# Graph invariants in the spin model

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**Abstract.** Given a symmetric $n \times n$ matrix $A$, we define, for any graph $G$,

$$f_A(G) := \sum_{\phi: VG \to \{1,\ldots,n\}} \prod_{uv \in EG} a_{\phi(u),\phi(v)}.$$

We characterize for which graph parameters $f$ there is a complex matrix $A$ with $f = f_A$, and similarly for real $A$. We show that $f_A$ uniquely determines $A$, up to permuting rows and (simultaneously) columns. The proofs are based on the Nullstellensatz and some elementary invariant-theoretic techniques.

## 1. Introduction

Let $\mathcal{G}$ denote the collection of all finite graphs, allowing loops and multiple edges, and considering two graphs the same if they are isomorphic. A *graph invariant* is a function $f : \mathcal{G} \to \mathbb{C}$.

We characterize the following type of graph invariants. Let $n \in \mathbb{N}$ and let $A = (a_{i,j})$ be a symmetric complex $n \times n$ matrix. Define $f_A : \mathcal{G} \to \mathbb{C}$ by

$$(1) \qquad f_A(G) := \sum_{\phi: VG \to [n]} \prod_{uv \in EG} a_{\phi(u),\phi(v)}.$$

Here $VG$ and $EG$ denote the sets of vertices and edges of $G$, respectively. Any edge connecting vertices $u$ and $v$ is denoted by $uv$. (So if there are $k$ parallel vertices connecting $u$ and $v$, the term $a_{\phi(u),\phi(v)}$ occurs $k$ times.) Moreover,

$$(2) \qquad [n] := \{1, \ldots, n\} \text{ for any } n \in \mathbb{N}.$$

We give characterizations for $A$ complex and for $A$ real.

The graph invariants $f_A$ are motivated by parameters coming from mathematical physics and from graph theory. For instance, if $A = J - I$, where $J$ is the $n \times n$ all-one matrix and $I$ is the $n \times n$ identity matrix, then $f_A(G)$ is equal to the number of proper $n$-colorings of the vertices of $G$. If $A = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}$, then $f_A(G)$ is equal to the number of independent sets of $G$.

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In terms of mathematical physics, these are graph invariants in the 'spin model', where vertices can be in $n$ 'states' and the value is determined by the values taken on edges. This is opposite to the 'vertex model' (sometimes called 'edge model'!), where the roles of vertex and edge are interchanged (cf. Szegedy [6]). For motivation and more examples, see de la Harpe and Jones [2]. For related work, see Freedman, Lovász, and Schrijver [1], Lovász and Schrijver [3,4], and Lovász and Szegedy [5].

## 2. Survey of results

In order to characterize the graph invariants $f_A$, we call a graph invariant $f$ *multiplicative* if

$$(3) \qquad f(K_0) = 1 \text{ and } f(GH) = f(G)f(H) \text{ for all } G, H \in \mathcal{G}.$$

Here $K_0$ is the graph $G$ with no vertices and edges. Moreover, $GH$ denotes the disjoint union of graphs $G$ and $H$.

In the characterization we also need the Möbius function on partitions. Let $P$ be a partition of a finite set $X$; that is, $P$ is an (unordered) collection of disjoint nonempty subsets of $X$, with union $X$. The sets in $P$ are called the *classes* of $P$. Let $\Pi_X$ denote the set of partitions of $X$. If $Q$ and $P$ are partitions of $X$, then we put $Q \leq P$ if for each class $C$ of $Q$ there is a class of $P$ containing $C$. The *Möbius function* is the unique function $\mu_P$ defined on partitions $P$ satisfying

$$(4) \qquad \sum_{Q \leq P} \mu_Q = \delta_{P,T_X}$$

for any partition $P$ of $X$. Here $T_X$ denotes the trivial partition $\{\{v\} \mid v \in X\}$ of $X$, and $\delta_{P,T_X} = 1$ if $P = T_X$, and $\delta_{P,T_X} = 0$ otherwise.[2]

For any graph $G$ and any partition $P$ of $VG$, the graph $G/P$ is defined to be the graph with vertex set $P$ and with for each edge $uv \in EG$ an edge $C_uC_v$, where $C_u$ and $C_v$ are the classes of $P$ containing $u$ and $v$ respectively. (So in $G/P$ generally several loops and multiple edges will arise.)

Now we can formulate our first characterization:

**Theorem 1.** *Let $f : \mathcal{G} \to \mathbb{C}$. Then $f = f_A$ for some $n \in \mathbb{N}$ and some symmetric matrix $A \in \mathbb{C}^{n\times n}$ if and only if $f$ is multiplicative and*

[2]It can be seen that $\mu_P := \prod_{C\in P}(-1)^{|C|-1}(|C|-1)!$, but we do not need this expression.

$$(5) \qquad \sum_{P \in \Pi_{VG}} \mu_P f(G/P) = 0$$

*for each graph $G$ with $|VG| > f(K_1)$.*

Here $K_1$ is the graph $G$ with one vertex and no edges.

