\lambda_U(x) \equiv 0$ .

*Claim 1.*  $A_V$  has a basis  $B_V$  consisting of self-adjoint idempotents with  $pq = 0$  for distinct  $p, q \in B_V$ . This basis is unique.

*Proof.* For each  $q \in A_V$  define  $\psi_q : A_V \rightarrow A_V$  by  $\psi_q(p) := qp$  for  $p \in A_V$ . Then the  $\psi_q$  are linear, and they commute. Moreover, for each  $q$ ,  $\psi_{q^*}$  is equal to the conjugate transformation of  $\psi_q$  (that is,  $\langle \psi_q(p), r \rangle = \langle p, \psi_{q^*}(r) \rangle$  for all  $p, q, r$ ).

Moreover, if  $\psi_q \equiv 0$ , then  $q = 0$ . Indeed, if  $\psi_q \equiv 0$ , then  $qe_V \in N$ , hence (since  $qe_V \equiv q$ )  $q \in N$ .

So the  $\psi_q$  form a space of commuting linear transformations, closed under conjugation. Hence the  $\psi_q$  have a common orthogonal basis of eigenvectors  $p_1, \dots, p_n$ , with  $n = \dim(A_V)$ . Then  $p_i p_j$  is a multiple of both  $p_i$  and  $p_j$ , hence if  $i \neq j$  it is 0. Moreover,  $p_i^2$  is nonzero, since otherwise  $\psi_{p_i} \equiv 0$ . So we can normalize the  $p_i$  such that  $p_i^2 = p_i$ . This makes the set

$$(37) \quad B_V := \{p_i \mid i = 1, \dots, n\}$$

unique.

Also,  $p^* = p$  for each  $p \in B_V$ , since for each  $q \in B_V$  with  $q \neq p$  one has  $\langle q, p^* \rangle = \langle qp, e_V \rangle = 0 = \langle q, p \rangle$ . Hence  $p^* = \lambda p$  for some nonzero  $\lambda \in \mathbb{C}$ . Taking squares at both sides, we see  $\lambda^2 = \lambda$ , hence  $\lambda = 1$ .  $\square$

It follows that

$$(38) \quad e_V = \sum_{p \in B_V} p,$$

since both terms are the unit of  $A_V$ .

So for  $p \in B_V$  we have  $f(p) > 0$ , since

$$(39) \quad f(p) = \langle p, 1 \rangle = \langle p^2, 1 \rangle = \langle p, p \rangle > 0.$$

(35) implies

$$(40) \quad \text{if } V \subseteq T \text{ then } A_V \subseteq A_T.$$

Indeed, for each  $s \in S_V$  we have  $s = e_T s \in A_T$ . So  $S_V \subseteq A_T$ , hence  $A_V \subseteq A_T$ .

Define for any  $p$ :

$$(41) \quad B_{T,p} = \{q \in B_T \mid pq = q\}.$$

Then for each  $p \in B_V$  with  $V \subseteq T$  one has

$$(42) \quad p = \sum_{q \in B_{T,p}} q.$$

Indeed, as  $p$  is in  $A_T$ , it is a linear combination of the elements of  $B_T$ , and as it is an idempotent, it is a sum of some of the elements in  $B_T$ , hence of those  $q \in B_T$  with  $pq = q$ .

For distinct  $p, p' \in B_V$ , one has  $pp' = 0$ , hence  $B_{T,p} \cap B_{T,p'} = \emptyset$ . Since  $\sum_{q \in B_T} q = 1 = \sum_{p \in B_V} p$ , the collection  $\{B_{T,p} \mid p \in B_V\}$  is a partition of  $B_T$ .

*Claim 2.* Let  $T, U \in F$ , and let  $V := T \cap U$ . Then for any  $p \in B_V$ ,  $q \in B_{T,p}$ , and  $r \in A_U$ :

$$(43) \quad f(qr) = \frac{f(q)}{f(p)} f(pr).$$

*Proof.* To prove this, we may assume that  $r \in S_U$ . Let  $\pi$  denote the orthogonal projection of  $A$  onto  $A_V$ . Then

$$(44) \quad f(qr) = f(\pi(q)r).$$

To see this, observe that for each  $s \in S_T$ ,  $\pi(s) = \lambda_V(s)$ . This follows from:

$$(45) \quad \langle s, t \rangle = f(s^*t) = f((\lambda_V(s^*))t) = \langle \lambda_V(s), t \rangle$$

for each  $t \in S_V$ . So  $\pi(s) = \lambda_V(s)$ , and hence, by (10),  $f(sr) = f(\pi(s)r)$ . (Indeed,  $f(sr) = f(\lambda_U(sr)) = f(\lambda_U(s)\lambda_U(r)) = f(\lambda_U(s)r) = f(\lambda_U(\lambda_T(s))r) = f(\lambda_{U \cap T}(s)r) = f(\lambda_V(s)r)$ .) As this holds for each  $s \in S_T$ , and as  $q \in A_T$  we have (44).

