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Generating connected and 2-edge connected graphs

Ângela Mestre[1]

[1]Doppler Institute & Department of Mathematics,
FNSPE, Czech Technical University
Trojanova 13, 120 00 Praha 2
Czech Republic
and
Centro de Física Teórica,
Departamento de Física da Universidade de Coimbra
P-3004-516 Coimbra, Portugal

Abstract

We focus on the algorithm underlying the main result of [6]. This is an algebraic formula to generate all connected graphs in a recursive and efficient manner. The key feature is that each graph carries a scalar factor given by the inverse of the order of its group of automorphisms. In the present paper, we revise that algorithm on the level of graphs. Moreover, we extend the result subsequently to further classes of connected graphs, namely, 2-edge connected, simple and loopless graphs. Our method consists of basic graph transformations only.

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E-mail address: mestre@langite.impmc.jussieu.fr (Ângela Mestre)

1 Introduction

The present paper is part of a program laid out in [5, 6] with the focus on the combinatorics of different kinds of connected graphs and problems of graph generation. In particular, the main result of [5] is a recursion formula to generate all trees. This result is generalized to all connected graphs (with loops and multiple edges allowed) in [6]. The underlying structure is a Hopf algebraic representation of graphs. In both cases, in a recursion step, the formulas yield linear combinations of graphs with rational coefficients. The essential property is that the coefficients of graphs are given by the inverses of the orders of their groups of automorphisms. Other problems in this context are considered in [3, 7], for instance.

In this paper, we express the algebraic recursion formula to generate all connected graphs given in [6], in terms of graphs. Moreover, we extend this result successively to 2-edge connected, simple connected and loopless connected graphs. Crucially, as in [5, 6], the exact coefficients of graphs are obtained.

Our method is based on three elementary graph transformations to produce a graph with, say, m edges from a graph with $m-1$ edges. Namely, (a) assigning a loop to a vertex; (b) connecting a pair of vertices with an edge; (c) splitting a vertex in two, distributing the ends of edges assigned to the split vertex, between the two new ones in a given way, and connecting the two new vertices with an edge. In particular, the last operation is (equivalently) defined for simple graphs in [2].

Furthermore, we consider a definition of graph which is more general than the one given in most textbooks on graph theory. In particular, we allow edges not to be connected to vertices at both ends. Clearly, all results hold when the number of these *external* edges vanishes and the standard definition of graph is recovered. However, as in [5, 6], external edges are fundamental for the (induction) proofs. This is due to the fact that vertices carrying (labeled) external edges are distinguishable and thus held fixed under any symmetry.

This paper is organized as follows: Section 2 reviews the basic concepts of graph theory underlying much of the paper. Section 3 contains the definitions of the basic linear maps to be used in the following sections. Section 4 translates the recursion formula to generate all connected graphs given in [6], to the language of graph theory. Section 5 extends this result to 2-edge connected, simple connected and loopless connected graphs.

2 Graphs

We briefly review the basic concepts of graph theory that are relevant for the following sections. For more information on these we refer the reader to standard textbooks such as [1].

Let A and B denote sets. By $[A, B]$, we denote the set of all unordered pairs of elements of A and B, $\{\{a, b\} | a \in A, b \in B\}$. In particular, by $[A]^2 := [A, A]$,

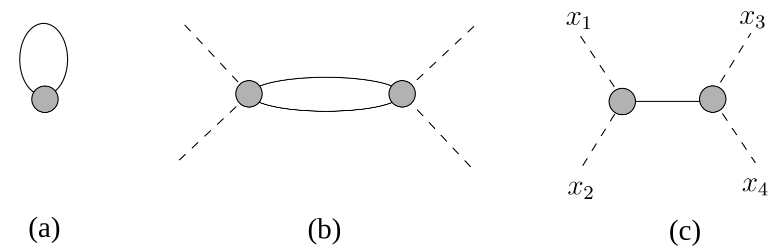


Figure 1: (a) A loop; (b) A graph with both internal and external edges; (c) A graph with labeled external edges. Internal edges are represented by continuous lines, while the external ones are represented by dashed lines.

we denote the set of all 2-element subsets of A. Also, by 2^A, we denote the power set of A, i.e., the set of all subsets of A. By $\mathrm{card}(A)$, we denote the cardinality of the set A. Finally, we recall that the symmetric difference of the sets A and B is given by $A \triangle B := (A \cup B) \backslash (A \cap B)$.

Let $\mathcal{V} = \{v_i\}_{i \in \mathbb{N}}$ and $\mathcal{K} = \{e_a\}_{a \in \mathbb{N}}$ be infinite sets so that $\mathcal{V} \cap \mathcal{K} = \emptyset$. Let $V \subset \mathcal{V}$; $V \neq \emptyset$ and $K \subset \mathcal{K}$ be finite sets. Let $E = E_{\text{int}} \cup E_{\text{ext}} \subseteq [K]^2$ and $E_{\text{int}} \cap E_{\text{ext}} = \emptyset$. Also, let the elements of E satisfy $\{e_a, e_{a'}\} \cap \{e_b, e_{b'}\} = \emptyset$. That is, $e_a, e_{a'} \neq e_b, e_{b'}$ and $e_a \neq e_{a'}$, $e_b \neq e_{b'}$. In this context, a *graph* is a triple $G = (V, K, E)$ together with the following maps:

(a) $\varphi_{\text{int}} := \eta \circ \zeta : E_{\text{int}} \to [V]^2 \cup V; \{e_a, e_{a'}\} \mapsto \{v_i, v_{i'}\}$, where

- $\zeta : E_{\text{int}} \to [K, V] \cup [K]^2$; $\zeta(\{e_a, e_{a'}\}) = \{e_a, v_{i'}\}$ or $\zeta(\{e_a, e_{a'}\}) = \{e_a, e_{a'}\}$;
- $\eta : [K, V] \cup [K]^2 \to [V]^2 \cup V$; $\eta(\{e_a, v_{i'}\}) = \eta(\{e_a, e_{a'}\}) = \{v_i, v_{i'}\}$;

(b) $\varphi_{\text{ext}} : E_{\text{ext}} \to [V, K]; \{e_a, e_{a'}\} \mapsto \{v_i, e_{a'}\}$.

The elements of V and E are called *vertices* and *edges*, respectively. In particular, the elements of E_{int} and E_{ext} are called *internal* edges and *external* edges, respectively. Both internal and external edges are unordered pairs of elements of K. The elements of these pairs are called *ends* of edges. In other words, internal edges are edges that are connected to vertices at both ends, while external edges have one free end. Internal edges with both ends assigned to the same vertex are also called *loops*. Two distinct vertices connected together by one or more internal edges, are said to be *adjacent*. Two or more internal edges connecting the same pair of distinct vertices together, are called *multiple edges*. For instance, Figure 1 (a) shows a loop, while Figure 1 (b) shows a graph with both multiple edges and external edges. A graph with no loops nor multiple edges is called *simple*. The *degree* of a vertex is the number of ends of edges assigned to the vertex. Clearly, a loop adds 2 to the degree of a vertex.

Let $G = (V, K, E)$; $E = E_{\text{int}} \cup E_{\text{ext}}$, $s := \text{card}(E_{\text{ext}})$, together with the maps φ_{int} and φ_{ext} denote a graph. The external edges of the graph G are said to be *labeled* if their free ends are assigned labels $x_1, \ldots, x_s$ from a *label set* $L = \{x_1, \ldots, x_s\}$. Labels on different ends of external edges are required to be distinct. More precisely, a *labeling* of the external edges of the graph G, is an injective map $l : E_{\text{ext}} \to [K, L]; \{e_a, e_{a'}\} \mapsto \{e_a, x_z\}$, where $z \in \{1, \ldots, s\}$. For instance, Figure 1 (c) shows a graph with two vertices and four labeled external edges.

A graph $G^* = (V^*, K^*, E^*)$; $E^* = E^*_{\text{int}} \cup E^*_{\text{ext}}$, together with the maps φ^*_{int} and φ^*_{ext} is called a *subgraph* of a graph $G = (V, K, E)$; $E = E_{\text{int}} \cup E_{\text{ext}}$, together with the maps φ_{int} and φ_{ext} if $V^* \subseteq V$, $K^* \subseteq K$, $E^* \subseteq E$ and $\varphi^*_{\text{int}} = \varphi_{\text{int}}|_{E^*_{\text{int}}}$, $\varphi^*_{\text{ext}} = \varphi_{\text{ext}}|_{E^*_{\text{ext}}}$.

A *path* is a graph $P = (V, K, E_{\text{int}})$; $V = \{v_1, \ldots, v_n\}$, $n := \text{card}(V) > 1$, together with the map φ_{int} so that $\varphi_{\text{int}}(E_{\text{int}}) = \{\{v_1, v_2\}, \{v_2, v_3\}, \ldots, \{v_{n-1}, v_n\}\}$ and the vertices v_1 and v_n have degree 1, while the vertices $v_2, \ldots, v_{n-1}$ have degree 2. In this context, the vertices v_1 and v_n are called the *end point* vertices, while the vertices $v_2, \ldots, v_{n-1}$ are called the *inner* vertices. A *cycle* is a graph $C = (V', K', E'_{\text{int}})$; $V' = \{v_1, \ldots, v_n\}$, together with the map φ'_{int} so that $\varphi'_{\text{int}}(E'_{\text{int}}) = \{\{v_1, v_2\}, \{v_2, v_3\}, \ldots, \{v_{n-1}, v_n\}, \{v_n, v_1\}\}$ and every vertex has degree 2. A graph is said to be *connected* if every pair of vertices is joined by a path. Otherwise, it is *disconnected*. Moreover, a *tree* is a connected graph with no cycles. A 2-*edge connected* graph (or *edge-biconnected* graph) is a connected graph that remains connected after erasing one and whichever internal edge. By definition, a graph consisting of a single vertex is 2-edge connected.

Furthermore, let $G = (V, K, E)$; $E = E_{\text{int}} \cup E_{\text{ext}}$, together with the maps φ_{int} and φ_{ext} denote a graph. The set $2^{E_{\text{int}}}$ is a vector space over the field $\mathbb{Z}_2$ so that vector addition is given by the symmetric difference. The *cycle space* $\mathcal{C}$ of the graph G is defined as the subspace of $2^{E_{\text{int}}}$ generated by all the cycles in G. The dimension of $\mathcal{C}$ is called the *cyclomatic number* of the graph G. Moreover, the cyclomatic number $k := \dim \mathcal{C}$ yields in terms of the vertex number $n := \text{card}(V)$ and the internal edge number $m := \text{card}(E_{\text{int}})$ as $k = m - n + c$, where c denotes the number of connected components of the graph G [4].

