Graph parameters and invariants of the orthogonal group
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Chapter 2
Preliminaries

In this chapter we introduce some important and probably not so well-known concepts such as labeled graphs, fragments and connection matrices. Moreover, we set up some basic notation.

2.1 Some notation and conventions

We set up some basic notation and conventions used throughout the thesis. We moreover give a few basic definitions.

Fields and sets
By $\mathbb{R}$, $\mathbb{C}$ we denote the set of real numbers and complex numbers respectively. Throughout this thesis, $\mathbb{F}$ denotes any field of characteristic zero, unless indicated otherwise. (Many definitions in this thesis make sense also in characteristic $p$, but for simplicity we just stick to characteristic zero throughout this thesis.) By $\overline{\mathbb{F}}$ we denote the algebraic closure of $\mathbb{F}$.

By $\mathbb{N}$ we denote the set of natural numbers including zero; $\mathbb{N} := \{0, 1, 2 \ldots \}$ and for $n \in \mathbb{N}$ we set
\[
[n] := \{1, \ldots, n\}.
\] (2.1)

Note that $[0]$ denotes the empty set. For $\alpha \in \mathbb{N}^k$, we denote by $x^\alpha \in \mathbb{F}[x_1, \ldots, x_k]$ the monomial $x_1^{\alpha_1} \cdots x_k^{\alpha_k}$. Furthermore, for $\alpha \in \mathbb{N}^k$ we set $|\alpha| := \sum_{j=1}^{k} \alpha_i$.

We will not only use $\delta$ to denote the set of edges incident with a vertex in a graph but also to define a certain set function: for a set $S$ and $s_1, s_2 \in S$, $\delta_{s_1, s_2} = 1$ if $s_1 = s_2$ and 0 otherwise; it is also known as the Kronecker delta function.
Linear algebra
For a vectorspace $V$ over $\mathbb{F}$ we denote by $V^*$ its dual space, the space of $\mathbb{F}$-linear functions $f : V \rightarrow \mathbb{F}$. However, by $\mathbb{F}^*$ we denote the nonzero entries of $\mathbb{F}$. The set $\text{End}(V)$ denotes the set of linear maps from $V$ to itself. By $I_V \in \text{End}(V)$ we denote the identity map; sometimes we just write $I$. For a (finite or infinite) matrix $M$ with values in $\mathbb{F}$ we denote by $M^T$ its transpose and by $M^*$ its conjugate transpose (if $\mathbb{F} = \mathbb{C}$). Moreover, we denote by $\text{rk}(M)$ the rank of the matrix $M$. For a subset $S$ of $V$, we denote by $\text{span}(S)$ the subspace of $V$ spanned by $S$.

Graphs
A graph $H$ is a pair $(V,E)$, with $V$ a finite set and $E$ a finite multiset of unordered pairs of elements of $V$. Elements of $V$ are called vertices and elements of $E$ are called edges. A loop of $H$ is an edge of the form $\{v,v\}$ for $v \in V$. A simple graph is a graph without loops and where each edge has multiplicity one. For a graph $H$ we denote by $V(H)$ its vertices and by $E(H)$ its edges. For $u,v \in V(H)$ we usually denote by $uv$ the set $\{u,v\}$. We say that $u,v$ are adjacent in $H$ if $uv \in E(H)$. For $v \in V(H)$, $\delta(v) \subset E(H)$ denotes the set of edges incident with $v$ (loops are counted twice); $d(v) := |\delta(v)|$ is the degree of $v$.

Let $\mathcal{G}$ denote the set of all graphs. By $\bigcirc$ we denote the circle (or vertex less loop). More precisely, $\bigcirc = (\emptyset, \{1\})$. According to the definition it is not a graph, but it will be convenient to think of it as a graph. We will write $\mathcal{G}'$ for the set consisting of elements that are the disjoint union of a graph and finitely many circles. A map $f : \mathcal{G}' \rightarrow \mathbb{F}$ is called a graph parameter or graph invariant if $f$ assigns the same values to isomorphic graphs. Sometimes $f$ will only be defined on a subset of $\mathcal{G}'$, but we will then nevertheless call $f$ a graph parameter.

