Graph invariants in the edge model

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Abstract. We sharpen the characterization of Szegedy of graph invariants

$$f_b(G) = \sum_{\phi:EG\to[n]} \prod_{v\in VG} b(\phi(\delta(v))),$$

where b is a real-valued function defined on the collection of all multisubsets of $[n] := \{1,\ldots,n\}$.

1. Introduction

Laci Lovász is a main inspirator of the new area of graph limits and graph connection matrices and their relations to graph parameters, partition functions, mathematical physics, reflection positivity, and extremal combinatorics. Prompted by Lovász's questions, Balázs Szegedy [5] characterized graph invariants in the 'edge model'. His proof is based on a highly original combination of methods from invariant theory and real algebraic geometry. It answers a question formulated in [1], which paper considers the corresponding 'vertex model'.

In this paper we give a sharpening of Szegedy's theorem and give a slightly shorter proof, although parts of our proof follow the scheme of Szegedy's proof. New elements of the present paper are the connections between linking of graphs and differentiation of polynomials and the use of a deep theorem of Procesi and Schwarz [4] in real invariant theory.

Let $\mathcal{G}$ be the collection of all finite graphs, where two graphs are considered to be the same if they are isomorphic. Graphs may have loops and multiple edges. Moreover, 'pointless' edges are allowed, that is, loops without a vertex. We use the notation

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

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

A *graph invariant* is any function $f : \mathcal{G} \to \mathbb{R}$. In this paper, as in Szegedy [5], we consider graph invariants obtained as follows. Let $n \in \mathbb{N}$ and let A_n be the collection of all multisubsets of $[n]$, that is, of all multisets with elements from $[n]$. (So each element of $[n]$ has a 'multiplicity' in any $\alpha \in A_n$. There is a one-to-one relation between A_n and $\mathbb{N}^n$, given by the multiplicities of $i \in [n]$ in a multiset $\alpha \in A_n$.)

For $b : A_n \to \mathbb{R}$ define $f_b : \mathcal{G} \to \mathbb{R}$ by

$$(2) \qquad f_b(G) = \sum_{\phi:EG\to[n]} \prod_{v\in VG} b(\phi(\delta(v)))$$

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for $G \in \mathcal{G}$. Here VG and EG denote the sets of vertices and edges of G, respectively, $\delta(v)$ is the set of edges incident with v, and $\phi(\delta(v))$ is the multiset of ϕ-values on $\delta(v)$, counting muytiplicities. (Actually, also $\delta(v)$ is a multiset, as loops at v occur twice in $\delta(v)$.)

Several graph invariants are equal to f_b for some appropriate b. For instance, the number of proper n-edge-colourings of a graph G is equal to $f_b(G)$, where, for $\alpha \in A_n$, $b(\alpha) = 1$ if all elements of $[n]$ have multiplicity 0 or 1 in α, and $b(\alpha) = 0$ otherwise. The number of perfect matchings in G is equal to $f_b(G)$ for $n = 2$ and $b(\alpha) = 1$ if the multiplicity of 1 in α is equal to 1, and $b(\alpha) = 0$ otherwise. For more background, see de la Harpe and Jones [3] and Freedman, Lovász, and Schrijver [1].

We characterize which graph invariants f satisfy $f = f_b$ for some $n \in \mathbb{N}$ and $b : A_n \to \mathbb{R}$, extending the characterizing of Szegedy [5]. We also prove that $f_b = f_c$ if and only if c arises from b by an orthogonal transformation. (Szegedy proved sufficiency here.)

2. The characterization

To describe the characterization, call a graph invariant f *multiplicative* if $f(K_0) = 1$ and $f(GH) = f(G)f(H)$ for any $G, H \in \mathcal{G}$. Here K_0 is the graph with no vertices and no edges, and GH denotes the disjoint union of G and H.

We also need the following operation. Let u and v be distinct vertices of a graph G, and let π be a bijection from $\delta(u)$ to $\delta(v)$. (This obviously requires that $\deg(u) = \deg(v)$.) Let $G_{u,v,\pi}$ be the graph obtained as follows (where we consider the graph as topological space). Delete u and v from G, and for each $e \in \delta(u)$, reconnect e to $\pi(e)$. So the open ends of e and $\pi(e)$ are glued together with a new topological point (which however will not be a vertex). It might be that $e = \pi(e)$ (so e connects u and v), in which case we create a pointless loop.