Now, let $L = \{x_1, \ldots, x_s\}$ be a finite label set. Let $G = (V, K, E)$; $E = E_{\text{int}} \cup E_{\text{ext}}$, $\text{card}(E_{\text{ext}}) = s$, together with the maps φ_{int} and φ_{ext}, and $G^* = (V^*, K^*, E^*)$; $E^* = E^*_{\text{int}} \cup E^*_{\text{ext}}$, $\text{card}(E^*_{\text{ext}}) = s$, together with the maps φ^*_{int} and φ^*_{ext} denote two graphs. Let $l : E_{\text{ext}} \to [K, L]$ and $l^* : E^*_{\text{ext}} \to [K^*, L]$ be labelings of the elements of E_{ext} and E^*_{ext}, respectively. An *isomorphism* between the graphs G and G^* is a bijection $\psi_V : V \to V^*$ and a bijection $\psi_K : K \to K^*$ which satisfy the following three conditions:

(a) $\varphi_{\text{int}}(\{e_a, e_{a'}\}) = \{v_i, v_{i'}\}$ iff $\varphi^*_{\text{int}}(\{\psi_K(e_a), \psi_K(e_{a'})\}) = \{\psi_V(v_i), \psi_V(v_{i'})\}$;

(b) $\varphi_{\text{ext}}(\{e_a, e_{a'}\}) = \{v_i, e_{a'}\}$ iff $\varphi^*_{\text{ext}}(\{\psi_K(e_a), \psi_K(e_{a'})\}) = \{\psi_V(v_i), \psi_K(e_{a'})\}$;

(c) $L \cap l(\{e_a, e_{a'}\}) = L \cap l^*(\{\psi_K(e_a), \psi_K(e_{a'})\})$.

Clearly, an isomorphism defines an equivalence relation on graphs. In particular, a *vertex* (resp. *edge*) isomorphism between the graphs G and G^* is an isomorphism so that ψ_K (resp. ψ_V) is the identity map. In this context, a *symmetry* of a graph G is an isomorphism of the graph onto itself (i.e, an *automorphism*). The order of the group of automorphisms of a graph G is called the *symmetry factor*. This is denoted by S^G. A *vertex symmetry* (resp. *edge symmetry*) of a graph G is a vertex (resp. edge) automorphism of the graph. The order of the group of vertex (resp. edge) automorphisms is called the *vertex symmetry factor* (resp. *edge symmetry factor*) of the graph. This is denoted by S^G_{vertex} (resp. S^G_{edge}). Furthermore, the orders of the groups of vertex and edge automorphisms of a graph G satisfy $S^G = S^G_{\text{vertex}} \cdot S^G_{\text{edge}}$ (a proof is given in [6], for instance).

3 Elementary linear transformations

We introduce some linear maps and prove their fundamental properties.

Given an arbitrary set X, by $\mathbb{Q}X$, we denote the free vector space on the set X over $\mathbb{Q}$. That is, (a) every vector in $\mathbb{Q}X$ yields a linear combination of the elements of X with coefficients in $\mathbb{Q}$; (b) the set X is linearly independent. Furthermore, by $\text{id}_X : X \to X; x \mapsto x$, we denote the identity map. By $\text{id}_{V\subseteq X} : V \to X; x \mapsto x$, we denote the identity embedding of the subset V of the set X into X. Finally, given maps $f : X \to X^*$ and $g : Y \to Y^*$, by $[f, g]$, we denote the map $[f, g] : [X, Y] \to [X^*, Y^*]; \{x, y\} \mapsto \{f(x), g(y)\}$ with $[f]^2 := [f, f]$.

Let $\mathcal{V} = \{v_i\}_{i\in\mathbb{N}}$ and $\mathcal{K} = \{e_a\}_{a\in\mathbb{N}}$ be infinite sets so that $\mathcal{V} \cap \mathcal{K} = \emptyset$. Fix integers $t, s, k \geq 0$ and $n \geq 1$. Let $L = \{x_1, \ldots, x_s\}$ be a label set. By $V^{n,k,s}$, we denote the set of all graphs with n vertices, cyclomatic number k and s external edges whose free ends are labeled $x_1, \ldots, x_s$. In all that follows, let $V = \{v_1, \ldots, v_n\} \subset \mathcal{V}$, $K = \{e_1, \ldots, e_t\} \subset \mathcal{K}$ and $E = E_{\text{int}} \cup E_{\text{ext}}$ be the sets of vertices, ends of edges and edges, respectively, of all elements of $V^{n,k,s}$. Also, let $l : E_{\text{ext}} \to [K, L]$ be a labeling of their external edges. Moreover, by $V^{n,k,s}_{\text{conn}}$ and $V^{n,k,s}_{\text{disconn}}$, we denote the subsets of $V^{n,k,s}$ whose elements are connected and disconnected graphs, respectively. Finally, by $V^{n,k,s}_{\text{2-edge}}$, $V^{n,k,s}_{\text{simple}}$ and $V^{n,k,s}_{\text{loopless}}$, we denote the subsets of $V^{n,k,s}_{\text{conn}}$ whose elements are 2-edge connected, simple and loopless graphs, respectively.

We now define the following linear transformations.

(i) *Assigning a loop to a vertex*: Let $G = (V, K, E)$; $E = E_{\text{int}} \cup E_{\text{ext}}$, together with the maps φ_{int} and φ_{ext} denote a graph in $V^{n,k,s}$. For all $i \in \{1, \ldots, n\}$, define

$$t_i : \mathbb{Q}V^{n,k,s} \to \mathbb{Q}V^{n,k+1,s}; G \mapsto G^* ,$$

where the graph $G^* = (V^*, K^*, E^*)$; $E^* = E^*_{\text{int}} \cup E^*_{\text{ext}}$, together with the maps φ^*_{int} and φ^*_{ext} satisfies the following conditions:

(a) $V^* = V$;

(b) $K^* = K \cup \{e_{t+1}, e_{t+2}\}$;

(c) $E^* = E^*_{\text{int}} \cup E^*_{\text{ext}}$, where $E^*_{\text{int}} = E_{\text{int}} \cup \{e_{t+1}, e_{t+2}\}$, $E^*_{\text{ext}} = E_{\text{ext}}$;

(d) $\varphi^*_{\text{int}}|_{E_{\text{int}}} = \varphi_{\text{int}}$ and $\varphi^*_{\text{int}}(\{e_{t+1}, e_{t+2}\}) = \{v_i\}$;

(e) $\varphi^*_{\text{ext}} = \varphi_{\text{ext}}$;

(f) $l^* = [\text{id}_{K \subset K^*}, \text{id}_L] \circ l : E^*_{\text{ext}} \to [K^*, L]$ is a labeling of the elements of E^*_{ext}.

The maps t_i are extended to the whole of $\mathbb{Q}V^{n,k,s}$ by linearity. Since the map $t_i : \mathbb{Q}V^{n,k,s} \to t_i(\mathbb{Q}V^{n,k,s})$ is injective, the operation of *erasing a loop* is given by ${t_i}^{-1}$.

(ii) *Connecting a pair of distinct vertices with an internal edge*: Let $G = (V, K, E)$; $E = E_{\text{int}} \cup E_{\text{ext}}$, together with the maps φ_{int} and φ_{ext} denote a graph in $V^{n,k,s}$; $n > 1$. For all $i, j \in \{1, \ldots, n\}$ with $i \neq j$, define

$$l_{i,j} : \mathbb{Q}V^{n,k,s} \to \mathbb{Q}V^{n,k+1,s} \cup \mathbb{Q}V^{n,k,s}; G \mapsto G^*,$$

where the graph $G^* = (V^*, K^*, E^*)$; $E^* = E^*_{\text{int}} \cup E^*_{\text{ext}}$, together with the maps φ^*_{int} and φ^*_{ext} satisfies the following conditions:

(a) $V^* = V$;

(b) $K^* = K \cup \{e_{t+1}, e_{t+2}\}$;

(c) $E^* = E^*_{\text{int}} \cup E^*_{\text{ext}}$, where $E^*_{\text{int}} = E_{\text{int}} \cup \{e_{t+1}, e_{t+2}\}$, $E^*_{\text{ext}} = E_{\text{ext}}$;

(d) $\varphi^*_{\text{int}}|_{E_{\text{int}}} = \varphi_{\text{int}}$ and $\varphi^*_{\text{int}}(\{e_{t+1}, e_{t+2}\}) = \{v_i, v_j\}$;

(e) $\varphi^*_{\text{ext}} = \varphi_{\text{ext}}$;

(f) $l^* = [\text{id}_{K \subset K^*}, \text{id}_L] \circ l : E^*_{\text{ext}} \to [K^*, L]$ is a labeling of the elements of E^*_{ext}.

The maps $l_{i,j}$ are extended to the whole of $\mathbb{Q}V^{n,k,s}$ by linearity. Since the map $l_{i,j} : \mathbb{Q}V^{n,k,s} \to l_{i,j}(\mathbb{Q}V^{n,k,s})$ is injective, the operation of *erasing an internal edge distinct from a loop* is given by ${l_{i,j}}^{-1}$. Furthermore, for $n > 1$ and for all $i, j \in \{1, \ldots, n\}$ with $i \neq j$, define $l^a_{i,j} := l_{i,j} \circ \delta_{i,j}$ and $l^b_{i,j} := l_{i,j} \circ (\text{id} - \delta_{i,j})$, where $\text{id} : \mathbb{Q}V^{n,k,s} \to \mathbb{Q}V^{n,k,s}$ is the identity map and

$$\delta_{i,j} : \mathbb{Q}V^{n,k,s} \to \mathbb{Q}V^{n,k,s}; G \mapsto \begin{cases} G & \text{if} \quad \{v_i, v_j\} \in \varphi_{\text{int}}(E_{\text{int}}) \\ 0 & \text{otherwise} \end{cases}$$

is a linear map.