From Theorem 1 we derive a characterization of those $f_A$ with $A$ real. For $i \in \mathbb{N}$, let $K_2^i$ denote the graph with vertex set $\{1, 2\}$ and $i$ parallel edges connecting the two vertices.

**Corollary 1a.** *Let $f : \mathcal{G} \to \mathbb{R}$. Then $f = f_A$ for some $n \in \mathbb{N}$ and some symmetric matrix $A \in \mathbb{R}^{n\times n}$ if and only if the conditions of Theorem 1 hold and moreover the matrix*

$$(6) \qquad L_f := \left( f(K_2^{i+j}) \right)_{i,j=0}^{\frac{1}{2}m(m+1)}$$

*is positive semidefinite, where $m := \lfloor f(K_1) \rfloor$.*

The method of proof of this theorem is inspired by Szegedy [6]. As consequence of Corollary 1a we will derive the following characterization in terms of labeled graphs, that relates to a characterization of Freedman, Lovász, and Schrijver [1].

A *$k$-labeled graph* is a pair $(G, u)$ of a graph $G$ and an element $u$ of $VG^k$, i.e., a $k$-tuple of vertices of $G$. (The vertices in $u$ need not be different.) Let $\mathcal{G}_k$ denote the collection of $k$-labeled graphs. For two $k$-labeled graphs $(G, u)$ and $(H, w)$, let the graph $(G, u) * (H, w)$ be obtained by taking the disjoint union of $G$ and $H$, and next identifying $u_i$ and $w_i$, for $i = 1, \ldots, k$. (In other words, add for each $i = 1, \ldots, k$ a new edge connecting $u_i$ and $w_i$, and next contract each new edge.) Then $M_{f,k}$ is the $\mathcal{G}_k \times \mathcal{G}_k$ matrix defined by

$$(7) \qquad (M_{f,k})_{(G,u),(H,w)} := f((G, u) * (H, w))$$

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

**Corollary 1b.** *Let $f : \mathcal{G} \to \mathbb{R}$. Then $f = f_A$ for some $n$ and some symmetric matrix $A \in \mathbb{R}^{n\times n}$ if and only if $f$ is multiplicative and $M_{f,k}$ is positive semidefinite for each $k \in \mathbb{N}$.*

Here an infinite matrix is positive semidefinite if each finite principal submatrix is positive semidefinite. The positive semidefiniteness of the matrices $M_{f,k}$ can be viewed as a form of 'reflection positivity' of $f$.

As a consequence of Corollary 1b the following can be derived (as was noticed by Laci Lovász). Let $\widetilde{\mathcal{G}}$ denote the collection of graphs without parallel edges, but loops are allowed — at most one at each vertex. Let $\widetilde{\mathcal{G}}_k$ be the collection of $k$-labeled graphs $(G, u)$ with

$G \in \widetilde{\mathcal{G}}$. For $(G,u),(H,w) \in \widetilde{\mathcal{G}}_k$, let the graph $(G,u)\tilde{*}(H,w)$ be obtained from $(G,u)*(H,w)$ by replacing parallel edges by one edge. Then the $\widetilde{\mathcal{G}}_k \times \widetilde{\mathcal{G}}_k$ matrix $\widetilde{M}_{f,k}$ is defined by

$$(8) \qquad (\widetilde{M}_{f,k})_{(G,u),(H,w)} := f((G,u)\tilde{*}(H,w))$$

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

For $G, H \in \widetilde{\mathcal{G}}$, let $\hom(G,H)$ denote the number of homomorphisms $G \to H$ (that is, adjacency preserving functions $VG \to VH$). Let $\hom(\cdot, H)$ denote the function $G \mapsto \hom(G,H)$ for $G \in \widetilde{\mathcal{G}}$.

**Corollary 1c.** *Let $f : \widetilde{\mathcal{G}} \to \mathbb{R}$. Then $f = \hom(\cdot, H)$ for some $H \in \widetilde{\mathcal{G}}$ if and only if $f$ is multiplicative and $\widetilde{M}_{f,k}$ is positive semidefinite for each $k \in \mathbb{N}$.*

This sharpens a theorem of Lovász and Schrijver [4], where, instead of multiplicativity, more strongly it is required that there exists an $n \in \mathbb{N}$ such that for each $k \in \mathbb{N}$, the matrix $\widetilde{M}_{f,k}$ has rank at most $n^k$. So Corollary 1c states that we need to stipulate this only for $k = 0$.

The derivation of Corollary 1c is by applying Corollary 1b to the function $\hat{f} : \mathcal{G} \to \mathbb{R}$ with $\hat{f}(G) = f(\widetilde{G})$ for $G \in \mathcal{G}$, where $\widetilde{G}$ arises from $G$ by replacing parallel edges by one edge.