We need a repeated application of this operation, denoted as follows. Let $u_1, v_1, \ldots, u_k, v_k$ be distinct vertices of graph G and let $\pi_i : \delta(u_i) \to \delta(v_i)$ be a bijection, for each $i = 1, \ldots, k$. Then we set

$$(3) \qquad G_{u_1,v_1,\pi_1,\ldots,u_k,v_k,\pi_k} := (\cdots(G_{u_1,v_1,\pi_1})\cdots)_{u_k,v_k,\pi_k}.$$

Now define the $\mathcal{G} \times \mathcal{G}$ matrix $M_{f,k}$ by

$$(4) \qquad (M_{f,k})_{G,H} := \sum_{u_1,v_1,\pi_1,\ldots,u_k,v_k,\pi_k} f((GH)_{u_1,v_1,\pi_1,\ldots,u_k,v_k,\pi_k})$$

for $G, H \in \mathcal{G}$, where the sum extends over all distinct $u_1, \ldots, u_k \in VG$, distinct $v_1, \ldots, v_k \in VH$, and bijections $\pi_i : \delta_G(u_i) \to \delta_H(v_i)$, for $i = 1, \ldots, k$.

Theorem 1. *Let $f : \mathcal{G} \to \mathbb{R}$. Then $f = f_b$ for some $n \in \mathbb{N}$ and some $b : A_n \to \mathbb{R}$ if and only if f is multiplicative and $M_{f,k}$ is positive semidefinite for each $k = 0, 1, \ldots$.*

The positive semidefiniteness of $M_{f,k}$ can be seen as a form of 'reflection positivity' of f. In Section 6, we derive Szegedy's characterization from Theorem 1. In Section 7 we prove that b is uniquely determined by f, up to certain orthogonal transformations.

3. Some framework

Let $\mathcal{Q}$ denote the collection of all formal real linear combinations $\sum_G \gamma_G G$ of graphs (with at most finitely many γ_G nonzero). These are called *quantum graphs*. By taking the disjoint union GH as multiplication, $\mathcal{Q}$ becomes a commutative algebra. The function f can be extended linearly to $\mathcal{Q}$.

For $G, H \in \mathcal{G}$ and $k \in \mathbb{N}$, define the quantum graph $\lambda_k(G, H)$ by

$$\lambda_k(G,H) := \sum_{u_1,v_1,\pi_1,\ldots,u_k,v_k,\pi_k} (GH)_{u_1,v_1,\pi_1,\ldots,u_k,v_k,\pi_k}, \tag{5}$$

where the sum is taken over the same set as in (4). We can extend $\lambda_k(G, H)$ linearly to a bilinear function $\mathcal{Q} \times \mathcal{Q} \to \mathcal{Q}$. As

$$M_{f,k}(G,H) = f(\lambda_k(G,H)), \tag{6}$$

the positive semidefiniteness of $M_{f,k}$ is equivalent to the fact that $f(\lambda_k(\gamma,\gamma)) \geq 0$ for each $\gamma \in \mathcal{Q}$.

For each $\alpha \in A_n$, we introduce a variable x_α. For each $G \in \mathcal{G}$, define the following polynomial in $\mathbb{R}[x_\alpha \mid \alpha \in A_n]$:

$$p_n(G) := \sum_{\phi: EG \to [n]} \prod_{v \in VG} x_{\phi(\delta(v))}. \tag{7}$$

So $f_b(G) = p_n(G)(b)$ for any $b : A_n \to \mathbb{R}$. We extend p_n linearly to $\mathcal{Q}$.