(iii) *Splitting a vertex in two and distributing the ends of edges assigned to the split vertex, between the two new ones in all possible ways*: Let $G = (V, K, E)$; $E = E_{\text{int}} \cup E_{\text{ext}}$, together with the maps $\varphi_{\text{int}} := \eta \circ \zeta$ and φ_{ext} denote a graph in $V^{n,k,s}$. Let $\mathcal{L}_i \subseteq E$ be the set of edges connected to the vertex $v_i \in V$; $i \in \{1, \ldots, n\}$. Also, let $\mathcal{L}_{\text{int},i}$ and $\mathcal{L}_{\text{ext},i}$ be the subsets of $\mathcal{L}_i$ whose elements are internal edges and external edges, respectively. Hence, $\mathcal{L}_i = \mathcal{L}_{\text{int},i} \cup \mathcal{L}_{\text{ext},i}$ and $\mathcal{L}_{\text{int},i} \cap \mathcal{L}_{\text{ext},i} = \emptyset$. Moreover, let $\mathcal{E}_i \subseteq K$ be the set of ends of edges assigned to the vertex v_i. Also, let $\mathcal{E}_{\text{int},i}$ and $\mathcal{E}_{\text{ext},i}$ be the subsets of $\mathcal{E}_i$ whose elements are ends of internal edges and ends of external edges, respectively. Thus, $\mathcal{E}_i = \mathcal{E}_{\text{int},i} \cup \mathcal{E}_{\text{ext},i}$ and $\mathcal{E}_{\text{int},i} \cap \mathcal{E}_{\text{ext},i} = \emptyset$. Let $[\mathcal{E}'_{\text{int},i}]^2 := \mathcal{L}_{\text{int},i} \cap [\mathcal{E}_{\text{int},i}]^2$ and $\mathcal{E}''_{\text{int},i} := \mathcal{E}_{\text{int},i} \backslash \mathcal{E}'_{\text{int},i}$. Furthermore, let $\mathcal{I}^2_{\mathcal{E}_i}$ denote the set of all ordered partitions of the set $\mathcal{E}_i$ into two disjoint sets: $\mathcal{I}^2_{\mathcal{E}_i} = \{(\mathcal{E}_i^{(1)}, \mathcal{E}_i^{(2)}) | \mathcal{E}_i^{(1)} \cup \mathcal{E}_i^{(2)} = \mathcal{E}_i \quad \text{and} \quad \mathcal{E}_i^{(1)} \cap \mathcal{E}_i^{(2)} = \emptyset\}$. Clearly, $\mathcal{E}_i^{(b)} = \mathcal{E}_{\text{int},i}^{(b)} \cup \mathcal{E}_{\text{ext},i}^{(b)}$; $b \in \{1, 2\}$. Also, a partition of the set $\mathcal{E}_{\text{ext},i}$ generates a partition of the set $\mathcal{L}_{\text{ext},i}$. Hence, $\mathcal{L}_{\text{ext},i}^{(b)} \subset [\mathcal{E}_{\text{ext},i}^{(b)}, K]$. Finally, let $V' \subseteq V \backslash \{v_i\}$ be so that $\varphi_{\text{int}}(\mathcal{L}_{\text{int},i} \backslash [\mathcal{E}'_{\text{int},i}]^2) = [v_i, V']$. In this context, for all $i \in \{1, \ldots, n\}$, define

$$s_i : \mathbb{Q}V^{n,k,s} \to \mathbb{Q}V^{n+1,k-1,s} \cup \mathbb{Q}V^{n+1,k,s}; G \mapsto \sum_{(\mathcal{E}_i^{(1)}, \mathcal{E}_i^{(2)}) \in \mathcal{I}^2_{\mathcal{E}_i}} G_{(\mathcal{E}_i^{(1)}, \mathcal{E}_i^{(2)})} ,$$

where the graphs $G_{(\mathcal{E}_i^{(1)}, \mathcal{E}_i^{(2)})} = (V^*, K^*, E^*)$; $E^* = E^*_{\text{int}} \cup E^*_{\text{ext}}$, together with the maps φ^*_{int} and φ^*_{ext} satisfy the following conditions:

(a) $V^* = V \cup \{v_{n+1}\}$;

(b) $K^* = K$;

(c) $E^* = E^*_{\text{int}} \cup E^*_{\text{ext}}$, where $E^*_{\text{int}} = E_{\text{int}}$, $E^*_{\text{ext}} = E_{\text{ext}}$;

(d) $\varphi^*_{\text{int}} = \eta^* \circ \zeta^*$, where

- $\zeta^*|_{E_{\text{int}} \backslash \mathcal{L}_{\text{int},i}} = \zeta|_{E_{\text{int}} \backslash \mathcal{L}_{\text{int},i}}$;
  $\zeta^*([\mathcal{E}'_{\text{int},i}]^2) = [\mathcal{E}'_{\text{int},i}]^2$;
  $\zeta^*(\mathcal{L}_{\text{int},i} \backslash [\mathcal{E}'_{\text{int},i}]^2) = [\mathcal{E}''_{\text{int},i}, V']$;

- $\eta^*|_{\zeta(E_{\text{int}} \backslash \mathcal{L}_{\text{int},i})} = \eta|_{\zeta(E_{\text{int}} \backslash \mathcal{L}_{\text{int},i})}$;
  $\eta^*([\mathcal{E}''^{(1)}_{\text{int},i}, V']) = [v_i, V']$, $\eta^*([\mathcal{E}''^{(2)}_{\text{int},i}, V']) = [v_{n+1}, V']$;
  $\eta^*([\mathcal{E}'^{(1)}_{\text{int},i}]^2) = \{v_i\}$, $\eta^*([\mathcal{E}'^{(2)}_{\text{int},i}]^2) = \{v_{n+1}\}$;
  $\eta^*([\mathcal{E}'^{(1)}_{\text{int},i}, \mathcal{E}'^{(2)}_{\text{int},i}]) = \{v_i, v_{n+1}\}$, where $\mathcal{E}'^{(b)}_{\text{int},i} \cup \mathcal{E}''^{(b)}_{\text{int},i} = \mathcal{E}^{(b)}_{\text{int},i}$; $b \in \{1, 2\}$;

(e) $\varphi^*_{\text{ext}}|_{E_{\text{ext}} \backslash \mathcal{L}_{\text{ext},i}} = \varphi_{\text{ext}}|_{E_{\text{ext}} \backslash \mathcal{L}_{\text{ext},i}}$;
$\varphi^*_{\text{ext}}(\mathcal{L}^{(1)}_{\text{ext},i}) \subset [v_i, K]$ and $\varphi^*_{\text{ext}}(\mathcal{L}^{(2)}_{\text{ext},i}) \subset [v_{n+1}, K]$;

(f) $l^* = l$ is a labeling of the elements of E^*_{ext}.

The maps s_i are extended to the whole of $\mathbb{Q}V^{n,k,s}$ by linearity. Moreover, we define the maps s_i^c (resp. s_i^d) by restricting the image of s_i to $\mathbb{Q}V^{n+1,k-1,s}_{\text{conn}}$ (resp. $\mathbb{Q}V^{n+1,k,s}_{\text{disconn}}$).

Now, let ${l_{i,j}}^{\rho} := \underbrace{l_{i,j} \circ \ldots \circ l_{i,j}}_{\rho \text{ times}}$, where $\rho \geq 1$ is an integer. We combine the maps ${l_{i,n+1}}^{\rho}$ and s_i to define the following maps:

$$q_i^{(\rho)} := \frac{1}{2(\rho - 1)!} {l_{i,n+1}}^{\rho} \circ s_i : \mathbb{Q}V^{n,k,s} \to \mathbb{Q}V^{n+1,k+\rho-1,s} .$$

For $\rho = 1$, the definition of $q_i^{(1)}$ generalizes the basic operation given in [2] to all partitions of the set $\mathcal{E}_i$ into two sets $\mathcal{E}_i^{(1)}$ and $\mathcal{E}_i^{(2)}$, and to all vertices of the graph. Analogously, the maps $q_i^{c(\rho)}$ (resp. $q_i^{d(\rho)}$) are given by the composition of ${l_{i,n+1}}^{\rho}$ with s_i^c (resp. s_i^d).

(iv) In addition, we revise the operation of *contracting an internal edge connecting two distinct vertices, and fusing the two vertices into one* [1]: Let $G = (V, K, E)$; $E = E_{\text{int}} \cup E_{\text{ext}}$, together with the maps φ_{int} and φ_{ext} denote a graph in $V^{n,k,s}$; $n > 1$. Let $\{e_a, e_{a'}\} \in E_{\text{int}}$; $a, a' \in \{1, \ldots, t\}$ with $a \neq a'$, denote an internal edge connecting two distinct vertices, say, $v_i, v_j \in V$; $i, j \in \{1, \ldots, n\}$ with $i < j$. Let $\mathcal{L}_{\text{int},j}$, $\mathcal{L}_{\text{ext},j}$ and $\mathcal{E}_{\text{int},j}$ denote the sets of internal edges, external edges and ends of internal edges, respectively, assigned to the vertex v_j. Let $[\mathcal{E}'_{\text{int},j}]^2 := \mathcal{L}_{\text{int},j} \cap [\mathcal{E}_{\text{int},j}]^2$. Also, let $V' \subseteq V \backslash \{v_j\}$ be so that $\varphi_{\text{int}}(\mathcal{L}_{\text{int},j} \backslash [\mathcal{E}'_{\text{int},j}]^2) = [v_j, V']$. Finally, let $\mathcal{E}_{\text{free},j}$ denote the set of free ends of the external edges in $\mathcal{L}_{\text{ext},j}$. In this context, define

$$c_{i,j} : \mathbb{Q}V^{n,k,s} \to \mathbb{Q}V^{n-1,k,s}; G \mapsto G^* ,$$

where the graph $G^* = (V^*, K^*, E^*)$; $E^* = E^*_{\text{int}} \cup E^*_{\text{ext}}$, together with the maps φ^*_{int} and φ^*_{ext} satisfies the following conditions:

(a) $V^* = \chi_v(V \backslash \{v_j\})$, where $\chi_v : v_l \mapsto \begin{cases} v_l & \text{if} \quad l \in \{1, \ldots, j-1\} \\ v_{l-1} & \text{if} \quad l \in \{j+1, \ldots, n\} \end{cases}$ is a bijection;

(b) $K^* = \chi_e(K \backslash \{e_a, e_{a'}\})$, where

$$\chi_e : e_b \mapsto \begin{cases} e_b & \text{if} \quad b \in \{1, \ldots, \min(a, a') - 1\} \\ e_{b-1} & \text{if} \quad b \in \{\min(a, a') + 1, \ldots, \max(a, a') - 1\} \\ e_{b-2} & \text{if} \quad b \in \{\max(a, a') + 1, \ldots, t\} \end{cases}$$

is a bijection;

(c) $E^* = E^*_{\text{int}} \cup E^*_{\text{ext}}$, where $E^*_{\text{int}} = [\chi_e]^2(E_{\text{int}} \backslash \{e_a, e_{a'}\})$, $E^*_{\text{ext}} = [\chi_e]^2(E_{\text{ext}})$;

(d) $\varphi^*_{\text{int}} \circ [\chi_e]^2|_{E_{\text{int}} \backslash \mathcal{L}_{\text{int},j}} = [\chi_v]^2 \circ \varphi_{\text{int}}|_{E_{\text{int}} \backslash \mathcal{L}_{\text{int},j}}$;
$\varphi^*_{\text{int}}([\chi_e]^2([\mathcal{E}'_{\text{int},j}]^2)) = \{v_i\}$;
$\varphi^*_{\text{int}}([\chi_e]^2(\mathcal{L}_{\text{int},j} \backslash ([\mathcal{E}'_{\text{int},j}]^2 \cup \{e_a, e_{a'}\}))) = [v_i, \chi_v(V')]$;

(e) $\varphi^*_{\text{ext}} \circ [\chi_e]^2|_{E_{\text{ext}} \backslash \mathcal{L}_{\text{ext},j}} = [\chi_v, \chi_e] \circ \varphi_{\text{ext}}|_{E_{\text{ext}} \backslash \mathcal{L}_{\text{ext},j}}$;
$\varphi^*_{\text{ext}}([\chi_e]^2(\mathcal{L}_{\text{ext},j})) = [v_i, \chi_e(\mathcal{E}_{\text{free},j})]$;

(f) $l^* = [\chi_e, \text{id}_L] \circ l \circ [{\chi_e}^{-1}]^2 : E^*_{\text{ext}} \to [K^*, L]$ is a labeling of the elements of E^*_{ext}.