An interesting question is how these results relate to the following theorem of Freedman, Lovász, and Schrijver [1]. For any $b \in \mathbb{R}_+^n$ and any symmetric matrix $A = (a_{i,j}) \in \mathbb{C}^{n\times n}$, let $f_{b,A} : \mathcal{G} \to \mathbb{C}$ be defined by

$$(9) \qquad f_{b,A}(G) := \sum_{\phi: VG \to [n]} \left( \prod_{v \in VG} b_{\phi(v)} \right) \left( \prod_{uv \in EG} a_{\phi(u),\phi(v)} \right)$$

for any graph $G$. So $f_A = f_{\mathbf{1},A}$, where $\mathbf{1}$ denotes the all-one function on $[n]$.

Let $\mathcal{G}'$ denote the set of loopless graphs (but multiple edges are allowed). Consider any function $f : \mathcal{G}' \to \mathbb{R}$. For any $k$, let $M'_{f,k}$ be the submatrix of $M_{f,k}$ induced by the rows and columns indexed by those $k$-labeled graphs $(G,u)$ for which $G$ is loopless and all vertices in $u$ are distinct. Then in [1] the following is proved:

(10) Let $n \in \mathbb{N}$ and $f : \mathcal{G}' \to \mathbb{R}$. Then $f = f_{b,A}|\mathcal{G}'$ for some $b \in \mathbb{R}_+^n$ and some symmetric matrix $A \in \mathbb{R}^{n\times n}$ if and only if $f(K_0) = 1$ and $M'_{f,k}$ is positive semidefinite and has rank at most $n^k$, for each $k \in \mathbb{N}$.

The proof in [1] is also algebraic (based on finite-dimensional commutative algebra and on idempotents), but rather different from the proof scheme given in the present paper (based on the Nullstellensatz and on invariant-theoretic methods). It is unclear if both results (Corollary 1b and (10)) can be proved by one common method.

Back to $\mathcal{G}$ and $f_A$, we will show as a side result that $f_A$ uniquely determines $A$, up to permuting rows and (simultaneously) columns:

**Theorem 2.** *Let $A \in \mathbb{C}^{n\times n}$ and $A' \in \mathbb{C}^{n'\times n'}$ be symmetric matrices. Then $f_A = f_{A'}$ if and only if $n = n'$ and $A' = P^{\mathsf{T}}AP$ for some $n \times n$ permutation matrix $P$.*

So if $H$ and $H'$ are graphs in $\widetilde{\mathcal{G}}$ with $\hom(\cdot, H) = \hom(\cdot, H')$, then $H$ and $H'$ are isomorphic.

The proofs of these theorems are based on the Nullstellensatz and on some elementary invariant-theoric methods. A basic tool is the following theorem. For $n \in \mathbb{N}$, introduce variables $x_{i,j}$ for $1 \le i \le j \le n$. If $i > j$, let $x_{i,j}$ denote the same variable as $x_{j,i}$. So, in fact, we introduce a symmetric variable matrix $X = (x_{i,j})$, and we can write $\mathbb{C}[X]$ for $\mathbb{C}[x_{1,1}, x_{1,2}, \dots, x_{n,n}]$. For any graph $G$, let $p_n(G)$ be the following polynomial in $\mathbb{C}[X]$:

$$p_n(G) := \sum_{\phi:VG\to[n]} \prod_{uv\in EG} x_{\phi(u),\phi(v)}. \tag{11}$$

So $p_n(G)(A) = f_A(G)$ for any symmetric matrix $A \in \mathbb{C}^{n\times n}$.

The symmetric group $S_n$ acts on $\mathbb{C}[X]$ by $x_{i,j} \mapsto x_{\pi(i),\pi(j)}$ for $i, j \in [n]$ and $\pi \in S_n$. As usual, $\mathbb{C}[X]^{S_n}$ denotes the set of polynomials in $\mathbb{C}[X]$ that are invariant under the action of $S_n$. In other words, $\mathbb{C}[X]^{S_n}$ consists of all polynomials $p(X)$ with $p(P^{\mathsf{T}}XP) = p(X)$ for each $n \times n$ permutation matrix $P$. It turns out to be equal to the linear hull of the polynomials $p_n(G)$:

**Theorem 3.** $\mathrm{lin}\{p_n(G) \mid G \in \mathcal{G}\} = \mathbb{C}[X]^{S_n}$.

We first prove Theorem 3 and after that Theorem 1, from which we derive Corollaries 1a, 1b, and 1c. Finally we show Theorem 2. Theorem 3 is used in the proof of Theorems 1 and 2. We start with a few sections with preliminaries.

## 3. Quantum graphs

A *quantum graph* is a formal linear combination of finitely many distinct graphs, i.e., it is

$$\sum_{G\in\mathcal{G}} \gamma_G G, \tag{12}$$

where $\gamma_G \in \mathbb{C}$ for each $G \in \mathcal{G}$, with $\gamma_G$ nonzero for only finitely many $G \in \mathcal{G}$. We identify any graph $H$ with the quantum graph (12) having $\gamma_G = 1$ if $G = H$, and $\gamma_G = 0$ otherwise.