Moreover,

$$(46) \quad \pi(q) = \frac{f(q)}{f(p)}p.$$

This follows from the facts that if  $p' \in B_V$  with  $p' \neq p$ , then  $\langle \frac{f(q)}{f(p)}p, p' \rangle = 0 = \langle q, p' \rangle$ , and that  $\langle \frac{f(q)}{f(p)}p, p \rangle = f(q) = \langle q, p \rangle$ . This proves (46), which together with (44) gives the claim.  $\square$

For any  $V \in F$  and any  $p \in B_V$ , denote  $\deg(p) = |B_{T,p}|$ , where  $T$  is any subset of  $Z$  with  $V \subseteq T$  and  $|T \setminus V| = 1$ . Note that (by the symmetry) the definition of  $\deg(p)$  is independent of the choice of  $T$ .

*Claim 3.* If  $q \in B_{T,p}$ , then  $\deg(q) \geq \deg(p)$ .

*Proof.* Consider a set  $W \supset T$  with  $|W \setminus T| = 1$ . Let  $T = V \cup \{t\}$  and  $W = T \cup \{u\}$ . Define  $U := V \cup \{u\}$ . Then for each  $r \in B_{U,p}$ ,  $qr$  is an idempotent in  $A_W$ , and it is the sum of the elements of  $B_{W,q} \cap B_{W,r}$ . Moreover,  $qr \neq 0$ , since (using Claim 2)

$$(47) \quad f(qr) = \frac{f(q)f(r)}{f(p)} \neq 0.$$

So  $B_{W,q} \cap B_{W,r} \neq \emptyset$  for each  $r \in B_{U,p}$ . Since these sets are disjoint (for distinct  $r \in B_{T,p}$ ), we have

$$(48) \quad \deg(q) = |B_{W,q}| \geq |B_{U,p}| = \deg(p),$$

proving the claim.  $\square$

This implies that  $\deg(p) \leq k$  for each  $V$  and  $p \in B_V$ , since

$$(49) \quad \deg(p)^{|T \setminus V|} \leq |B_{T,p}| \leq |B_T| = \dim(A_T) \leq k^{|T|}$$

for each  $T \supseteq V$ .

So we can choose a set  $V \in F$  and  $p \in B_V$  with  $\deg(p)$  maximal, and we can assume that  $\deg(p) = k$  (as the conclusion of the theorem is maintained if we increase  $k$ ). For the remainder of this proof we fix  $V$  and  $p$ .

Let  $W := Z \setminus V$  and, for each  $v \in W$ , let

$$(50) \quad B_{V \cup \{v\}, p} = \{q_{v,1}, \dots, q_{v,k}\},$$

choosing indices such that  $q_{v,i}$  arises from  $q_{u,i}$  by mapping  $u$  to  $v$ , leaving  $V$  invariant. For  $i \in [k]$ , define (choosing an arbitrary  $v \in W$ )

$$(51) \quad \alpha_i := \frac{f(q_{v,i})}{f(p)}.$$

This is independent of the choice of  $v \in W$ . Since  $f(q_{v,i}) > 0$  and  $f(p) > 0$  we have  $\alpha_i > 0$ .

For any finite subset  $U$  of  $W$  and any  $\phi : U \rightarrow [k]$ , consider

$$(52) \quad r_\phi := p \prod_{v \in U} q_{v, \phi(v)}.$$

(The factor  $p$  is superfluous if  $U \neq \emptyset$ .) Since  $r_\phi^2 = r_\phi$  and  $pr_\phi = r_\phi$ , we know that  $r_\phi = \sum_{q \in L_\phi} q$  for some subset  $L_\phi$  of  $B_{V \cup U, p}$ . Also,  $r_\phi \neq 0$ , since (using Claim 2 repeatedly)

$$(53) \quad f(r_\phi) = f\left(p \prod_{v \in U} q_{v, \phi(v)}\right) = \left(\prod_{v \in U} \alpha_{\phi(v)}\right) f(p) \neq 0.$$

So  $r_\phi \neq 0$ , implying  $L_\phi \neq \emptyset$ .