The maps $c_{i,j}$ are extended to the whole of $\mathbb{Q}V^{n,k,s}$ by linearity.

(v) *Distributing external edges between all elements of a given subset of vertices in all possible ways*: Let $G = (V, K, E)$; $E = E_{\text{int}} \cup E_{\text{ext}}$, together with the maps φ_{int} and φ_{ext} denote a graph in $V^{n,k,s}$. Let $V' = \{v_{z_1}, \ldots, v_{z_{n'}}\} \subseteq V$; with $1 \leq z_1 < \cdots < z_{n'} \leq n$. Let $K' \subset \mathcal{K}$ be a finite set so that $K \cap K' = \emptyset$.

Also, let $E'_{\text{ext}} \subseteq [K']^2$; $s' := \text{card}(E'_{\text{ext}})$. Assume that the elements of E'_{ext} satisfy $\{e_a, e_{a'}\} \cap \{e_b, e_{b'}\} = \emptyset$. Let $L' = \{x_{s+1}, \ldots, x_{s+s'}\}$ be a label set so that $L \cap L' = \emptyset$. Let $l' : E'_{\text{ext}} \to [K', L']$ be a labeling of the elements of E'_{ext}. Finally, let $\mathcal{I}^{n'}_{E'_{\text{ext}}}$ denote the set of all ordered partitions of the set E'_{ext} into n' disjoint subsets: $\mathcal{I}^{n'}_{E'_{\text{ext}}} = \{(E'^{(1)}_{\text{ext}}, \ldots, E'^{(n')}_{\text{ext}}) | E'^{(1)}_{\text{ext}} \cup \ldots \cup E'^{(n')}_{\text{ext}} = E'_{\text{ext}}$ and $E'^{(i)}_{\text{ext}} \cap E'^{(j)}_{\text{ext}} = \emptyset, \forall i, j \in \{1, \ldots, n'\}$ with $i \neq j\}$. In this context, define

$$\xi_{E'_{\text{ext}}, V'} : \mathbb{Q}V^{n,k,s} \to \mathbb{Q}V^{n,k,s+s'}; G \mapsto \sum_{(E'^{(1)}_{\text{ext}}, \ldots, E'^{(n')}_{\text{ext}}) \in \mathcal{I}^{n'}_{E'_{\text{ext}}}} G_{(E'^{(1)}_{\text{ext}}, \ldots, E'^{(n')}_{\text{ext}})} ,$$

where the graphs $G_{(E'^{(1)}_{\text{ext}}, \ldots, E'^{(n')}_{\text{ext}})} = (V^*, K^*, E^*)$; $E^* = E^*_{\text{int}} \cup E^*_{\text{ext}}$, together with the maps φ^*_{int} and φ^*_{ext} satisfy the following conditions:

(a) $V^* = V$;

(b) $K^* = K \cup K'$;

(c) $E^* = E^*_{\text{int}} \cup E^*_{\text{ext}}$, where $E^*_{\text{int}} = E_{\text{int}}$, $E^*_{\text{ext}} = E_{\text{ext}} \cup E'_{\text{ext}}$;

(d) $\varphi^*_{\text{int}} = \varphi_{\text{int}}$;

(e) $\varphi^*_{\text{ext}}|_{E_{\text{ext}}} = \varphi_{\text{ext}}$ and $\varphi^*_{\text{ext}}(E'^{(i)}_{\text{ext}}) \subset [v_{z_i}, K']$ for all $i \in \{1, \ldots, n'\}$;

(f) $l^* : E^*_{\text{ext}} \to [K^*, L \cup L']$, with $l^*|_{E_{\text{ext}}} = l$ and $l^*|_{E'_{\text{ext}}} = l'$, is a labeling of the elements of E^*_{ext}.

The maps $\xi_{E'_{\text{ext}}, V'}$ are extended to the whole of $\mathbb{Q}V^{n,k,s}$ by linearity.

(vi) *Assigning external edges to vertices which have none*: Let $G = (V, K, E)$; $E = E_{\text{int}} \cup E_{\text{ext}}$, together with the maps φ_{int} and φ_{ext} denote a graph in $V^{n,k,s}$. Assume that there exists a set $V' \subseteq V$; $s' := \text{card}(V')$ so that $V' \cap \varphi_{\text{ext}}(E_{\text{ext}}) = \emptyset$. Moreover, let $K' \subset \mathcal{K}$ be a finite set so that $K \cap K' = \emptyset$. Let $E'_{\text{ext}} \subseteq [K']^2$; $\text{card}(E'_{\text{ext}}) = s'$. Assume that the elements of E'_{ext} satisfy $\{e_a, e_{a'}\} \cap \{e_b, e_{b'}\} = \emptyset$. Let $L' = \{x_{s+1}, \ldots, x_{s+s'}\}$ be a label set so that $L \cap L' = \emptyset$. Finally, let $l' : E'_{\text{ext}} \to [K', L']$ be a labeling of the elements of E'_{ext}. In this context, define

$$\epsilon_{E'_{\text{ext}}} : \mathbb{Q}V^{n,k,s} \to \mathbb{Q}V^{n,k,s+s'}; G \mapsto G^* ,$$

where the graph $G^* = (V^*, K^*, E^*)$; $E^* = E^*_{\text{int}} \cup E^*_{\text{ext}}$, together with the maps φ^*_{int} and φ^*_{ext} satisfies the following conditions:

(a) $V^* = V$;

(b) $K^* = K \cup K'$;

(c) $E^* = E^*_{\text{int}} \cup E^*_{\text{ext}}$, where $E^*_{\text{int}} = E_{\text{int}}$, $E^*_{\text{ext}} = E_{\text{ext}} \cup E'_{\text{ext}}$;

(d) $\varphi^*_{\text{int}} = \varphi_{\text{int}}$;

(e) $\varphi^*_{\text{ext}}|_{E_{\text{ext}}} = \varphi_{\text{ext}}$ and $\varphi^*_{\text{ext}}(E'_{\text{ext}}) \subset [V', K']$ so that $V' \cap \varphi^*_{\text{ext}}(E'_{\text{ext}}) = V'$;

(f) $l^* : E^*_{\text{ext}} \to [K^*, L \cup L']$, with $l^*|_{E_{\text{ext}}} = l$ and $l^*|_{E'_{\text{ext}}} = l'$, is a labeling of the elements of E^*_{ext}.

The maps $\epsilon_{E'_{\text{ext}}}$ are extended to the whole of $\mathbb{Q}V^{n,k,s}$ by linearity.

The following lemmas are now established.

Lemma 1 *Fix integers $k, s \geq 0$ and $n, \rho \geq 1$. Then, for all $i, j \in \{1, \ldots, n\}$ with $i \neq j$, the following statements hold:*

(a) $t_i(\mathbb{Q}V^{n,k,s}_{conn}) \subseteq \mathbb{Q}V^{n,k+1,s}_{conn}$;

(b) $l_{i,j}(\mathbb{Q}V^{n,k,s}_{conn}) \subseteq \mathbb{Q}V^{n,k+1,s}_{conn}$;

(c) $q_i^{(\rho)}(\mathbb{Q}V^{n,k,s}_{conn}) \subseteq \mathbb{Q}V^{n+1,k+\rho-1,s}_{conn}$.

Proof: (a), (b) Clearly, the statements hold. (c) Let $G = (V, K, E)$; $E = E_{\text{int}} \cup E_{\text{ext}}$, together with the maps φ_{int} and φ_{ext} denote a graph in $V^{n,k,s}_{\text{conn}}$. Apply the map $q_i^{(\rho)} := \frac{1}{2(\rho-1)!} {l_{i,n+1}}^{\rho} \circ s_i$ to the graph G. In particular, $s_i(G)$ is a linear combination of graphs, each of which is either connected or disconnected with two components. Applying the map ${l_{i,n+1}}^{\rho}$ to $s_i(G)$ yields connected graphs. This completes the proof. □

Lemma 2 *Fix integers $s \geq 0$, $k > 0$ and $n \geq 1$. Let $G = (V, K, E)$; $E = E_{int} \cup E_{ext}$, together with the maps φ_{int} and φ_{ext} denote a graph in $V^{n,k,s}_{conn}$ which is not simple. Then, for all $i, j \in \{1, \ldots, n\}$ with $i \neq j$, the following statements hold:*

(a) $l_{i,j}(G) \notin \mathbb{Q}V^{n,k+1,s}_{simple}$;

(b) $q_i^{d(1)}(G) \notin \mathbb{Q}V^{n+1,k,s}_{simple}$.

Proof: (a) Clearly, the statement holds. (b) By assumption, the graph G has at least either one loop or multiple edges. Apply the map $q_i^{d(1)} := \frac{1}{2} l_{i,n+1} \circ s_i^d$ to the graph G. In particular, $s_i^d(G)$ is a linear combination of disconnected graphs, each of which is produced from the graph G by assigning all ends of internal edges belonging to the same cycles, from the vertex $v_i \in V$ to either v_i or v_{n+1}. Therefore, at least one of the two components of the graphs in $s_i^d(G)$ is not simple. Applying the map $l_{i,n+1}$ to $s_i^d(G)$ cannot produce simple graphs. This completes the proof. □

Lemma 3 *Fix integers $k, s \geq 0$ and $n \geq 1$. Then, for all $i, j \in \{1, \ldots, n\}$ with $i \neq j$, the following statements hold:*

(a) $l^b_{i,j}(\mathbb{Q}V^{n,k,s}_{simple}) \subseteq \mathbb{Q}V^{n,k+1,s}_{simple}$;

(b) $q_i^{(1)}(\mathbb{Q}V^{n,k,s}_{simple}) \subseteq \mathbb{Q}V^{n+1,k,s}_{simple}$.