Let $\mathcal{QG}$ denote the collection of quantum graphs. This is a commutative algebra, with multiplication given by

$$(13) \qquad \left(\sum_{G\in\mathcal{G}} \gamma_G G\right)\left(\sum_{H\in\mathcal{G}} \beta_H H\right) = \sum_{G\in\mathcal{G}}\sum_{H\in\mathcal{G}} \gamma_G \beta_H GH.$$

(As before, $GH$ denotes the disjoint union of $G$ and $H$.) In other words, $\mathcal{QG}$ is the semigroup algebra asociated with the semigroup $\mathcal{G}$, taking disjoint union as multiplication. Then $K_0$ is the unit element.

The function $p_n$ can be extended linearly to $\mathcal{QG}$. Note that for all $G, H \in \mathcal{G}$:

$$(14) \qquad p_n(GH) = p_n(G)p_n(H).$$

Hence $p_n$ is an algebra homomorphism $\mathcal{QG} \to \mathbb{C}[X]$, and $p_n(\mathcal{QG})$ is a subalgebra of $\mathbb{C}[X]$. (An algebra homomorphism is a linear function maintaining the unit and multiplication.)

## 4. The Möbius transform of a graph

Choose $G \in \mathcal{G}$. The *Möbius transform* $M(G)$ of $G$ is defined to be the quantum graph

$$(15) \qquad M(G) := \sum_{P\in\Pi_{VG}} \mu_P G/P.$$

This can be extended linearly to the Möbius transform $M(\gamma)$ of any quantum graph $\gamma \in \mathcal{QG}$.

The Möbius transform has an inverse determined by the *zeta transform*

$$(16) \qquad Z(G) = \sum_{Q\in\Pi_{VG}} G/Q.$$

Indeed,

$$(17) \qquad Z(M(G)) = \sum_{P}\sum_{Q\geq P} \mu_P G/Q = \sum_{Q}\sum_{P\leq Q} \mu_P G/Q = \sum_{Q} \delta_{Q,T_{VG}} G/Q = G/T_{VG} = G.$$

As $M$ is surjective (since $M(G)$ is a linear combination of $G$ and graphs smaller than $G$), we also know $M(Z(G)) = G$ for each $G \in \mathcal{G}$. (Indeed, $G = M(\gamma)$ for some $\gamma$, and $\gamma = Z(M(\gamma)) = Z(G)$.) So

$$Z \circ M = \mathrm{id}_{\mathcal{QG}} = M \circ Z. \tag{18}$$

We can now describe the polynomial $p_n(M(G))$. This is equal to the following polynomial $q_n(G) \in \mathbb{C}[X]$:

$$q_n(G) := \sum_{\phi : VG \rightarrowtail [n]} \prod_{uv \in EG} x_{\phi(u),\phi(v)}. \tag{19}$$

Het $\rightarrowtail$ means that the function is injective. Again, $q_n$ can be extended linearly to $\mathcal{QG}$.

To prove that $q_n(G) = p_n(M(G))$, note that

$$p_n(G) = \sum_{Q \in \Pi_{VG}} q_n(G/Q) \tag{20}$$

(since each $\phi : VG \to [n]$ can be factorized to an injective function $Q \to [n]$ for some unique partition $Q$ of $VG$). Hence $p_n(G) = q_n(Z(G))$ by (16). So $p_n = q_n \circ Z$, and hence, by (18), $q_n = p_n \circ M$. This implies that $p_n(\mathcal{QG}) = q_n(\mathcal{QG})$.

## 5. Proof of Theorem 3

**Theorem 3.** $\mathrm{lin}\{p_n(G) \mid G \in \mathcal{G}\} = \mathbb{C}[X]^{S_n}$.

**Proof.** Trivially, $p_n(G) \in \mathbb{C}[X]^{S_n}$ for any graph $G$, hence $p_n(\mathcal{QG}) \subseteq \mathbb{C}[X]^{S_n}$. To see the reverse inclusion, each monomial $m$ in $\mathbb{C}[X]$ is equal to $\prod_{ij \in EG} x_{i,j}$ for some graph $G$ with $VG = [n]$. Then, by definition of $q_n$, $q_n(G) = \sum_{\pi \in S_n} m^\pi$, where $m^\pi$ is obtained from $m$ by replacing any $x_{i,j}$ by $x_{\pi(i),\pi(j)}$. Since each polynomial in $\mathbb{C}[X]^{S_n}$ is a linear combination of polynomials $\sum_{\pi \in S_n} m^\pi$, we have $\mathbb{C}[X]^{S_n} \subseteq q_n(\mathcal{QG})$. As $p_n(\mathcal{QG}) = q_n(\mathcal{QG})$, this proves Theorem 3. ∎

## 6. A lemma on the Möbius transform

In the proof of Theorem 1, we need the following equality in the algebra $\mathcal{QG}$:

**Lemma 1.** *For any graph $G$: $M(K_1 G) = (K_1 - |VG|)M(G)$.*

**Proof.** Let $\phi$ be the linear function $\mathcal{QG} \to \mathcal{QG}$ determined by

$$\phi(G) := (K_1 + |VG|)G \tag{21}$$

for $G \in \mathcal{G}$. Then one has for any $\gamma \in \mathcal{QG}$:

$$\phi(Z(\gamma)) = Z(K_1\gamma), \tag{22}$$

since for any $H \in \mathcal{G}$,

$$\phi(Z(H)) = \phi(\sum_{P\in\Pi_{VH}} H/P) = \sum_{P\in\Pi_{VH}} \phi(H/P) = \sum_{P\in\Pi_{VH}} (K_1 + |P|)H/P = Z(K_1H). \tag{23}$$

The last equality follows from the fact that sum (16) giving $Z(K_1H)$ can be split into those $Q$ containing $VK_1$ as a singleton, and those $Q$ not containing $VK_1$ as a singleton — hence $VK_1$ is added to some class in some partition $P$ of $VH$.