2.2 Labeled graphs and fragments
In this section we introduce the concept of labeled graphs and fragments.

2.2.1 Labeled graphs
For $l \in \mathbb{N}$, an $l$-labeled graph is a graph $H = (V,E)$ with an injective map $\lambda : [l] \rightarrow V$. For an $l$-labeled graph $H = (V,E)$ we think of $[l]$ as a subset of $V$, identifying $1, \ldots, l$ with the labeled vertices of $H$. See Figure 2.1 for some

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1Two graphs $H_1, H_2$ are isomorphic if there exists a bijection $\tau : V(H_1) \rightarrow V(H_2)$ such that $\tau(u)\tau(v) \in E(H_2)$ if and only if $uv \in E(H_2)$. 

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2.2. Labeled graphs and fragments

examples. We denote the set of \( l \)-labeled graphs by \( \mathcal{G}_l \) and we identify \( \mathcal{G} \) with \( \mathcal{G}_0 \).

Schrijver \cite{60} introduced a different kind of labeled graphs, where the map \( \lambda : [l] \to V \) is not required to be injective. See Lovász \cite{40} for other examples.

When \( f : \mathcal{G} \to \mathcal{F} \) is a graph parameter, we can simply extend \( f \) to \( \mathcal{G}_l \) for any \( l \) by letting \( f(H) := f([H]) \) for \( H \in \mathcal{G}_l \), where \([H]\) is the graph obtained from \( H \) by deleting its labels.

![Figure 2.1: Some examples of labeled graphs.](image)

The labeled vertex will be denoted by \( K_1^\bullet \), the labeled loop will be denoted by \( C_1^\bullet \) and the 2-labeled edge will be denoted by \( K_2^{\bullet\bullet} \). See Figure 2.2.

![Figure 2.2: The labeled graphs \( K_1^\bullet, C_1^\bullet \) and \( K_2^{\bullet\bullet} \).](image)

Let \( H_1 \) and \( H_2 \) be two \( l \)-labeled graphs. We define their gluing product \( H_1 \cdot H_2 \) by taking their disjoint union, and then identifying nodes with equal labels. See Figure 2.3 for an example. We sometimes just write \( H_1 H_2 \) instead of \( H_1 \cdot H_2 \). In particular, for two ordinary (unlabeled) graphs \( H_1, H_2, H_1 H_2 \) denotes their disjoint union. Note that with this gluing product, \( \mathcal{G}_l \) becomes a semigroup for any \( l \).

2.2.2 Fragments

For \( l \in \mathbb{N} \), an \( l \)-fragment is an \( l \)-labeled graph such that all the labeled vertices have degree one. (Lovász \cite{40} calls them \( l \)-broken graphs.) These labeled vertices are called open ends and the edge connected to an open end is called a half edge. So in Figure 2.1 the first labeled graph is not a fragment whereas the
second one is. We sometimes refer to $K^{**}_2$ as the open edge. By $F_1$ we denote the set of all $l$-fragments. We will identify $G'$ with $F_0$. Define a gluing operation $\star : F_1 \times F_1 \to G'$ as follows: for $F_1$ and $F_2 \in F_1$, take their disjoint union and connect the half edges incident with open ends with equal labels to form single edges (with the labeled vertices erased); the resulting graph is denoted by $F_1 \star F_2 \in G'$. See Figure 2.4 for an example. Note that $K^{**}_2 \star K^{**}_2 = \bigcirc$. This explains why it is useful to consider $\bigcirc$ as a graph.

Note that the gluing operation does not make $F_1$ into a semigroup for $l \geq 1$. We can however make $F_{2l}$ into a (noncommutative) semigroup as follows. Consider $F_1, F_2 \in F_{2l}$. Think of the labels $1, \ldots, l$ as the left labels and $l + 1, \ldots, 2l$ as the right labels. Define $F_1 \cdot F_2$ to be the $2l$-fragment obtained from the disjoint union of $F_1$ and $F_2$ by gluing the right open end of $F_1$ labeled $l + i$ to the left open end of $F_2$ labeled $i$, for $i = 1, \ldots, l$. This operation should not be confused with the gluing product for labeled graphs. Note that the identity element in $F_{2l}$ is the matching connecting $i$ to $l + i$ for $i \in [l]$. See Figure 2.5 for an example of this gluing product.
2.3 Connection matrices