Let $\mathcal{O}(n)$ be the group of (real) orthogonal $n \times n$ matrices. The group $\mathcal{O}(n)$ acts (linearly) on $\mathbb{R}[y_1, \ldots, y_n]$, and via the bijection

$$x_\alpha \leftrightarrow \prod_{i \in \alpha} y_i \tag{8}$$

between the variables x_α and monomials in $\mathbb{R}[y_1, \ldots, y_n]$, $\mathcal{O}(n)$ also acts on $\mathbb{R}[x_\alpha \mid \alpha \in A_n]$. Then, by the First Fundamental Theorem of invariant theory for the orthogonal group $\mathcal{O}(n)$ (cf. Goodman and Wallach [2]), we have

$$p_n(\mathcal{Q}) = \mathbb{R}[x_\alpha \mid \alpha \in A_n]^{\mathcal{O}(n)}. \tag{9}$$

(The latter denotes as usual the set of polynomials in $\mathbb{R}[x_\alpha \mid \alpha \in A_n]$ invariant under $\mathcal{O}(n)$.) This can be seen using the connection (8).

4. Derivatives

For any polynomial $p \in \mathbb{R}[x_\alpha \mid \alpha \in A_n]$, let dp be its derivative, being an element of $\mathbb{R}[x_\alpha \mid \alpha \in A_n] \otimes_{\mathbb{R}} L_n$, where L_n is the space of linear functions in $\mathbb{R}[x_\alpha \mid \alpha \in A_n]$. Then $d^k p \in \mathbb{R}[x_\alpha \mid \alpha \in A_n] \otimes_{\mathbb{R}} L_n^{\otimes k}$.

Let $\langle .,. \rangle$ be the inner product on L_n given by

$$\langle x_\alpha, x_\beta \rangle := c_\alpha \delta_{\alpha,\beta} \tag{10}$$

for $\alpha, \beta \in A_n$, where

$$c_\alpha := \prod_{i=1}^{n} \mu_i(\alpha)!, \tag{11}$$

where $\mu_i(\alpha)$ denotes the multiplicity of i in α. This induces an inner product on $L_n^{\otimes k}$ for each k. With the usual product of polynomials in $\mathbb{R}[x_\alpha \mid \alpha \in A_n]$, this gives an inner product on $\mathbb{R}[x_\alpha \mid \alpha \in A_n] \otimes_{\mathbb{R}} L_n^{\otimes k}$ with values in $\mathbb{R}[x_\alpha \mid \alpha \in A_n]$.

The following lemma is basic to our proof, and is used several times in it.

Lemma 1. *For all graphs G, H and $k, n \in \mathbb{N}$:*

$$p_n(\lambda_k(G,H)) = \langle d^k p_n(G), d^k p_n(H) \rangle. \tag{12}$$

Proof. We expand $d^k p_n(G)$:

$$\begin{aligned} d^k p_n(G) &= \sum_{\alpha_1,\ldots,\alpha_k \in A_n} \sum_{\phi: EG \to [n]} \frac{d}{dx_{\alpha_1}} \cdots \frac{d}{dx_{\alpha_k}} \left(\prod_{v \in VG} x_{\phi(\delta(v))} \right) \otimes x_{\alpha_1} \otimes \cdots \otimes x_{\alpha_k} = \\ & \sum_{\alpha_1,\ldots,\alpha_k \in A_n} \sum_{\phi: EG \to [n]} \sum_{\substack{u_1,\ldots,u_k \in VG \\ \forall i: \phi(\delta(u_i)) = \alpha_i}} \left(\prod_{v \in VG \setminus \{u_1,\ldots,u_k\}} x_{\phi(\delta(v))} \right) \otimes x_{\alpha_1} \otimes \cdots \otimes x_{\alpha_k} = \\ & \sum_{u_1,\ldots,u_k \in VG} \sum_{\phi: EG \to [n]} \left(\prod_{v \in VG \setminus \{u_1,\ldots,u_k\}} x_{\phi(\delta(v))} \right) \otimes x_{\phi(\delta(u_1))} \otimes \cdots \otimes x_{\phi(\delta(u_k))}. \end{aligned} \tag{13}$$

Here $u_1, \ldots, u_k$ are distinct. Now for any $\phi : EG \to [n]$ and $\psi : EH \to [n]$ and any $u \in VG$ and $v \in VH$, $\langle x_{\phi(\delta(u))}, x_{\psi(\delta(v))} \rangle$ is equal to the number of bijections $\pi : \delta(u) \to \delta(v)$ such that $\psi \circ \pi = \phi | \delta(u)$. This implies (12). ☐

5. Proof of Theorem 1

To see necessity, let $b : A_n \to \mathbb{R}$ and $f = f_b$. Then, trivially, f is multiplicative. Positive semidefiniteness of $M_{f,k}$ follows from

$$f_b(\lambda_k(G,H)) = p_n(\lambda_k(G,H))(b) = \langle d^k p_n(G)(b), d^k p_n(H)(b) \rangle, \tag{14}$$

using Lemma 1.