This proves (22), which implies, setting $\gamma := M(G)$, that $\phi(G) = Z(K_1M(G))$, and hence $M(\phi(G)) = K_1M(G)$. Therefore with (21) we obtain

$$M(K_1G) = M(\phi(G)) - |VG|M(G) = (K_1 - |VG|)M(G). \tag{24}$$

∎

## 7. A lemma on the Möbius inverse function of partitions

For $P, Q \in \Pi_V$, let $P \vee Q$ denote the smallest (with respect to $\leq$) partition satisfying $P, Q \leq P \vee Q$.

**Lemma 2.** *Let $V$ be a set with $|V| = k$. Then for each $x \in \mathbb{C}$ and $t \geq 1$ one has*

$$\sum_{P_1,\ldots,P_t\in\Pi_V} \mu_{P_1}\cdots\mu_{P_t} x^{|P_1\vee\cdots\vee P_t|} = x(x-1)\cdots(x-k+1). \tag{25}$$

**Proof.** Since both sides in (25) are polynomials, it suffices to prove it for $x \in \mathbb{N}$. For any function $\phi : [k] \to [x]$, let $Q_\phi$ be the partition

$$Q_\phi := \{\phi^{-1}(i) \mid i \in [x], \phi^{-1}(i) \neq \emptyset\}. \tag{26}$$

Then

$$\sum_{P_1,\ldots,P_t\in\Pi_V} \mu_{P_1}\cdots\mu_{P_t} x^{|P_1\vee\cdots\vee P_t|} = \sum_{P_1,\ldots,P_t\in\Pi_V} \mu_{P_1}\cdots\mu_{P_t} \sum_{\substack{\phi:[k]\to[x] \\ P_1\vee\cdots\vee P_t\leq Q_\phi}} 1 = \tag{27}$$

$$\sum_{\phi:[k]\to[x]} \sum_{P_1,\ldots,P_t\le Q_\phi} \mu_{P_1}\cdots\mu_{P_t} = \sum_{\phi:[k]\to[x]} (\sum_{P\le Q_\phi}\mu_P)^t = \sum_{\phi:[k]\to[x]} \delta_{Q_\phi,T_{[k]}} =$$
$$\sum_{\phi:[k]\rightarrowtail[x]} 1 = x(x-1)\cdots(x-k+1). \qquad \blacksquare$$

## 8. Proof of Theorem 1

**Theorem 1.** *Let $f:\mathcal{G}\to\mathbb{C}$. Then $f=f_A$ for some $n\in\mathbb{N}$ and some symmetric matrix $A\in\mathbb{C}^{n\times n}$ if and only if $f$ is multiplicative and*

$$\sum_{P\in\Pi_{VG}} \mu_P f(G/P) = 0 \tag{28}$$

*for each graph $G$ with $|VG|>f(K_1)$.*

**Proof.** To see necessity, suppose $f=f_A$ for some $n\in\mathbb{N}$ and some symmetric matrix $A\in\mathbb{C}^{n\times n}$. Then trivially $f$ is multiplicative. Moreover, $f(M(G))=0$ if $|VG|>f(K_1)$, since $f(K_1)=n$, and

$$f(M(G)) = p_n(M(G))(A) = q_n(G)(A) = 0, \tag{29}$$

as $q_n(G)=0$ if $|VG|>n$ (since then there is no injective function $VG\to[n]$).

We next show sufficiency. First, $f(K_1)$ is a nonnegative integer. For if not, there is a nonnegative integer $k>f(K_1)$ with $\binom{f(K_1)}{k}\neq 0$. Let $N_k$ be the graph with vertex set $[k]$ and no edges. Then, by the condition in Theorem 1,

$$0 = \sum_{P\in\Pi_{[k]}} \mu_P f(N_k/P) = \sum_{P\in\Pi_{[k]}} \mu_P f(K_1)^{|P|} = \binom{f(K_1)}{k} k! \tag{30}$$

(by Lemma 2), a contradiction. So $f(K_1)\in\mathbb{N}$. Define $n:=f(K_1)$.