Moreover, if  $\phi \neq \phi'$ , then  $r_\phi r_{\phi'} = 0$  (since if  $\phi(v) \neq \phi'(v)$ , then  $q_{v,\phi(v)} q_{v,\phi'(v)} = 0$ ). So if  $\phi \neq \phi'$ , then  $L_\phi \cap L_{\phi'} = \emptyset$ . Hence, since  $|B_{V \cup U, p}| = k^{|U|}$  (by Claim 3), we know that  $|L_\phi| = 1$  for each  $\phi : U \rightarrow [k]$ . Therefore,

$$(54) \quad B_{V \cup U, p} = \{r_\phi \mid \phi : U \rightarrow [k]\}.$$

Now, for any  $s \in S$  with  $C(s) \subseteq W$ , we can express  $ps$  in the elements of  $B_{V \cup C(s), p}$ :

$$(55) \quad ps = \sum_{\phi: C(s) \rightarrow [k]} \beta_s(\phi) r_\phi.$$

This is possible, since for any  $r \in B_{V \cup C(s)}$  with  $r \notin B_{V \cup C(s), p}$  one has  $rps = 0$ , since  $rp = 0$ .

By the symmetry, this definition of  $\beta_s$  extends to all  $s \in S$ . We show that the  $\beta_s$  satisfy (11).

To see (11)(i), we have

$$(56) \quad \begin{aligned} f(p)f(s) &= f(ps) = f\left(\sum_{\phi: C(s) \rightarrow [k]} \beta_s(\phi) r_\phi\right) = \\ &= \sum_{\phi: C(s) \rightarrow [k]} \beta_s(\phi) f(r_\phi) = \sum_{\phi: C(s) \rightarrow [k]} \beta_s(\phi) \left(\prod_{v \in C(s)} \alpha_{\phi(v)}\right) f(p) = \\ &= f(p) \sum_{\phi: C(s) \rightarrow [k]} \left(\prod_{v \in C(s)} \alpha_{\phi(v)}\right) \beta_s(\phi) \end{aligned}$$

(the first equality follows from (20), using the facts that  $p \in A_V$  and that  $V \cap C(s) = \emptyset$ ). Since  $f(p) \neq 0$ , this gives (11)(i).

To see (11)(ii), first note that if  $\phi : C(st) \rightarrow [k]$ , then

$$(57) \quad r_\phi = r_{\phi|C(s)} r_{\phi|C(t)},$$

as follows from (52). Hence, for all  $s, t \in S$  one has

$$(58) \quad \begin{aligned} \sum_{\phi: C(st) \rightarrow [k]} \beta_s(\phi|C(s)) \beta_t(\phi|C(t)) r_\phi &= \\ \sum_{\phi: C(st) \rightarrow [k]} \beta_s(\phi|C(s)) \beta_t(\phi|C(t)) r_{\phi|C(s)} r_{\phi|C(t)} &= \end{aligned}$$

$$\left( \sum_{\phi': C(s) \rightarrow [k]} \beta_s(\phi') r_{\phi'} \right) \left( \sum_{\phi'': C(t) \rightarrow [k]} \beta_t(\phi'') r_{\phi''} \right) = (ps)(pt) = p(st)$$

(note that  $r_{\phi'} r_{\phi''} = 0$  if  $\phi'|C(s) \cap C(t) \neq \phi''|C(s) \cap C(t)$ ). Hence for each  $\phi : C(st) \rightarrow [k]$  one has

$$(59) \quad \beta_{st}(\phi) = \beta_s(\phi|C(s))\beta_t(\phi|C(t)),$$

which is (11)(ii). Condition (11)(iii) follows from the symmetry and uniqueness of the  $\beta_s(\phi)$ . Finally, we have  $\beta_{s^*}(\phi) = \overline{\beta_s(\phi)}$  from (55), since  $p^* = p$  and  $r_{\phi}^* = r_{\phi}$ .  $\blacksquare$

## 11. Applications to graph and hypergraph parameters

We apply Theorem 1 to the Examples 1–5 mentioned above. First we derive the theorem given in Freedman, Lovász, and Schrijver [4].