Let \( f : \mathcal{G}' \rightarrow \mathcal{F} \) be a graph parameter. The \( l \)-th vertex-connection matrix of \( f \) is the \( \mathcal{G}_l \times \mathcal{G}_l \) matrix defined by:

\[
N_{f,l}(H_1, H_2) = f(H_1 \cdot H_2),
\]

for \( H_1, H_2 \in \mathcal{G}_l \). Vertex-connection matrices were introduced by Freedman Lovász and Schrijver [24], to characterize partition functions of real vertex-coloring models (cf. Theorem 5.1).

The \( l \)-th edge-connection matrix of \( f \) is the \( \mathcal{F}_l \times \mathcal{F}_l \) matrix defined by:

\[
M_{f,l}(F_1, F_2) = f(F_1 \ast F_2),
\]

for \( F_1, F_2 \in \mathcal{F}_l \). The edge-connection matrices were used by Szegedy [66] to characterize partition functions of edge-coloring models over \( \mathbb{R} \) (cf. Theorem 5.2).

Clearly, these connection matrices contain a lot of information about the graph parameter \( f \). There are various other ways to define connection matrices based on different kinds of labeling and gluing. Makowski [47] introduced several variants of gluing operations which he used to study questions about definability of graph parameters in monadic second order logic.

For \( H_1, H_2 \in \mathcal{G}' \), we will refer to the disjoint union of \( H_1 \) and \( H_2 \), \( H_1 H_2 \) as the product of \( H_1 \) and \( H_2 \). Let \( f : \mathcal{G}' \rightarrow \mathcal{F} \) be a graph parameter. Let \( \mathcal{S} \subset \mathcal{G}' \) be subset that is closed under multiplication and that contains \( \emptyset \). We call \( f \) multiplicative on \( \mathcal{S} \) if \( f(H_1 H_2) = f(H_1)f(H_2) \) for all \( H_1, H_2 \in \mathcal{S} \) and \( f(\emptyset) = 1 \). Equivalently, \( f \) is multiplicative on \( \mathcal{S} \) if the submatrix of \( M_{f,0} \) indexed by \( \mathcal{S} \)

\[\text{Figure 2.5: Gluing two 6-fragments into a 6-fragment.}\]
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has rank 1 and \( f(\emptyset) = 1 \). We will often omit the reference to \( S \) and just call \( f \) multiplicative.

When \( F = \mathbb{R} \), we call \( f \) reflection positive if \( N_{f,1} \) is positive semidefinite for all \( l \); we call \( f \) edge-reflection positive if \( M_{f,1} \) is positive semidefinite for all \( l \). An infinite matrix is positive semidefinite if all its finite principal submatrices are positive semidefinite. So \( N_{f,1} \) is positive semidefinite if and only if \( \sum_{i=1,j=1}^{n} \lambda_i \lambda_j f(H_i H_j) \geq 0 \) for all \( H_1, \ldots, H_n \in \mathcal{G}_l \) and \( \lambda_1, \ldots, \lambda_n \in \mathbb{R} \). Similarly, \( M_{f,1} \) is positive semidefinite if and only if \( \sum_{i=1,j=1}^{n} \lambda_i \lambda_j f(F_i \ast F_j) \geq 0 \) for all \( F_1, \ldots, F_n \in \mathcal{F}_l \) and \( \lambda_1, \ldots, \lambda_n \in \mathbb{R} \).

Let us end this section with an example to illustrate these definitions.

Example 2.1. For \( x \in \mathbb{R} \), define \( f_x : \mathcal{G} \rightarrow \mathbb{R} \) by

\[
f_x(H) = \begin{cases} x^c(H) & \text{if } H \text{ is 2-regular} \\ 0 & \text{otherwise,} \end{cases}
\]

where \( c(H) \) denotes the number of connected components of \( H \).