We next show sufficiency. First we have:

Claim 1. Let γ be a quantum graph consisting of k-vertex graphs. If $f(\lambda_k(\gamma,\gamma))=0$ then $f(\gamma)=0$.

Proof. We prove the claim by induction on k. So assume that the claim holds for all quantum graphs made of graphs with less than k vertices.

We can assume that all graphs occurring in γ with nonzero coefficient have the same degree sequence $d_1,\ldots,d_k$, since if we would write $\gamma=\gamma_1+\gamma_2$, where all graphs in γ_1 have degree sequence different from those in γ_2, then $\lambda_k(\gamma_1,\gamma_2)=0$, whence $f(\lambda_k(\gamma_i,\gamma_i))=0$ for $i=1,2$.

Now $f(\lambda_k(\gamma,\gamma))=0$ implies, by the positive semidefiniteness of $M_{f,k}$:

$$f(\lambda_k(\gamma,H))=0 \text{ for each graph } H. \tag{15}$$

Let P be the graph with $2k$ vertices $1,1',\ldots,k,k'$, where for each $i=1,\ldots,k$, there are d_i parallel edges connecting i and i'. If $d_1,\ldots,d_k$ are all distinct, we are done, since then γ is a multiple of $\lambda_k(\gamma,P)$, implying with (15) that $f(\gamma)=0$ — but generally there can be vertices of equal degrees.

The sum in (5) for $\lambda_k(\gamma,P)$ can be decomposed according to the set I of those components of P with both vertices chosen among $v_1,\ldots,v_k$ and to the set J of those components of P with no vertices chosen among $v_1,\ldots,v_k$ (necessarily $|I|=|J|$). Let K denote the set of components of P, and for $J\subseteq K$, let P_J be the union of the components in J. Then

$$\lambda_k(\gamma,P)=\sum_{\substack{I,J\subseteq K\\ I\cap J=\emptyset,|I|=|J|}}\alpha_{I,J}\gamma_I P_J, \tag{16}$$

where $\alpha_{I,J}\in\mathbb{N}$ with $\alpha_{\emptyset,\emptyset}\neq 0$, and where

$$\gamma_I:=\lambda_{2|I|}(\gamma,P_I). \tag{17}$$

Now for each $I\subseteq K$, we have $\lambda_{k-2|I|}(\gamma_I,\gamma_I)=\lambda_k(\gamma,\gamma_I P_I)$. Hence

$$f(\lambda_{k-2|I|}(\gamma_I,\gamma_I))=f(\lambda_k(\gamma,\gamma_I P_I))=0, \tag{18}$$

by (15). So by induction, if $I\neq\emptyset$ then $f(\gamma_I)=0$. Therefore, by (16), since $f(\lambda_k(\gamma,P))=0$ and $\alpha_{\emptyset,\emptyset}\neq 0$, $f(\gamma)=f(\gamma_\emptyset P_\emptyset)=0$. □

Let O be the graph just consisting of the pointless loop.

Claim 2. $f(O)\in\mathbb{N}$.

Proof. Suppose not. Then we can choose a $k\in\mathbb{N}$ with $\binom{f(O)}{k}<0$. For each $\pi\in S_k$, let G_π be the graph with vertex set $[k]$ and edges $\{i,\pi(i)\}$ for $i=1,\ldots,k$. (So G_π is 2-regular.) Define

$$\gamma := \sum_{\pi \in S_k} \operatorname{sgn}(\pi) G_\pi. \tag{19}$$

Then for any n:

$$p_n(\gamma) = \sum_{\pi \in S_k} \operatorname{sgn}(\pi) p_n(G_\pi) = \sum_{\pi \in S_k} \operatorname{sgn}(\pi) \sum_{\phi: EG_\pi \to [n]} \prod_{v \in VG_\pi} x_{\phi(\delta(v))} = \tag{20}$$
$$\sum_{\pi \in S_k} \operatorname{sgn}(\pi) \sum_{\phi:[k]\to[n]} \prod_{v\in[k]} x_{\{\phi(v),\phi\circ\pi^{-1}(v)\}} = \sum_{\phi:[k]\to[n]} \sum_{\pi\in S_k} \operatorname{sgn}(\pi) \prod_{v\in[k]} x_{\{\phi(v),\phi\circ\pi(v)\}}.$$