Proof: Applying the maps $l^b_{i,j}$ or $q^{(1)}_i$ to a simple graph cannot introduce loops nor multiple edges. □

Lemma 4 *Fix integers $k, s \geq 0$ and $n \geq 1$. Let $G = (V, K, E)$; $E = E_{int} \cup E_{ext}$, together with the maps φ_{int} and φ_{ext} denote a graph in $V^{n,k,s}_{conn}$ which is not 2-edge connected. Then, for all $i \in \{1, \dots, n\}$, the following statements hold:*

(a) $t_i(G) \notin \mathbb{Q}V^{n,k+1,s}_{2\text{-edge}}$;

(b) $q^{(1)}_i(G) \notin \mathbb{Q}V^{n+1,k,s}_{2\text{-edge}}$.

Proof: (a) Clearly, the statement holds. (b) First, by definition all connected graphs with only one vertex are 2-edge connected. Consequently, the maps $q^{(1)}_i$ produce 2-edge connected graphs with two vertices only from 2-edge connected ones. Now, let $n > 1$. By assumption, the graph G has at least one internal edge which does not belong to any cycle. Therefore, it connects two (distinct) vertices that must be connected together with only one internal edge. Let these vertices be $v_i, v_j \in V$; $i, j \in \{1, \dots, n\}$ with $i \neq j$. Apply the map $q^{(1)}_i := \frac{1}{2} l_{i,n+1} \circ s_i$ to the graph G. In particular, $q^{(1)}_i(G)$ is a linear combination of graphs, each of which is so that the vertex v_j is connected with only one internal edge either to v_i or v_{n+1} (but not to both). Clearly, only cycles containing the vertex v_i, are affected by the map $q^{(1)}_i$. That is, the vertex v_j cannot share a cycle with neither of the vertices v_i or v_{n+1}. Hence, the graphs in $q^{(1)}_i(G)$ are not 2-edge connected. This completes the proof. □

Lemma 5 *Fix integers $k, s \geq 0$ and $n \geq 1$. Then, for all $i \in \{1, \dots, n\}$, the following statements hold:*

(a) $t_i(\mathbb{Q}V^{n,k,s}_{2\text{-edge}}) \subseteq \mathbb{Q}V^{n,k+1,s}_{2\text{-edge}}$;

(b) $q^{c(1)}_i(\mathbb{Q}V^{n,k,s}_{2\text{-edge}}) \subseteq \mathbb{Q}V^{n+1,k,s}_{2\text{-edge}}$.

Proof: (a) Clearly, the statement holds. (b) Let $G = (V, K, E)$; $E = E_{\text{int}} \cup E_{\text{ext}}$, together with the maps φ_{int} and φ_{ext} denote a graph in $V^{n,k,s}_{2\text{-edge}}$. Apply the map $q^{c(1)}_i := \frac{1}{2} l_{i,n+1} \circ s^c_i$ to the graph G. In particular, $s^c_i(G)$ is a linear combination of graphs, each of which is produced from the graph G by transforming one or more cycles containing the vertex $v_i \in V$, into paths whose end point vertices are v_i and v_{n+1}. Moreover, every way to assign the remaining ends of internal edges in the process, from v_i to either v_i or v_{n+1}, defines new cycles. Therefore, applying the map $l_{i,n+1}$ to $s^c_i(G)$ restores the broken cycles and yields 2-edge connected graphs. This completes the proof. □

4 Arbitrary connected graphs

The present section has substantial overlap with Section II of [6]. Its main result is a recursion formula to generate all connected graphs directly in the algebraic representation rooted in [5]. Here, we formulate that formula on the level of graphs. In a recursion step, the formula yields the linear combination of all graphs having the same vertex and cyclomatic numbers. Moreover, the sum of the coefficients of all graphs in the same equivalence class, corresponds to the inverse of the order of their group of automorphisms.

We use the maps t_i and $q_i^{(1)}$ defined in the preceding section to recursively generate all connected graphs following [6].

Theorem 6 *Fix an integer $s \geq 0$. Let $L = \{x_1, \ldots, x_s\}$ be a label set. For all integers $k \geq 0$ and $n \geq 1$, define $\omega^{n,k,s} \in \mathbb{Q}V_{conn}^{n,k,s}$ by the following recursion relation:*

- *$\omega^{1,0,s}$ is a single vertex with s external edges whose free ends are labeled $x_1, \ldots, x_s$, and unit coefficient;*
-

$$\omega^{n,k,s} := \frac{1}{k+n-1} \left(\sum_{i=1}^{n-1} q_i^{(1)}(\omega^{n-1,k,s}) + \frac{1}{2} \sum_{i=1}^{n} t_i(\omega^{n,k-1,s}) \right). \qquad (1)$$

Then, for fixed values of n and k, $\omega^{n,k,s} = \sum_{G \in V_{conn}^{n,k,s}} \alpha_G \, G$; $\alpha_G \in \mathbb{Q}$ and $\alpha_G > 0$ for all $G \in V_{conn}^{n,k,s}$. Moreover, $\sum_{G \in \mathscr{C}} \alpha_G = 1/S^{\mathscr{C}}$, where $\mathscr{C} \subseteq V_{conn}^{n,k,s}$ denotes an arbitrary equivalence class of graphs and $S^{\mathscr{C}}$ denotes their symmetry factor.

In the recursion equation above, the t_i summand does not appear when $k = 0$. Theorem 6 and formula (1) correspond to Theorem 10 and formula (11) of [6], respectively. In particular, for $k = 0$, the former theorem and formula correspond to Lemma 10 and formula (12) of [5], respectively. Moreover, formula (1) is an instance of a double recursion. Therefore, its algorithmic implementation is that of any recursive function that makes two calls to itself, such as the defining recurrence of the binomial coefficients.

Proof: The proof is nearly the same as that of Theorem 10 of [6]. The procedure is also very analogous to the one given in [5]. We translate every lemma given in Section II of the former paper to the present setting.

Lemma 7 *Fix integers $s, k \geq 0$ and $n \geq 1$. Let $\omega^{n,k,s} = \sum_{G \in V_{conn}^{n,k,s}} \alpha_G \, G \in \mathbb{Q}V_{conn}^{n,k,s}$ be defined by formula (1). Then, $\alpha_G > 0$ for all $G \in V_{conn}^{n,k,s}$.*

Proof: The proof proceeds by induction on the internal edge number m. Clearly, the statement holds for $m = 0$. We assume the statement to hold for a general number of internal edges $m - 1$. Let $G = (V, K, E)$; $E = E_{\text{int}} \cup E_{\text{ext}}$, $m := \text{card}(E_{\text{int}})$, together with the maps φ_{int} and φ_{ext} denote an arbitrary graph in $V_{\text{conn}}^{n,k,s}$, where $m = k + n - 1$. We now show that the graph G is generated by applying the maps t_i to graphs occurring in $\omega^{n,k-1,s} = \sum_{G^* \in V_{\text{conn}}^{n,k-1,s}} \gamma_{G^*} G^*$; $\gamma_{G^*} \in \mathbb{Q}$, or the maps $q_i^{(1)} := \frac{1}{2} l_{i,n} \circ s_i$ to graphs occurring in $\omega^{n-1,k,s} = \sum_{G' \in V_{\text{conn}}^{n-1,k,s}} \beta_{G'} G'$; $\beta_{G'} \in \mathbb{Q}$.

(i) Suppose that the graph G has at least one vertex with one or more loops. Let this vertex be $v_i \in V$; $i \in \{1, \ldots, n\}$, for instance. Erasing any loop yields a graph ${t_i}^{-1}(G) \in V_{\text{conn}}^{n,k-1,s}$. By induction assumption, $\gamma_{{t_i}^{-1}(G)} > 0$. Hence, applying the map t_i to the graph ${t_i}^{-1}(G)$ produces again the graph G. That is, $\alpha_G > 0$.

(ii) Suppose that the graph G has no loops. There exists $i \in \{1, \ldots, n-1\}$ so that $\{v_i, v_n\} \in \varphi_{\text{int}}(E_{\text{int}})$. Applying the map $c_{i,n}$ to the graph G yields a graph $c_{i,n}(G) \in V_{\text{conn}}^{n-1,k,s}$. By induction assumption, $\beta_{c_{i,n}(G)} > 0$. Hence, applying the map $q_i^{(1)}$ to the graph $c_{i,n}(G)$ produces a linear combination of graphs, one of which is the graph G. That is, $\alpha_G > 0$.

□

What remains in order to prove Theorem 6 is to show that the sum of the coefficients of all graphs in the same equivalence class, is given by the inverse of their symmetry factor. We start with a more restricted result.

Lemma 8 *Fix integers $k \geq 0$, $n \geq 1$ and $s \geq n$. Let $\mathscr{C} \subseteq V_{\text{conn}}^{n,k,s}$ denote an equivalence class. Let $G = (V, K, E)$; $E = E_{\text{int}} \cup E_{\text{ext}}$, together with the maps φ_{int} and φ_{ext} denote a graph in $\mathscr{C}$. Assume that $V \cap \varphi_{\text{ext}}(E_{\text{ext}}) = V$. Let $\omega^{n,k,s} = \sum_{G \in V_{\text{conn}}^{n,k,s}} \alpha_G \, G \in \mathbb{Q}V_{\text{conn}}^{n,k,s}$ be defined by formula (1). Then, $\sum_{G \in \mathscr{C}} \alpha_G = 1/S^{\mathscr{C}}$, where $S^{\mathscr{C}}$ denotes the symmetry factor of every graph in $\mathscr{C}$.*

Proof: The proof proceeds by induction on the internal edge number m. Clearly, the statement holds for $m = 0$. We assume the statement to hold for a general number of internal edges $m-1$. Consider the graph $G = (V, K, E) \in \mathscr{C}$; $E = E_{\text{int}} \cup E_{\text{ext}}$, $m := \text{card}(E_{\text{int}}) = k + n - 1$, together with the maps φ_{int} and φ_{ext}. By Lemma 7, the coefficient of the graph G in $\omega^{n,k,s}$ is positive, i.e., $\alpha_G > 0$. Moreover, the graph $G \in \mathscr{C}$ is so that every one of its vertices has at least one (labeled) external edge. Hence, the graph G has no non-trivial vertex symmetries: $S_{\text{vertex}}^{\mathscr{C}} = 1$. That is, $S^{\mathscr{C}} = S_{\text{edge}}^{\mathscr{C}}$ for any symmetry is an edge symmetry. We proceed to show that $\sum_{G \in \mathscr{C}} \alpha_G = 1/S^{\mathscr{C}}$. To this end, we check from which graphs with $m-1$ internal edges, the graphs in the equivalence class $\mathscr{C}$ are generated by the recursion formula (1), and how many times they are generated. Choose any one of the m internal edges of the graph $G \in \mathscr{C}$.