Let  $f$  be a real-valued function defined on the collection of undirected graphs, invariant under isomorphisms. Define, for each natural number  $n$ , the matrix  $M_{f,n}$  as follows. Fix  $n \geq 0$ , and let  $\mathcal{G}_n$  be the set of all undirected graphs  $G$  with  $VG \cap Z = Z_n$ . Let  $M_{f,n}$  be the  $\mathcal{G}_n \times \mathcal{G}_n$  matrix with entry  $f(G \cup G')$  in position  $G, G'$ . Here, in making the union, we first make the vertex sets of  $G$  and  $G'$  disjoint outside  $Z_n$ .

For any integer  $k \geq 0$ , any vector  $\alpha \in \mathbb{R}_+^k$ , and any  $k \times k$  real symmetric matrix  $(\beta_{i,j})$ , define the undirected graph parameter  $f_{\alpha,\beta}$  as in (1).

**Corollary 1.** *Let  $f$  be a complex-valued undirected graph parameter and  $k \geq 0$ . Then  $f = f_{\alpha,\beta}$  for some  $\alpha \in \mathbb{R}_+^k$  and some symmetric real-valued  $k \times k$  matrix  $(\beta_{i,j})$  if and only if  $f(K_0) = 1$  and, for each  $n$ ,  $M_{f,n}$  is positive semidefinite and has rank at most  $k^n$ .*

**Proof.** Apply the theorem to the  $*$ -semigroup consisting of all undirected graphs, with multiplication  $GG' := G \cup G'$  and conjugation  $G^* := G$ .

Note that  $K_2$  and its images under automorphisms generate the  $*$ -semigroup, so the functions  $\beta_G$  are determined by the function  $\beta_{K_2}$ , which can be described by a  $k \times k$  matrix. The fact that  $\beta_{K_2}$  is real follows from the fact that  $\beta_{K_2} = \beta_{K_2^*} = \overline{\beta_{K_2}}$ .  $\blacksquare$

The property that  $M_{f,n}$  is positive semidefinite for each  $n$  is called *re-*

*flection positivity* of  $f$ . Moreover, the property that there is an integer  $k$  such that for each  $n$ ,  $M_{f,n}$  has rank at most  $k^n$ , is called *rank connectivity* of  $f$ .

For simple graphs we obtain a similar characterization if we restrict  $\beta$  to  $0, 1$  matrices. For a function  $f$  defined on the collection  $\tilde{\mathcal{G}}$  of *simple* finite undirected graphs, let (for  $n \in \mathbb{N}$ )  $\tilde{M}_{f,n}$  be the  $\tilde{\mathcal{G}} \times \tilde{\mathcal{G}}$  matrix with entry  $f(G \cup G')$  in position  $G, G'$ , where now we do not take multiplicities into account. Then we obtain:

**Corollary 2.** *Let  $f$  be a complex-valued undirected simple graph parameter and  $k \geq 0$ . Then  $f = f_{\alpha,\beta}$  for some  $\alpha \in \mathbb{R}_+^k$  and some symmetric  $k \times k$   $0, 1$  matrix  $(\beta_{i,j})$  if and only if  $f(K_0) = 1$  and, for each  $n$ ,  $\tilde{M}_{f,n}$  is positive semidefinite and has rank at most  $k^n$ .*

**Proof.** The proof is similar to that of Corollary 1. Now we have that the graph  $K_2$  on vertices  $1, 2$  (say) satisfies, for any  $\phi : \{1, 2\} \rightarrow [k]$ :

$$(60) \quad (\beta_{K_2}(\phi))^2 = \beta_{K_2}(\phi)\beta_{K_2}(\phi) = \beta_{K_2K_2}(\phi) = \beta_{K_2}(\phi).$$

Hence  $\beta_{K_2}(\phi) \in \{0, 1\}$ . ■

We next turn to directed graphs. Let  $f$  be a complex-valued function defined on the collection of directed graphs, invariant under isomorphisms. Define, for each natural number  $n$ , matrices  $M_{f,n}$  and  $M'_{f,n}$  as follows. Fix  $n \geq 0$ , and let  $\mathcal{G}_n$  be the set of all directed graphs  $G$  with  $VG \cap Z = Z_n$ . For any directed graph  $G$ , let  $G^{-1}$  be the directed graph obtained from  $G$  by reversing all arcs. Let  $M_{f,n}$  be the  $\mathcal{G}_n \times \mathcal{G}_n$  matrix with entry  $f(G \cup G')$  in position  $G, G'$ . Let  $M'_{f,n}$  be the  $\mathcal{G}_n \times \mathcal{G}_n$  matrix with entry  $f(G^{-1} \cup G')$  in position  $G, G'$ . Again, in making the union, we first make the vertex sets of  $G$  and  $G'$  disjoint outside  $Z_n$ .