Now if ϕ is not injective, then $\phi = \phi \circ \pi$ for some $\pi \in S_k$ with $\operatorname{sgn}(\pi) = -1$, and hence the last inner sum is 0. So if $n < k$ then $p_n(\gamma) = 0$. If $n = k$, then $p_n(\gamma)$ contains the term $x_{\{1,1\}} \cdots x_{\{k,k\}}$ with nonzero coefficient, so $p_k(\gamma) \neq 0$.

Since $\lambda_k(\gamma, \gamma)$ is a sum of graphs with no vertices, we know that $\lambda_k(\gamma, \gamma) = q(O)$ for some polynomial $q \in \mathbb{R}[y]$, of degree at most k. Then, if $n < k$,

$$q(n) = q(p_n(O)) = p_n(q(O)) = p_n(\lambda_k(\gamma, \gamma)) = 0, \tag{21}$$

with Lemma 1, as $p_n(\gamma) = 0$. Moreover, $q(k) = p_k(\lambda_k(\gamma, \gamma)) > 0$, as $p_k(\gamma) \neq 0$ (again using Lemma 1). So $q(y) = c\binom{y}{k}$ for some $c > 0$. Therefore,

$$f(\lambda_k(\gamma, \gamma)) = f(q(O)) = q(f(O)) = c\binom{f(O)}{k} < 0, \tag{22}$$

contradicting the positive semidefiniteness condition. □

This gives us n:

$$n := f(O). \tag{23}$$

Then Claim 1 implies:

(24) there is linear function $\hat{f} : p_n(\mathcal{Q}) \to \mathbb{R}$ such that $f = \hat{f} \circ p$.

Otherwise, there is a quantum graph γ with $p_n(\gamma) = 0$ and $f(\gamma) \neq 0$. We can assume that $p_n(\gamma)$ is homogeneous, that is, all graphs in γ have the same number of vertices, k say. Hence, since $\lambda_k(\gamma, \gamma)$ is a polynomial in O, and since $f(O) = n = p_n(O)$,

$$f(\lambda_k(\gamma, \gamma)) = p_n(\lambda_k(\gamma, \gamma)) = 0, \tag{25}$$

by Lemma 1. So by Claim 1, $f(\gamma) = 0$. This proves (24).

In fact, $\hat{f}$ is an algebra homomorphism, since for all $G, H \in \mathcal{G}$:

$$\hat{f}(p_n(G)p_n(H)) = \hat{f}(p_n(GH)) = f(GH) = f(G)f(H) = \hat{f}(p_n(G))\hat{f}(p_n(H)). \tag{26}$$

Then for all $G, H \in \mathcal{G}$, using Lemma 1:

$$\hat{f}(\langle dp_n(G), dp_n(H)\rangle) = \hat{f}(p_n(\lambda_1(G,H))) = f(\lambda_1(G,H)) = (M_{f,1})_{G,H}. \tag{27}$$

Since $M_{f,1}$ is positive semidefinite, (27) implies that for each $q \in p_n(\mathcal{Q})$:

$$\hat{f}(\langle dq, dq\rangle) \geq 0. \tag{28}$$

Now choose $\Delta \in \mathbb{N}$. Let $\mathcal{G}_\Delta$ be the set of graphs of maximum degree at most Δ, and let $\mathcal{Q}_\Delta$ be the set of all formal linear combinations of graphs in $\mathcal{G}_\Delta$. Define

$$A_{n,\Delta} := \{\alpha \in A_n \mid |\alpha| \leq \Delta\}. \tag{29}$$

By (28) and since the inner product $\langle .,. \rangle$ on L_n is $\mathcal{O}(n)$-invariant, the theorem of Procesi and Schwarz [4] (which we can apply in view of (9)) implies the existence of a $b \in \mathbb{R}^{A_{n,\Delta}}$ such that $\hat{f}(p) = p(b)$ for each $p \in p_n(\mathcal{Q}_\Delta)$. So

$$f(G) = \hat{f}(p_n(G)) = p_n(G)(b) = f_b(G) \tag{30}$$

for each $G \in \mathcal{G}_\Delta$.