(i) If that internal edge is a loop, let this be assigned to the vertex $v_i \in V$; $i \in \{1, \ldots, n\}$, for instance. Also, assume that the vertex v_i has exactly $1 \leq \tau \leq k$ loops as well as $x \geq 1$ external edges whose free ends are labeled $x_{a_1}, \ldots, x_{a_x}$, with $1 \leq a_1 < \cdots < a_x \leq s$. Erasing any one of these loops yields a graph ${t_i}^{-1}(G) \in V_{\text{conn}}^{n,k-1,s}$ whose symmetry factor is related to that of $G \in \mathscr{C}$ via $S^{{t_i}^{-1}(G)} = S^{\mathscr{C}}/(2\tau)$. Let $\omega^{n,k-1,s} = \sum_{G^* \in V_{\text{conn}}^{n,k-1,s}} \gamma_{G^*} G^* \, ; \gamma_{G^*} \in \mathbb{Q}$. Also, let $\mathscr{A} \subseteq V_{\text{conn}}^{n,k-1,s}$ denote the equivalence class containing ${t_i}^{-1}(G)$. The map t_i produces the graph G from the graph ${t_i}^{-1}(G)$ with coefficient $\alpha_G^* = \gamma_{{t_i}^{-1}(G)} \in \mathbb{Q}$. Each vertex of the graph ${t_i}^{-1}(G)$ has at least one labeled external edge. Hence, by induction assumption, $\sum_{G^*\in\mathscr{A}}\gamma_{G^*} = 1/S^{t_i^{-1}(G)} = 1/S^{\mathscr{A}}$. Now, take one graph (distinct from the graph G) in $\mathscr{C}$ in turn, choose any one of the τ loops of the vertex having x external edges whose free ends are labeled $x_{a_1},\ldots,x_{a_x}$, and repeat the procedure above. We obtain

$$\sum_{G\in\mathscr{C}}\alpha^*_G = \sum_{G^*\in\mathscr{A}}\gamma_{G^*} = \frac{1}{S^{\mathscr{A}}} = \frac{2\tau}{S^{\mathscr{C}}}.$$

Therefore, according to formula (1), the contribution to $\sum_{G\in\mathscr{C}}\alpha_G$ is $\tau/(m\cdot S^{\mathscr{C}})$. Distributing this factor between the τ loops considered yields $1/(m\cdot S^{\mathscr{C}})$ for each loop.

(ii) If that internal edge is not a loop, let this edge be connected to the vertices, $v_i, v_j\in V$; $i,j\in\{1,\ldots,n\}$ with $i<j$, for instance. Also, assume that v_i has $\tau'\geq 0$ loops as well as $r\geq 1$ external edges whose free ends are labeled $x_{a_1},\ldots,x_{a_r}$, with $1\leq a_1<\cdots<a_r\leq s$, while v_j has $\tau''\geq 0$ loops as well as $r'\geq 1$ external edges whose free ends are labeled $x_{b_1},\ldots,x_{b_{r'}}$, with $1\leq b_1<\cdots<b_{r'}\leq s$ and $a_z\neq b_{z'}$ for all $z\in\{1,\ldots,r\}, z'\in\{1,\ldots,r'\}$. Finally, assume that the two vertices are connected together with $\rho\geq 1$ internal edges, so that $1\leq\tau'+\tau''+\rho\leq k+1$. Contracting any one of these internal edges yields a graph $c_{i,j}(G)\in V^{n-1,k,s}_{\text{conn}}$ whose vertex v_i has $\mu:=\tau'+\tau''+\rho-1$ loops as well as $r+r'$ external edges whose free ends are labeled $x_{a_1},\ldots,x_{a_r},x_{b_1},\ldots,x_{b_{r'}}$. Consequently, the symmetry factor of the graph $c_{i,j}(G)$ is related to that of $G\in\mathscr{C}$ via

$$\frac{1}{2^\mu}\frac{1}{\mu!}S^{c_{i,j}(G)} = \frac{1}{2^{\tau'}\tau'!}\frac{1}{2^{\tau''}\tau''!}\frac{1}{\rho!}S^{\mathscr{C}}\,.$$

Let $\omega^{n-1,k,s} = \sum_{G'\in V^{n-1,k,s}_{\text{conn}}}\beta_{G'}G'\,;\beta_{G'}\in\mathbb{Q}$. Let $\mathscr{B}\subseteq V^{n-1,k,s}_{\text{conn}}$ denote the equivalence class containing $c_{i,j}(G)$. Apply the map $q^{(1)}_i := \frac{1}{2}l_{i,n}\circ s_i$ to $c_{i,j}(G)$. Notice that there are two ways to distribute the $r+r'$ external edges assigned to the vertex v_i of the graph $c_{i,j}(G)$ between the vertices v_i and v_n, so that one vertex is assigned with r external edges whose free ends are labeled $x_{a_1},\ldots,x_{a_r}$, while the other is assigned with r' external edges whose free ends are labeled $x_{b_1},\ldots,x_{b_{r'}}$. Therefore, there are two graphs in the linear combination of graphs $q^{(1)}_i(c_{i,j}(G))$ which are isomorphic to the graph $G\in\mathscr{C}$. To calculate the coefficient $\alpha'_G\in\mathbb{Q}$ of each of these graphs in that linear combination, we need to count the number of ways to distribute the 2μ ends of internal edges assigned to the vertex v_i of the graph $c_{i,j}(G)\in V^{n-1,k,s}_{\text{conn}}$, between the vertices v_i and v_n, so that the vertex with the given r external edges is assigned with τ' loops, the vertex with the given r' external edges is assigned with τ'' loops, while the remaining $\rho-1$ internal edges are employed to connect the two vertices together. Now, there are $\binom{\mu}{\tau'} = \frac{\mu!}{(\mu-\tau')!\tau'!}$ ways to assign both ends of τ' internal edges chosen among the μ internal edges in the process, to the vertex with the aforesaid r external edges. Besides, there are $\binom{\mu-\tau'}{\tau''} = \frac{(\mu-\tau')!}{(\mu-\tau'-\tau'')!\tau''!}$ ways to assign both ends of τ'' internal edges chosen among the $\mu-\tau'$ internal edges in the process, to the vertex with the aforesaid r' external edges. Finally, there are two ways to distribute one end of each of the remaining $\rho-1$ internal edges, per vertex. This yields $2^{\rho-1}$ ways to connect the two vertices together with $\rho-1$ internal edges. The final result is given by the product of all these factors. Hence, there are

$$2^{\rho-1}\frac{\mu!}{(\mu-\tau')!\tau'!}\cdot\frac{(\mu-\tau')!}{(\mu-\tau'-\tau'')!\tau''!}=2^{\rho-1}\frac{\mu!}{\tau'!\,\tau''!\,(\rho-1)!}$$

ways to distribute the 2μ ends of internal edges between the vertices v_i and v_n so as to produce a graph in the equivalence class $\mathscr{C}$. Consequently, $\alpha'_G = 2^{\rho-2}\frac{\mu!}{\tau'!\,\tau''!\,(\rho-1)!}\beta_{c_{i,j}(G)}$ for the map $q_i^{(1)}$ carries the factor 1/2. Moreover, each vertex of the graph $c_{i,j}(G)$ has at least one labeled external edge. Therefore, by induction assumption, $\sum_{G'\in\mathscr{B}}\beta_{G'} = 1/S^{c_{i,j}(G)} = 1/S^{\mathscr{B}}$. Now, take one graph (distinct from G) in $\mathscr{C}$ in turn, choose any one of the ρ internal edges connecting together the pair of vertices so that one vertex has r external edges whose free ends are labeled $x_{a_1},\ldots,x_{a_r}$, while the other has r' external edges whose free ends are labeled $x_{b_1},\ldots,x_{b_{r'}}$, and repeat the procedure above. We obtain

$$\begin{aligned}\sum_{G\in\mathscr{C}}\alpha'_G &= 2\cdot 2^{\rho-2}\frac{\mu!}{\tau'!\,\tau''!\,(\rho-1)!}\sum_{G'\in\mathscr{B}}\beta_{G'}\\ &= 2^{\rho-1}\frac{\mu!}{\tau'!\,\tau''!\,(\rho-1)!}\frac{1}{S^{\mathscr{B}}}\\ &= 2^{\rho-1}\frac{\mu!}{\tau'!\,\tau''!\,(\rho-1)!}\cdot\frac{\tau'!\,\tau''!\,\rho!}{\mu!}\cdot\frac{1}{2^{\rho-1}S^{\mathscr{C}}}\\ &= \frac{\rho}{S^{\mathscr{C}}},\end{aligned}$$

where the factor 2 on the right hand side of the first equality, is due to the fact that each graph in the equivalence class $\mathscr{B}$ generates two graphs in $\mathscr{C}$. Therefore, according to formula (1), the contribution to $\sum_{G\in\mathscr{C}}\alpha_G$ is $\rho/(m\cdot S^{\mathscr{C}})$. Distributing this factor between the ρ internal edges considered yields $1/(m\cdot S^{\mathscr{C}})$ for each edge.

We conclude that every one of the m internal edges of the graph G contributes $1/(m\cdot S^{\mathscr{C}})$ to $\sum_{G\in\mathscr{C}}\alpha_G$. Hence, the overall contribution is exactly $1/S^{\mathscr{C}}$. This completes the proof. □

$\omega^{n,k,s}$ satisfies the following property.