Next we show:

$$f=\hat{f}\circ p_n \text{ for some algebra homomorphism } \hat{f}:p_n(\mathcal{Q}\mathcal{G})\to\mathbb{C}. \tag{31}$$

We first show that there exists a linear function $\hat{f}:p_n(\mathcal{Q}\mathcal{G})\to\mathbb{C}$ with $\hat{f}\circ p_n=f$. For this we must show that, for any $\gamma\in\mathcal{Q}\mathcal{G}$, if $p_n(\gamma)=0$ then $f(\gamma)=0$. Equivalently, if $p_n(M(\gamma))=0$ then $f(M(\gamma))=0$. That is, since $p_n\circ M=q_n$,

(32) $\quad$ if $q_n(\gamma) = 0$ then $f(M(\gamma)) = 0$.

Suppose not. Choose $\gamma$ with $q_n(\gamma) = 0$ and $f(M(\gamma)) \neq 0$, minimizing the sum of $|VG|$ over those graphs $G$ with $\gamma_G \neq 0$. If $|VG| > n$, then $q_n(G) = 0$ and $f(M(G)) = 0$ (by assumption). So, by the minimality, if $\gamma_G \neq 0$, then $|VG| \leq n$.

Suppose next that some $G$ with $\gamma_G \neq 0$ has an isolated vertex. So $G = K_1 H$ for some graph $H$. Then $q_n(G) = (n - |VH|)q_n(H)$, by definition (19), and $f(M(G)) = (n-|VH|)f(M(H))$, by Lemma 1. So we could replace $G$ in $\gamma$ by $(n-|VH|)H$, contradicting our minimality condition.

Now for any graph $G$ with $|VG| \leq n$, say $VG = [k]$, $q_n(G)$ is a scalar multiple of the polynomial $\sum_{\pi\in S_n} m^\pi$, where $m$ is the monomial $\prod_{ij\in EG} x_{i,j}$. If $G$ and $G'$ are such graphs and have no isolated vertices, these polynomials have no monomials in common. Since $q_n(\gamma) = 0$, this implies $\gamma = 0$, hence $f(M(\gamma)) = 0$, proving (32).

So there is a linear function $\hat{f} : p_n(\mathcal{QG}) \to \mathbb{C}$ with $\hat{f} \circ p_n = f$. Then $\hat{f}$ is an algebra homomorphism, since

(33) $$\hat{f}(p_n(\beta)p_n(\gamma)) = \hat{f}(p_n(\beta\gamma)) = f(\beta\gamma) = f(\beta)f(\gamma) = \hat{f}(p_n(\beta))\hat{f}(p_n(\gamma))$$

for $\beta, \gamma \in \mathcal{QG}$. This proves (31).

Now let $I$ be the following ideal in $p_n(\mathcal{QG})$:

(34) $$I := \{p \in p_n(\mathcal{QG}) \mid \hat{f}(p) = 0\}.$$

Then the polynomials in $I$ have a common zero. For if not, by Hilbert's Nullstellensatz (saying that an ideal in $\mathbb{C}[X]$ not containing 1 has a common zero) there exist $r_1, \ldots, r_k \in I$ and $s_1, \ldots, s_k \in \mathbb{C}[X]$ with

(35) $$r_1 s_1 + \cdots + r_k s_k = 1.$$

We can assume that the $s_i$ in fact belong to $p_n(\mathcal{QG})$. For let $\sigma$ be the Reynolds operator $\mathbb{C}[X] \to \mathbb{C}[X]^{S_n}$, that is,

(36) $$\sigma(p)(X) := n!^{-1} \sum_P p(P^\mathsf{T} X P),$$

where $P$ extends over the $n \times n$ permutation matrices. Then, since $r_i(P^\mathsf{T} X P) = r_i(X)$ for each $i$ and each $P$,

(37) $$1 = \sigma(r_1 s_1 + \cdots + r_k s_k) = r_1 \sigma(s_1) + \cdots + r_k \sigma(s_k).$$

So we can assume that $s_i = \sigma(s_i)$ for each $i$. Hence $s_i \in \mathbb{C}[X]^{S_n}$. So, by Theorem 3, $s_i \in p_n(\mathcal{Q}\mathcal{G})$ for each $i$. As $I$ is an ideal in $p_n(\mathcal{Q}\mathcal{G})$, this implies $1 \in I$. This however gives the contradiction $1 = f(K_0) = \hat{f}(p_n(K_0)) = \hat{f}(1) = 0$.

So the polynomials in $I$ have a common zero, $A$ say. Now for each $G \in \mathcal{G}$, the polynomial $p_n(G) - f(G)$ belongs to $I$ (where $f(G)$ is the constant polynomial with value $f(G)$). So $p_n(G)(A) - f(G) = 0$, that is $f_A(G) = f(G)$, as required. ∎

# 9. Derivation of Corollary 1a from Theorem 1

**Corollary 1a.** *Let $f : \mathcal{G} \to \mathbb{R}$. Then $f = f_A$ for some $n \in \mathbb{N}$ and some symmetric matrix $A \in \mathbb{R}^{n\times n}$ if and only if the conditions of Theorem 1 hold and moreover the matrix*

$$(38) \qquad L_f := \Big(f(K_2^{i+j})\Big)_{i,j=0}^{\frac{1}{2}m(m+1)}$$

*is positive semidefinite, where $m := \lfloor f(K_1) \rfloor$.*

**Proof.** For necessity it suffices (in view of Theorem 1) to show that $L_f$ is positive semidefinite. Suppose $f = f_A$ for some $n \in \mathbb{N}$ and some symmetric matrix $A = (a_{i,j}) \in \mathbb{R}^{n\times n}$. Then

$$(39) \qquad (L_f)_{k,l} = f(K_2^{k+l}) = \sum_{i,j=1}^{n} a_{i,j}^{k+l}.$$

So $L_f$ is positive semidefinite.