Note that \( f_x \) is clearly multiplicative for any \( x \). However, for any nonzero \( x \), \( f_x \) is not reflection positive. As \( f_x \) is only nonzero on 2-regular graphs, \( f_x((K^+_{1,1} \pm C_{1,1}^*)^2) = \pm 2 f_x(K^+_{1,1} C_{1,1}^*) = \pm 2 x \). So \( N_{f_x,1} \) is not positive semidefinite and hence \( f_x \) is not reflection positive. For \( x \in \mathbb{N} \), \( f_x \) is edge-reflection positive however. This follows from the fact that for \( x \in \mathbb{N} \), \( f_x \) is the partition function of an \( x \)-color edge-coloring model over \( \mathbb{R} \), as we will see in Section 5.2. Combined with Szegedy’s characterization (cf. Theorem 5.2) it follows that \( f_x \) is edge-reflection positive (this is actually the easy part of Szegedy’s theorem and we recover this in Section 6.2).

Clearly, \( f_x \) is not edge-reflection positive for \( x < 0 \). Indeed, consider the path on three vertices with both its endpoint labeled and denote it by \( K_{1,2}^{\bullet \bullet} \). Then \( f_x(K_{1,2}^{\bullet \bullet} \ast K_{1,2}^{\bullet \bullet}) = f(C_2) = x < 0 \). In fact, for any \( x \in \mathbb{R} \setminus \mathbb{N} \), \( f_x \) is not edge-reflection positive. As, by Proposition 5.6, \( f_x \) is not the partition function of any complex-valued edge-coloring model. Hence by Szegedy’s theorem, \( f_x \) is not edge-reflection positive.

2.4 Graph algebras

With the gluing product, the set of all \( l \)-labeled graphs \( \mathcal{G}_l \) becomes a semigroup with unit element the disjoint union of \( l \) copies of \( K^*_{1} \). Let \( F \mathcal{G}_l \) be the semigroup algebra of \( (\mathcal{G}_l, \cdot) \), i.e., elements of \( F \mathcal{G}_l \) are finite formal \( F \)-linear combinations of \( l \)-labeled graphs; they are called \( l \)-labeled quantum graphs (if \( l = 0 \) they are just
2.4. Graph algebras

called quantum graphs\footnote{In the terminology we follow Freedman, Lovász and Schrijver. It should be noted that the term quantum graph has been used elsewhere in mathematics with a different meaning.}

Let \( f : \mathcal{G} \to \mathbb{F} \) be a graph parameter. Extend \( f \) linearly to \( \mathbb{F}\mathcal{G} \). Note that \( f : \mathbb{F}\mathcal{G} \to \mathbb{F} \) is multiplicative if and only if \( f \) is a homomorphism of algebras. (In this thesis a homomorphism of algebras always maps the unit to the unit).

Let \( \mathcal{I}_I(f) \) be the ideal in \( \mathbb{F}\mathcal{G}_I \) generated by the kernel of \( f \), i.e.,

\[
\mathcal{I}_I(f) := \{ x \in \mathbb{F}\mathcal{G}_I \mid f(x \cdot y) = 0 \text{ for all } y \in \mathbb{F}\mathcal{G}_I \}.
\] (2.5)

Equivalently, \( \mathcal{I}_I(f) \) is the kernel of \( N_{f,I} \). Then define the quotient algebra by

\[
\mathcal{Q}_I(f) := \mathbb{F}\mathcal{G}_I / \mathcal{I}_I(f).
\] (2.6)

We will indicate elements of \( \mathcal{Q}_I(f) \) by representatives in \( \mathbb{F}\mathcal{G}_I \). We say that \( x, y \in \mathcal{Q}_I(f) \) are equivalent modulo \( f \) if \( x - y \in \mathcal{I}_I(f) \). These algebras were introduced by Freedman, Lovász and Schrijver \cite{24} and they are called graph algebras.

These graph algebras carry the same information about the parameter \( f \) as the vertex connection matrices, but they provide more structure and are somehow more convenient to work with. In particular, we have:

**Proposition 2.1.** The dimension of \( \mathcal{Q}_I(f) \) is equal to the rank of \( N_{f,I} \).

We can of course define similar objects for fragments. In particular, \( \mathbb{F}\mathcal{F}_{2I} \) denotes the semigroup algebra of \( (\mathcal{F}_{2I}, \cdot) \). In Section 6.2 we will show that we can equip the space of linear combinations of all fragments with the structure of an associative algebra.