This can be extended to the collection $\mathcal{G}$ of all graphs. For each d, let $K_2^{(d)}$ be the graph with two vertices, connected by d parallel edges. Then any $b : A_n \to \mathbb{R}$ with $f = f_b$ satisfies

$$b(\alpha)^2 \leq f(K_2^{(|\alpha|)}) \tag{31}$$

for $\alpha \in A_n$.

For each $\Delta \in \mathbb{N}$, define

$$B_\Delta := \{b : A_n \to \mathbb{R} \mid f(G) = f_b(G) \text{ for each } G \in \mathcal{G}_\Delta,\ b(\alpha)^2 \leq f(K_2^{(|\alpha|)}) \text{ for each } \alpha \in A_n\}. \tag{32}$$

By the above, $B_\Delta \neq \emptyset$ for each Δ. As each B_Δ is compact by Tychonoff's theorem, and as $B_\Delta \supseteq B_{\Delta'}$ if $\Delta \leq \Delta'$, we know $\bigcap_\Delta B_\Delta \neq \emptyset$. Any b in this intersection satisfies $f = f_b$. ∎

Note that the positive semidefiniteness of $M_{f,k}$ for $k \neq 1$ is only used to prove Claims 2 and 1. If we know that $f = \hat{f} \circ p_n$ for some linear function $\hat{f} : p_n(\mathcal{Q}) \to \mathbb{R}$ and some n, then it suffices to require that $M_{f,1}$ is positive semidefinite and f is multiplicative.

6. Derivation of Szegedy's theorem

We now derive as a consequence the theorem of Szegedy [5]. 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 (H,v) are k-exit graphs, then $(G,u)\cdot(H,v)$ is the undirected graph obtained by taking the disjoint union of G and H, and, for each $i=1,\ldots,k$, deleting u_i and v_i and adding a new point connecting the ends left by u_i and v_i.

Let $\mathcal{G}_k$ be the collection of k-exit graphs. For $f:\mathcal{G}\to\mathbb{R}$, define the $\mathcal{G}_k\times\mathcal{G}_k$ matrix $N_{f,k}$ by

$$(N_{f,k})_{(G,u),(H,v)} := f((G,u)\cdot(H,v)) \tag{33}$$

for $(G,u),(H,v)\in\mathcal{G}_k$. Then ([5]):

Corollary 1a. *Let $f:\mathcal{G}\to\mathbb{R}$. Then $f=f_b$ for some $n\in\mathbb{N}$ and some $b:A_n\to\mathbb{R}$ if and only if f is multiplicative and $N_{f,k}$ is positive semidefinite for each $k\in\mathbb{N}$.*

Proof. Necessity follows similarly as in Theorem 1. To see sufficiency, let for any graph G and any $d\in\mathbb{N}$, G_d be the quantum d-exit graph being the sum of all d-exit graphs obtained as follows. Choose a vertex v of degree d, delete v topologically from G, and add vertices of degree 1 to the loose ends. Let F be the graph obtained this way. Order these new vertices in a vector in $u\in VF^d$. The sum of these (F,u) makes G_d. So G_d is a sum of precisely $d!m$ d-exit graphs, where m is the number of vertices of degree d in G.