For any integer  $k \geq 0$ , any vector  $\alpha \in \mathbb{C}^k$ , and any  $k \times k$  complex matrix  $(\beta_{i,j})$ , define the directed graph function  $f_{\alpha,\beta}$  by:

$$(61) \quad f_{\alpha,\beta}(G) = \sum_{\phi: VG \rightarrow [k]} \left( \prod_{v \in VG} \alpha_{\phi(v)} \right) \left( \prod_{(u,v) \in EG} \beta_{\phi(u), \phi(v)} \right).$$

**Corollary 3.** *Let  $f$  be a directed graph parameter and  $k \geq 0$ . Then  $f = f_{\alpha,\beta}$  for some  $\alpha \in \mathbb{R}_+^k$  and some real-valued  $k \times k$  matrix  $(\beta_{i,j})$  if and only if  $f(K_0) = 1$  and, for each  $n$ ,  $M_{f,n}$  is positive semidefinite and has rank at*

most  $k^n$ .

**Proof.** Apply the theorem to the \*-semigroup consisting of all directed graphs, with multiplication  $GG' := G \cup G'$  and conjugation  $G^* := G$ . In this case,  $\beta_{i,j}$  is real, since  $\beta_{\vec{K}_2} = \beta_{\vec{K}_2^*} = \overline{\beta_{\vec{K}_2}}$ .  $\blacksquare$

**Corollary 4.** *Let  $f$  be a directed graph parameter and  $k \geq 0$ . Then  $f = f_{\alpha,\beta}$  for some  $\alpha \in \mathbb{R}_+^k$  and some Hermitian  $k \times k$  matrix  $(\beta_{i,j})$  if and only if  $f(K_0) = 1$  and, for each  $n$ ,  $M'_{f,n}$  is positive semidefinite and has rank at most  $k^n$ .*

**Proof.** Apply the theorem to the \*-semigroup consisting of all directed graphs, with multiplication  $GG' := G \cup G'$  and conjugation  $G^* := G^{-1}$ .

In this case we have  $\beta_{j,i} = \overline{\beta_{i,j}}$ , since  $\beta_{\vec{K}_2^{-1}} = \beta_{\vec{K}_2^*} = \overline{\beta_{\vec{K}_2}}$ .  $\blacksquare$

Finally we consider applying Theorem 1 to hypergraphs. Let  $\mathcal{H}$  be the collection of  $m$ -uniform hypergraphs and let  $f : \mathcal{H} \rightarrow \mathbb{C}$ . Choose  $k \in \mathbb{Z}_+$ . Let  $\alpha : [k] \rightarrow \mathbb{R}_+$  and let  $\beta : [k]^m \rightarrow \mathbb{R}$  be symmetric (that is, invariant under permuting coordinates of  $[k]^m$ ). Define

$$(62) \quad f_{\alpha,\beta}(H) := \sum_{\phi: VH \rightarrow [k]} \left( \prod_{v \in VH} \alpha_{\phi(v)} \right) \left( \prod_{e \in EH} \beta_{\phi(e)} \right)$$

where  $\beta_{\phi(\{v_1, \dots, v_m\})} := \beta(\phi(v_1), \dots, \phi(v_m))$ .

For any complex-valued hypergraph parameter  $f$  and any  $n \in \mathbb{Z}_+$ , let  $M_{f,n}$  be the following matrix. Let  $\mathcal{H}_n$  be the collection of hypergraphs  $H$  with  $VH \cap Z = Z_n$ . For  $H, H' \in \mathcal{H}_n$  let  $H \cup H'$  be the union of  $H$  and  $H'$ , assuming that  $VH \cap VH' = Z_n$  and  $EH \cap EH' = \emptyset$  (that is, edges of  $H$  and  $H'$  that span the same subset of  $VH \cap VH'$ , are considered to be distinct and give multiple edges in  $H \cup H'$ ). Let  $M_{f,n}$  be the  $\mathcal{H}_n \times \mathcal{H}_n$  matrix with  $(M_{f,n})_{H,H'} := f(H \cup H')$  for  $H, H' \in \mathcal{H}_n$ .