We next show sufficiency. By Theorem 1 we know that $f = f_A$ for some $n$ and some symmetric matrix $A = (a_{i,j}) \in \mathbb{C}^{n\times n}$. We prove that $A$ is real.

Suppose $A$ is not real, say $a_{i',j'} \notin \mathbb{R}$. Then there is a polynomial $p \in \mathbb{C}[x]$ of degree at most $t := \frac{1}{2}n(n+1)$ such that $p(a_{i',j'}) = \mathrm{i}$, $p(\overline{a}_{i',j'}) = -\mathrm{i}$, and $p(a_{i,j}) = 0$ for all $i, j$ with $a_{i,j} \notin \{a_{i',j'}, \overline{a}_{i',j'}\}$. [3] Note that this implies $\overline{p}(a_{i',j'}) = \overline{p(\overline{a}_{i',j'})} = \mathrm{i}$ and $\overline{p}(\overline{a}_{i',j'}) = \overline{p(a_{i',j'})} = -\mathrm{i}$.

Write $p = \sum_{k=0}^{t} p_k x^k$ and $q := (p_0, \ldots, p_t)^{\mathsf{T}}$. Then

$$(40) \qquad q^{\mathsf{T}} L_f \overline{q} = \sum_{k,l=0}^{t} p_k \overline{p}_l f(K_2^{k+l}) = \sum_{k,l=0}^{t} p_k \overline{p}_l \sum_{i,j=1}^{n} a_{i,j}^{k+l} = \sum_{i,j=1}^{n} p(a_{i,j})\overline{p}(a_{i,j}) < 0.$$

[3] Observe the typographical difference between i (the imaginary unit) and $i$ (an index).

This contradicts the positive semidefiniteness of $L_f$. ∎

## 10. Derivation of Corollary 1b from Corollary 1a

**Corollary 1b.** *Let $f : \mathcal{G} \to \mathbb{R}$. Then $f = f_A$ for some $n$ and some symmetric matrix $A \in \mathbb{R}^{n\times n}$ if and only if $f$ is multiplicative and $M_{f,k}$ is positive semidefinite for each $k \in \mathbb{N}$.*

**Proof.** To see necessity it suffices to show that $M_{f_A,k}$ is positive semidefinite for each symmetric matrix $A \in \mathbb{R}^{n\times n}$ and each $k \in \mathbb{N}$. This follows from

$$(41)\qquad (M_{f_A,k})_{(G,u),(H,w)} = f_A((G,u)*(H,w)) = \sum_{\chi:[k]\to[n]} \left( \sum_{\substack{\phi:VG\to[n]\\ \forall j\in[k]:\phi(u_j)=\chi(j)}} \prod_{uv\in EG} a_{\phi(u),\phi(v)} \right) \left( \sum_{\substack{\psi:VH\to[n]\\ \forall j\in[k]:\psi(w_j)=\chi(j)}} \prod_{uv\in EH} a_{\psi(u),\psi(v)} \right)$$

for $k$-labeled graphs $(G,u),(H,w)$. So $M_{f_A,k}$ is a Gram matrix, hence positive semidefinite.

To see sufficiency, if $M_{f,2}$ is positive semidefinite, then $L_f$ is positive semidefinite. Indeed,

$$(42)\qquad (L_f)_{k,l} = f(K_2^{k+l}) = f((K_2^k,(1,2))*(K_2^l,(1,2))) = (M_{f,2})_{(K_2^k,(1,2)),(K_2^l,(1,2))}.$$

So the positive semidefiniteness of $M_{f,2}$ implies that of $L_f$.

We finally show that if $|VG| > f(K_1)$ then $f(M(G)) = 0$. First choose any $k > f(K_1)$. Let $N_k$ be the graph with vertex set $[k]$ and no edges. For any partition $P$ of $[k]$, let $P(i)$ denote the class of $P$ containing $i$ (for $i \in [k]$), and let

$$(43)\qquad u_P := (P(1),\dots,P(k)).$$

So $u_P \in V(N_k/P)^k$, and hence $(N_k/P, u_P)$ is a $k$-labeled graph. Then

$$(44)\qquad \sum_{P,Q\in\Pi_{[k]}} \mu_P\mu_Q f((N_k/P,u_P)*(N_k/Q,u_Q)) = \sum_{P,Q\in\Pi_{[k]}} \mu_P\mu_Q f(K_1)^{|P\vee Q|} = \binom{f(K_1)}{k}k!,$$

by Lemma 2. Hence, since $M_{f,k}$ is positive semidefinite, $\binom{f(K_1)}{k} \geq 0$, and therefore, as this holds for each $k > f(K_1)$, we have $f(K_1) \in \mathbb{N}$. Hence, for $k > f(K_1)$, $\binom{f(K_1)}{k} = 0$, and so (44) implies

$$(45) \qquad \sum_{P,Q \in \Pi_{[k]}} \mu_P \mu_Q f((N_k/P, u_P) * (N_k/Q, u_Q)) = 0.$$