Lemma 9 *Fix integers $s,k\geq 0$ and $n\geq 1$. Let V, K and $E=E_{int}\cup E_{ext}$ be the sets of vertices, ends of edges and edges, respectively, of all graphs in $V^{n,k,s}$. Let $L=\{x_1,\ldots,x_s\}$ be a label set and let $l:E_{ext}\to[K,L]$ be a labeling of the elements of E_{ext}. Let $\omega^{n,k,s}=\sum_{G\in V_{conn}^{n,k,s}}\alpha_G\,G\in\mathbb{Q}V_{conn}^{n,k,s}$ be defined* *by formula (1). Moreover, let $K' \subset \mathcal{K}$ be a finite set so that $K \cap K' = \emptyset$. Let $E'_{ext} \subseteq [K']^2$; $s' := \mathrm{card}(E'_{\mathrm{ext}})$. Assume that the elements of E'_{ext} satisfy $\{e_a, e_{a'}\} \cap \{e_b, e_{b'}\} = \emptyset$. Also, let $L' = \{x_{s+1}, \ldots, x_{s+s'}\}$ be a label set so that $L \cap L' = \emptyset$. Let $l' : E'_{ext} \to [K', L']$ be a labeling of the elements of E'_{ext}. Then, $\omega^{n,k,s+s'} = \xi_{E'_{ext},V}(\omega^{n,k,s})$.*

Proof: Clearly, $\xi_{E'_{\mathrm{ext}},V} = \sum_{\mathcal{L}_{\mathrm{ext}} \subseteq E'_{\mathrm{ext}}} \xi_{E'_{\mathrm{ext}} \setminus \mathcal{L}_{\mathrm{ext}}, V \setminus \{v_i, v_n\}} \circ \xi_{\mathcal{L}_{\mathrm{ext}}, \{v_i, v_n\}} : \mathbb{Q}V^{n,k,s} \to \mathbb{Q}V^{n,k,s+s'}$; $i \in \{1, \ldots, n-1\}$. Also, $\xi_{\mathcal{L}_{\mathrm{ext}}, \{v_i, v_n\}} \circ s_i = s_i \circ \xi_{\mathcal{L}_{\mathrm{ext}}, \{v_i\}} : \mathbb{Q}V^{n-1,k,s} \to \mathbb{Q}V^{n,k-1,s+s^*} \cup \mathbb{Q}V^{n,k,s+s^*}$, where $s^* = \mathrm{card}(\mathcal{L}_{\mathrm{ext}})$. Therefore, the equality $\omega^{n,k,s+s'} = \xi_{E'_{\mathrm{ext}},V}(\omega^{n,k,s})$ follows immediately from the recursive definition (1). □

We proceed to show that $\sum_{G \in \mathscr{C}} \alpha_G = 1/S^{\mathscr{C}}$, where $\mathscr{C} \subseteq V^{n,k,s}_{\mathrm{conn}}$ denotes any equivalence class.

Lemma 10 *Fix integers $s, k \geq 0$ and $n \geq 1$. Let $\mathscr{C} \subseteq V^{n,k,s}_{conn}$ denote an arbitrary equivalence class. Let $\omega^{n,k,s} = \sum_{G \in V^{n,k,s}_{conn}} \alpha_G \, G \in \mathbb{Q}V^{n,k,s}_{conn}$ be defined by formula (1). Then, $\sum_{G \in \mathscr{C}} \alpha_G = 1/S^{\mathscr{C}}$, where $S^{\mathscr{C}}$ denotes the symmetry factor of every graph in $\mathscr{C}$.*

Proof: Choose a graph $G = (V, K, E) \in \mathscr{C}$; $E = E_{\mathrm{int}} \cup E_{\mathrm{ext}}$, together with the maps φ_{int} and φ_{ext}. Let $L = \{x_1, \ldots, x_s\}$ be a label set and let $l : E_{\mathrm{ext}} \to [K, L]$ be a labeling of the elements of E_{ext}. If $\varphi_{\mathrm{ext}}(E_{\mathrm{ext}}) = V$, we simply recall Lemma 8. Thus, we may assume that there exists a set $V' \subseteq V$; $s' := \mathrm{card}(V')$ so that $V' \cap \varphi_{\mathrm{ext}}(E_{\mathrm{ext}}) = \emptyset$. Let $K' \subset \mathcal{K}$ be a finite set so that $K \cap K' = \emptyset$. Let $E'_{\mathrm{ext}} \subseteq [K']^2$; $\mathrm{card}(E'_{\mathrm{ext}}) = s'$. Assume that the elements of E'_{ext} satisfy $\{e_a, e_{a'}\} \cap \{e_b, e_{b'}\} = \emptyset$. Also, let $L' = \{x_{s+1}, \ldots, x_{s+s'}\}$ be a label set so that $L \cap L' = \emptyset$. Finally, let $l' : E'_{\mathrm{ext}} \to [K', L']$ be a labeling of the elements of E'_{ext}. Now, apply a map $\epsilon_{E'_{\mathrm{ext}}}$ to the graph G. Let $\mathscr{D} \subseteq V^{n,k,s+s'}_{\mathrm{conn}}$ denote the equivalence class containing $\epsilon_{E'_{\mathrm{ext}}}(G)$. Let $\omega^{n,k,s+s'} = \sum_{G' \in V^{n,k,s+s'}_{\mathrm{conn}}} \beta_{G'} G'$; $\beta_{G'} \in \mathbb{Q}$. By Lemma 8, $\sum_{G' \in \mathscr{D}} \beta_{G'} = 1/S^{\epsilon_{E'_{\mathrm{ext}}}(G)} = 1/S^{\mathscr{D}}$. Since, in general, the maps $\epsilon_{E'_{\mathrm{ext}}}$ are not uniquely defined, assume that there are T distinct maps $\epsilon^{(l)}_{E'_{\mathrm{ext}}}$; $l \in \{1, \ldots, T\}$ so that $\epsilon^{(l)}_{E'_{\mathrm{ext}}}(G) \in \mathscr{D}$. Clearly, $\beta_{\epsilon^{(l)}_{E'_{\mathrm{ext}}}(G)} = \alpha_G > 0$. Therefore, repeating the same procedure for every graph in $\mathscr{C}$ and recalling Lemma 9, we obtain

$$\sum_{G' \in \mathscr{D}} \beta_{G'} = \sum_{l=1}^{T} \sum_{G \in \mathscr{C}} \beta_{\epsilon^{(l)}_{E'_{\mathrm{ext}}}(G)} = T \sum_{G \in \mathscr{C}} \alpha_G = \frac{1}{S^{\mathscr{D}}} \,.$$

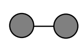
That is, $\sum_{G \in \mathscr{C}} \alpha_G = 1/(T \cdot S^{\mathscr{D}})$. Now, every map $\epsilon^{(l)}_{E'_{\mathrm{ext}}}$ defines a vertex symmetry of the graph G. This can have no more than these vertex symmetries, since the vertices that already carry (labeled) external edges, are distinguishable and thus held fixed under any symmetry. Hence, $S^{G}_{\mathrm{vertex}} = S^{\mathscr{C}}_{\mathrm{vertex}} = T$. Moreover, $S^{\mathscr{D}} = S^{\mathscr{D}}_{\mathrm{edge}} = S^{\mathscr{C}}_{\mathrm{edge}}$. Finally, from the identity $S^{\mathscr{C}} = S^{\mathscr{C}}_{\mathrm{vertex}} \cdot S^{\mathscr{C}}_{\mathrm{edge}}$, follows that $\sum_{G \in \mathscr{C}} \alpha_G = 1/S^{\mathscr{C}}$. □

This completes the proof of Theorem 6. □

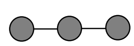
4.1 Examples

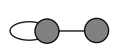
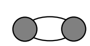
The present section overlaps the appendix of [6]. We show the result of computing all mutually non-isomorphic connected graphs without external edges as contributions to $\omega^{n,k,0}$ via formula (1), up to order $n+k \leq 4$. The coefficients in front of graphs are the inverses of the orders of their groups of automorphisms.

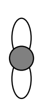
$n = 1, k = 0$ 

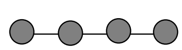
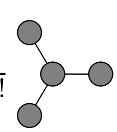
$n = 2\,, k = 0$ $\frac{1}{2}$ 

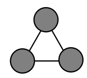
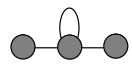
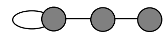
$n = 1\,, k = 1$ $\frac{1}{2}$ 

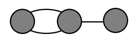
$n = 3\,, k = 0$ $\frac{1}{2}$ 

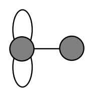
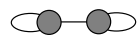
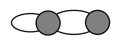
$n = 2\,, k = 1$ $\frac{1}{2}$  $+ \frac{1}{2^2}$ 

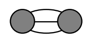
$n = 1\,, k = 2$ $\frac{1}{2^3}$ 

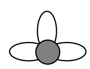
$n = 4\,, k = 0$ $\frac{1}{2}$  $+ \frac{1}{3!}$ 

$n = 3\,, k = 1$ $\quad \frac{1}{3!}$  $+ \frac{1}{2^2}$  $+ \frac{1}{2}$  $+$

$+ \frac{1}{2}$ 

$n = 2\,, k = 2$ $\quad \frac{1}{2^3}$  $+ \frac{1}{2^3}$  $+ \frac{1}{2^2}$  $+$

$+ \frac{1}{2 \cdot 3!}$ 

$n = 1\,, k = 3$ $\quad \frac{1}{2^3 \cdot 3!}$ 

5 Extensions

We generalize Theorem 6 to 2-edge connected, simple connected and loopless connected graphs. These three results were not obtained in previous papers using the Hopf algebraic approach given in [5, 6].

5.1 2-edge connected graphs

By Lemmas 4 and 5, Theorem 6 specializes to 2-edge connected graphs by replacing the maps $q_i^{(1)}$ by the maps $q_i^{c(1)}$ in formula (1).

Theorem 11 *Fix an integer $s \geq 0$. Let $L = \{x_1, \ldots, x_s\}$ be a label set. For all integers $k \geq 0$ and $n \geq 1$, define $\beta^{n,k,s} \in \mathbb{Q}V^{n,k,s}_{\text{2-edge}}$ by the following recursion relation:*

- *$\beta^{1,0,s}$ is a single vertex with s external edges whose free ends are labeled $x_1, \ldots, x_s$, and unit coefficient;*
- $$\beta^{n,k,s} := \frac{1}{k+n-1}\left(\sum_{i=1}^{n-1} q_i^{c(1)}(\beta^{n-1,k,s}) + \frac{1}{2}\sum_{i=1}^{n} t_i(\beta^{n,k-1,s})\right), k > 0\,. \tag{2}$$

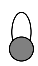
Then, for fixed values of n and k, $\beta^{n,k,s} = \sum_{G \in V^{n,k,s}_{\text{2-edge}}} \alpha_G\, G$; $\alpha_G \in \mathbb{Q}$ and $\alpha_G > 0$ for all $G \in V^{n,k,s}_{\text{2-edge}}$. Moreover, $\sum_{G \in \mathscr{C}} \alpha_G = 1/S^{\mathscr{C}}$, where $\mathscr{C} \subseteq V^{n,k,s}_{\text{2-edge}}$ denotes an arbitrary equivalence class of graphs and $S^{\mathscr{C}}$ denotes their symmetry factor.