Then (where  $H_0$  denotes the hypergraph with no vertices and edges):

**Corollary 5.** *Let  $f$  be a complex-valued parameter on  $m$ -uniform hypergraphs and  $k \geq 0$ . Then  $f = f_{\alpha,\beta}$  for some  $\alpha : [k] \rightarrow \mathbb{R}_+$  and some symmetric  $\beta : [k]^m \rightarrow \mathbb{R}$  if and only if  $f(H_0) = 1$  and for each  $n$ , the matrix  $M_{f,n}$  is positive semidefinite and has rank at most  $k^n$ .*

**Proof.** Apply the theorem to the \*-semigroup consisting of all hypergraphs, with multiplication  $HH' := H \cup H'$  and conjugation  $H^* := H$ .

Now the  $\beta_H$  are determined by  $\beta_{H_m}$ . Moreover,  $\beta_{H_m}$  is real-valued, since  $\beta_{H_m} = \beta_{H_m^*} = \overline{\beta_{H_m}}$ . ■

We leave it to the reader to formulate the application of Theorem 1 to Example 5.

## 12. Application to positive definite \*-semigroup functions

Let  $S$  be a commutative \*-semigroup with unit 1. For any function  $f : S \rightarrow \mathbb{C}$ , define the  $S \times S$  matrix  $M_f$  by:

$$(63) \quad (M_f)_{s,t} := f(s^*t)$$

for  $s, t \in S$ . The function  $f : S \rightarrow \mathbb{C}$  is called *positive definite* if  $M_f$  is positive semidefinite. This implies that  $f(s^*) = \overline{f(s)}$  for each  $s \in S$ , since positive semidefiniteness of  $M_f$  implies that  $M_f$  is Hermitian.

It can be checked easily that each \*-semicharacter is positive definite. Under certain conditions, all positive definite functions on  $S$  can be obtained from \*-semicharacters as follows ([5], [1], and [3] (cf. [2])).

We can equip  $S^*$  with the topology of pointwise convergence. Let  $f : S \rightarrow \mathbb{C}$ . Then there exists a Radon measure  $\mu$  on  $S^*$  with compact support such that

$$(64) \quad f = \int_{S^*} \chi d\mu(\chi)$$

if and only if  $f$  is positive definite and is *exponentially bounded* — this means that there exists a function  $|\cdot| : S \rightarrow \mathbb{R}_+$  satisfying  $|1| = 1$ ,  $|st| \leq |s||t|$ ,  $|s^*| = |s|$ , and  $|f(s)| \leq |s|$  for all  $s, t \in S$ .

It can be shown moreover that if  $M_f$  has finite rank  $k$ , then  $\mu$  is a sum of  $k$  Dirac measures. This follows directly from our method of proof. But it can also be derived from Theorem 1, as follows. Let  $S$  be a commutative \*-semigroup  $S$  with unit 1. Let

$$(65) \quad S' := \{\phi \mid \phi : V \rightarrow S \text{ for some } V \in F\}.$$

Let  $\text{dom}(\phi)$  denote the domain of any function  $\phi$ . For  $\phi, \psi \in S'$ , define  $\phi\psi$  be the function from  $\text{dom}(\phi) \cup \text{dom}(\psi) \rightarrow S$  defined by  $\phi\psi(i) := \phi(i)\psi(i)$ ,

taking  $\phi(i)$  or  $\psi(i)$  to be equal to 1 if it is undefined. Define a carrier  $C : S' \rightarrow \mathcal{P}(Z)$  by  $C(\phi) := \text{dom}(\phi)$  for  $\phi \in S'$ . For any function  $f : S \rightarrow \mathbb{C}$  define  $f' : S' \rightarrow \mathbb{C}$  by  $f'(\phi) := \prod_{i \in \text{dom}(\phi)} f(\phi(i))$ . Then  $M_f$  is positive semidefinite and has rank at most  $k$  if and only if  $f$  satisfies the conditions in Theorem 1. The conclusion then gives the characterization mentioned above.

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