Consider now any graph $G$ with $k := |VG| > n$ vertices, say $VG = [k]$. Define $u := (1, \ldots, k)$. Then by the positive semidefiniteness of $M_{f,k}$, (45) implies

$$(46) \qquad 0 = \sum_{P \in \Pi_{[k]}} \mu_P f((N_k/P, u_P) * (G, u)) = \sum_{P \in \Pi_{[k]}} \mu_P f(G/P) = f(M(G)).$$

So $f(M(G)) = 0$, as required. ∎

## 11. Derivation of Corollary 1c from Corollary 1b

**Corollary 1c.** *Let $f : \widetilde{\mathcal{G}} \to \mathbb{R}$. Then $f = \hom(\cdot, H)$ for some $H \in \widetilde{\mathcal{G}}$ if and only if $f$ is multiplicative and $\widetilde{M}_{f,k}$ is positive semidefinite for each $k \in \mathbb{N}$.*

**Proof.** Necessity is shown as before. Sufficiency is derived from Corollary 1b as follows.

Let $f : \widetilde{\mathcal{G}} \to \mathbb{R}$ be multiplicative with $\widetilde{M}_{f,k}$ positive semidefinite for each $k \in \mathbb{N}$. Define $\hat{f} : \mathcal{G} \to \mathbb{R}$ by $\hat{f}(G) := f(\widetilde{G})$, for $G \in \mathcal{G}$, where $\widetilde{G}$ arises from $G$ by replacing parallel edges by one edge. Then $\hat{f}$ is multiplicative and the matrix $M_{\hat{f},k}$ is positive semidefinite for each $k \in \mathbb{N}$. Hence by Corollary 1b, $\hat{f} = f_A$ for some $n \in \mathbb{N}$ and some real symmetric $n \times n$ matrix $A = (a_{i,j})$. Now it suffices to show that all entries of $A$ belong to $\{0, 1\}$, since then $A$ is the adjacency matrix of a graph $H$, implying $f_A(G) = \hom(G, H)$ for each $G \in \mathcal{G}$.

Now, as $f_A = \hat{f}$, we know $f_A(K_2^t) = f_A(K_2^1)$ for each $t \geq 1$. So $\sum_{i,j} a_{i,j}^t = \sum_{i,j} a_{i,j}$ for each $t \geq 1$. Hence $\sum_{i,j}(a_{i,j}^2 - a_{i,j})^2 = \sum_{i,j}(a_{i,j}^4 - 2a_{i,j}^3 + a_{i,j}^2) = 0$. Therefore $a_{i,j}^2 - a_{i,j} = 0$ for all $i, j$. So $a_{i,j} \in \{0, 1\}$ for all $i, j$. ∎

## 12. Proof of Theorem 2

**Theorem 2.** *Let $A \in \mathbb{C}^{n \times n}$ and $A' \in \mathbb{C}^{n' \times n'}$ be symmetric matrices. Then $f_A = f_{A'}$ if and only if $n = n'$ and $A' = P^\mathsf{T} A P$ for some $n \times n$ permutation matrix $P$.*

**Proof.** Sufficiency being direct, we prove necessity. Suppose $f_A = f_{A'}$. Then $n = n'$, since $n = f_A(K_1) = f_{A'}(K_1) = n'$.

Let $\Pi$ denote the collection of $n \times n$ permutation matrices. Suppose $A' \neq P^\mathsf{T} A P$ for all $P \in \Pi$. Then the sets

$$Y := \{P^\mathsf{T} A P \mid P \in \Pi\} \text{ and } Y' := \{P^\mathsf{T} A' P \mid P \in \Pi\} \tag{47}$$

are disjoint finite subsets of $\mathbb{C}^{n\times n}$. Hence there is a polynomial $p \in \mathbb{C}[X]$ such that $p(X) = 0$ for each $X \in Y$ and $p(X) = 1$ for each $X \in Y'$. Let $q$ be the polynomial

$$q(X) := n!^{-1} \sum_{P\in\Pi} p(P^\mathsf{T} X P). \tag{48}$$

So $q \in \mathbb{C}[X]^{S_n}$. Hence, by Theorem 3, $q \in p_n(\mathcal{QG})$, say $q = p_n(\gamma)$ for $\gamma \in \mathcal{QG}$. This gives the contradiction

$$0 = q(A) = p_n(\gamma)(A) = f_A(\gamma) = f_{A'}(\gamma) = p_n(\gamma)(A') = q(A') = 1. \tag{49}$$

∎

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