We can repeat this to define the quantum $d_1+\cdots+d_k$-exit graph $G_{d_1,\ldots,d_k}$ for any $d_1,\ldots,d_k\in\mathbb{N}$, where we concatenate the exit vectors. Then

$$\lambda_k(G,H)=\sum_{d_1,\ldots,d_k} c_{d_1,\ldots,d_k} G_{d_1,\ldots,d_k}\cdot H_{d_1,\ldots,d_k} \tag{34}$$

for some $c_{d_1,\ldots,d_k}>0$ (namely, the inverse of the number of permutations $\pi\in S_k$ with $d_{\pi(i)}=d_i$ for each $i\in[k]$). Hence for any quantum graph γ:

$$f(\lambda_k(\gamma,\gamma))=\sum_{d_1,\ldots,d_k} c_{d_1,\ldots,d_k} f(\gamma_{d_1,\ldots,d_k}\cdot\gamma_{d_1,\ldots,d_k})\geq 0, \tag{35}$$

by the positive semidefiniteness of the $N_{f,l}$. ∎

7. Uniqueness of b

We finally consider the uniqueness of b, and extend a theorem of Szegedy [5] (who showed sufficiency). As usual, b^U denotes the result of the action of U on b.

Theorem 2. *Let $b:A_n\to\mathbb{R}$ and $c:A_m\to\mathbb{R}$. Then $f_b=f_c$ if and only if $n=m$ and $c=b^U$ for some $U\in\mathcal{O}(n)$.*

Proof. Sufficiency can be seen as follows. Let $n=m$ and $c=b^U$ for some $U\in\mathcal{O}(n)$. Then for any graph G, using (9),

$$f_b(G)=p_n(G)(b)=p_n(G)^{U^{-1}}(b)=p_n(G)(b^U)=f_{b^U}(G)=f_c(G). \tag{36}$$

Conversely, let $f_b(G) = f_c(G)$ for each graph G. Then $n = f_b(O) = f_c(O) = m$. We show that for each $\Delta \in \mathbb{N}$, there exists $U \in \mathcal{O}(n)$ such that $c|A_{n,\Delta} = b^U|A_{n,\Delta}$, where $A_{n,\Delta}$ is as in (29). As $\mathcal{O}(n)$ is compact, this implies that there exists $U \in \mathcal{O}(n)$ with $c = b^U$.

Suppose that $c|A_{n,\Delta} \neq b^U|A_{n,\Delta}$ for each $U \in \mathcal{O}(n)$. Then the sets

$$S := \{b^U|A_{n,\Delta} \mid U \in \mathcal{O}(n)\} \text{ and } T := \{c^U|A_{n,\Delta} \mid U \in \mathcal{O}(n)\} \tag{37}$$

are compact and disjoint subsets of $\mathbb{R}^{A_{n,\Delta}}$. So, by the Stone-Weierstrass theorem, there exists a polynomial $q \in \mathbb{R}[x_\alpha \mid \alpha \in A_{n,\Delta}]$ such that $q(s) \leq 0$ for each $s \in S$ and $q(t) \geq 1$ for each $t \in T$. Replacing q by

$$\int_{\mathcal{O}(n)} q^U d\mu(U) \tag{38}$$

(where μ is the normalized Haar measure on $\mathcal{O}(n)$), we can assume that $q^U = q$ for each $U \in \mathcal{O}(n)$. Hence by (9), $q \in p_n(\mathcal{Q})$, say $q = p_n(\gamma)$ with $\gamma \in \mathcal{Q}$. Then $f_b(\gamma) = p_n(\gamma)(b) = q(b) \leq 0$ and $f_c(\gamma) = p_n(\gamma)(c) = q(c) \geq 1$. This contradicts $f_b = f_c$. ∎

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References

[1] M.H. Freedman, L. Lovász, A. Schrijver, Reflection positivity, rank connectivity, and homomorphisms of graphs, *Journal of the American Mathematical Society* 20 (2007) 37–51.

[2] R. Goodman, N.R. Wallach, *Representations and Invariants of the Classical Groups*, Cambridge University Press, Cambridge, 1998.

[3] P. de la Harpe, V.F.R. Jones, Graph invariants related to statistical mechanical models: examples and problems, *Journal of Combinatorial Theory, Series B* 57 (1993) 207–227.

[4] C. Procesi, G. Schwarz, Inequalities defining orbit spaces, *Inventiones Mathematicae* 81 (1985) 539–554.

[5] B. Szegedy, Edge coloring models and reflection positivity, *Journal of the American Mathematical Society* 20 (2007) 969–988.