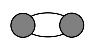
For $k = 1$ and $n > 1$, formula (2) specializes to recursively generate a cycle with n vertices, s external edges whose free ends are labeled $x_1, \ldots, x_s$, and coefficient $1/(2n)$, from a cycle with $n-1$ vertices, the given external edges and coefficient $1/(2(n-1))$.

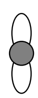
5.1.1 Examples

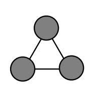
We show the result of computing all mutually non-isomorphic 2-edge connected graphs without external edges as contributions to $\beta^{n,k,0}$ via formula (2), up to order $n+k \leq 5$. The coefficients in front of graphs are the inverses of the orders of their groups of automorphisms.

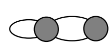
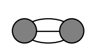
$n = 1, k = 0$ 

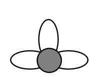
$n = 1\,, k = 1$ $\frac{1}{2}$ 

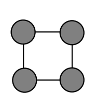
$n = 2\,, k = 1$ $\frac{1}{2^2}$ 

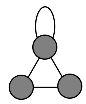
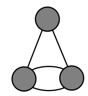
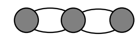
$n = 1\,, k = 2$ $\frac{1}{2^3}$ 

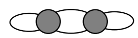
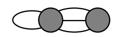
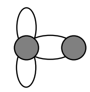
$n = 3\,, k = 1$ $\frac{1}{3!}$ 

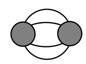
$n = 2\,, k = 2$ $\frac{1}{2^2}$  $+ \frac{1}{2 \cdot 3!}$ 

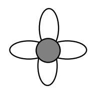
$n = 1\,, k = 3$ $\frac{1}{2^3 \cdot 3!}$ 

$n = 4\,, k = 1$ $\frac{1}{8}$ 

$n = 3\,, k = 2$ $\quad \frac{1}{2^2}$  $+ \frac{1}{2^2}$  $+ \frac{1}{2^3}$ 

$n = 2\,, k = 3$ $\quad \frac{1}{2^4}$  $+ \frac{1}{2 \cdot 3!}$  $+ \frac{1}{2^4}$  $+$

$+ \frac{1}{2 \cdot 4!}$ 

$n = 1\,, k = 4$ $\quad \frac{1}{2^4 \cdot 4!}$ 

5.2 Simple connected graphs

We generalize Theorem 6 to simple connected graphs. To this end, we combine the maps $q_i^{d(1)}$ with the maps $l_{i,j}^b$ in formula (1).

Theorem 12 *Fix an integer $s \geq 0$. Let $L = \{x_1, \ldots, x_s\}$ be a label set. For all integers $k \geq 0$ and $n \geq 1$, define $\sigma^{n,k,s} \in \mathbb{Q}V_{\text{simple}}^{n,k,s}$ by the following recursion relation:*

- *$\sigma^{1,0,s}$ is a single vertex with s external edges whose free ends are labeled $x_1, \ldots, x_s$, and unit coefficient;*
-
$$\sigma^{n,k,s} := \frac{1}{k+n-1} \left(\sum_{i=1}^{n-1} q_i^{d(1)}(\sigma^{n-1,k,s}) + \sum_{i=1}^{n} \sum_{j=1}^{i-1} l_{i,j}^b(\sigma^{n,k-1,s}) \right) , n > 1\,. \tag{3}$$

Then, for fixed values of n and k, $\sigma^{n,k,s} = \sum_{G \in V_{\text{simple}}^{n,k,s}} \alpha_G\, G$; $\alpha_G \in \mathbb{Q}$ and $\alpha_G > 0$ for all $G \in V_{\text{simple}}^{n,k,s}$. Moreover, $\sum_{G \in \mathscr{C}} \alpha_G = 1/S^{\mathscr{C}}$, where $\mathscr{C} \subseteq V_{\text{simple}}^{n,k,s}$ denotes an arbitrary equivalence class of graphs and $S^{\mathscr{C}}$ denotes their symmetry factor.

In the recursion equation above, the $l_{i,j}^b$ summand does not appear when $k = 0$.

Proof: The proof is very analogous to that of Theorem 6. Actually, every lemma given in the preceding section remains valid by replacing $\omega^{n,k,s}$ by $\sigma^{n,k,s}$. Here, we only state and prove the two lemmas corresponding to Lemmas 7 and 8. The rest of the proof is implied by analogy.

Lemma 13 *Fix integers $s, k \geq 0$ and $n \geq 1$. Let $\sigma^{n,k,s} = \sum_{G \in V^{n,k,s}_{simple}} \alpha_G\, G \in \mathbb{Q}V^{n,k,s}_{simple}$ be defined by formula (3). Then, $\alpha_G > 0$ for all $G \in V^{n,k,s}_{simple}$.*

Proof: The proof proceeds by induction on the internal edge number m. Clearly, the statement holds for $m = 0$. We assume the statement to hold for a general number of internal edges $m - 1$. Let $G = (V, K, E)$; $E = E_{\text{int}} \cup E_{\text{ext}}$, $m := \text{card}(E_{\text{int}})$, together with the maps φ_{int} and φ_{ext} denote an arbitrary graph in $V^{n,k,s}_{\text{simple}}$, where $m = k + n - 1$. We now show that the graph G is generated by applying the maps $q_i^{d(1)} := \frac{1}{2} l_{i,n} \circ s_i^d$ to graphs occurring in $\sigma^{n-1,k,s} = \sum_{G' \in V^{n-1,k,s}_{\text{simple}}} \beta_{G'} G'$; $\beta_{G'} \in \mathbb{Q}$, or the maps $l^b_{i,j} := l_{i,j} \circ (\text{id} - \delta_{i,j})$ to graphs occurring in $\sigma^{n,k-1,s} = \sum_{G^* \in V^{n,k-1,s}_{\text{simple}}} \gamma_{G^*} G^*$; $\gamma_{G^*} \in \mathbb{Q}$.

(i) If $k = 0$, by Lemma 7, $\alpha_G > 0$.

(ii) If $k > 0$, choose any one of the internal edges of the graph G which belong at least to one cycle. Let this edge be connected to the vertices $v_i, v_j \in V$; $i, j \in \{1, \ldots, n\}$ with $i \neq j$. Erasing such internal edge yields a graph ${l_{i,j}}^{-1}(G) \in V^{n,k-1,s}_{\text{simple}}$. By induction assumption, $\gamma_{{l_{i,j}}^{-1}(G)} > 0$. Hence, applying the map $l^b_{i,j}$ to ${l_{i,j}}^{-1}(G)$ produces again the graph G. That is, $\alpha_G > 0$.

□

Lemma 14 *Fix integers $k \geq 0$, $n \geq 1$ and $s \geq n$. Let $\mathscr{C} \subseteq V^{n,k,s}_{simple}$ denote an equivalence class. Let $G = (V, K, E)$; $E = E_{int} \cup E_{ext}$, together with the maps φ_{int} and φ_{ext} denote a graph in $\mathscr{C}$. Assume that $V \cap \varphi_{ext}(E_{ext}) = V$. Let $\sigma^{n,k,s} = \sum_{G \in V^{n,k,s}_{simple}} \alpha_G\, G \in \mathbb{Q}V^{n,k,s}_{simple}$ be defined by formula (3). Then, $\sum_{G \in \mathscr{C}} \alpha_G = 1$.*

Proof: The proof proceeds by induction on the internal edge number m. Clearly, the statement holds for $m = 0$. We assume the statement to hold for a general number of internal edges $m - 1$. Consider the graph $G = (V, K, E) \in \mathscr{C}$; $E = E_{\text{int}} \cup E_{\text{ext}}$, $m := \text{card}(E_{\text{int}}) = k + n - 1$, together with the maps φ_{int} and φ_{ext}. By Lemma 13, the coefficient of the graph G in $\sigma^{n,k,s}$ is positive: $\alpha_G > 0$. Moreover, $S^{\mathscr{C}} = 1$ for the graph $G \in \mathscr{C}$ is simple and has no non-trivial vertex symmetries. We proceed to show that $\sum_{G \in \mathscr{C}} \alpha_G = 1$. To this end, choose any one of the m internal edges of the graph $G \in \mathscr{C}$.

(i) If that internal edge does not belong to any cycle, by Lemma 8, it adds $1/m$ to $\sum_{G \in \mathscr{C}} \alpha_G$.

(ii) If that internal edge belongs at least to one cycle, let this edge be connected to the vertices $v_i, v_j \in V$; $i, j \in \{1, \ldots, n\}$ with $i \neq j$. Also, assume that v_i has $r \geq 1$ external edges whose free ends are labeled $x_{a_1}, \ldots, x_{a_r}$, with $1 \leq a_1 < \cdots < a_r \leq s$, while v_j has $r' \geq 1$ external edges whose free ends are labeled $x_{b_1}, \ldots, x_{b_{r'}}$, with $1 \leq b_1 < \cdots < b_{r'} \leq s$ and $a_z \neq b_{z'}$ for all $z \in \{1, \ldots, r\}, z' \in \{1, \ldots, r'\}$. Erasing such internal edge yields a graph ${l_{i,j}}^{-1}(G) \in V^{n,k-1,s}_{\text{simple}}$ so that $S^{{l_{i,j}}^{-1}(G)} = 1$. Let $\sigma^{n,k-1,s} = \sum_{G^* \in V^{n,k-1,s}_{\text{simple}}} \gamma_{G^*} G^*\,; \gamma_{G^*} \in \mathbb{Q}$. Also, let $\mathscr{A} \subseteq V^{n,k-1,s}_{\text{simple}}$ denote the equivalence class containing ${l_{i,j}}^{-1}(G)$. The map $l^b_{i,j} := l_{i,j} \circ (\text{id} - \delta_{i,j})$ produces the graph G from the graph ${l_{i,j}}^{-1}(G)$ with coefficient $\alpha^*_G = \gamma_{{l_{i,j}}^{-1}(G)} \in \mathbb{Q}$. Each vertex of the graph ${l_{i,j}}^{-1}(G)$ has at least one labeled external edge. Hence, by induction assumption, $\sum_{G^* \in \mathscr{A}} \gamma_{G^*} = 1$. Now, take one graph (distinct from G) in $\mathscr{C}$ in turn, choose the internal edge connected to the vertex having r external edges whose free ends are labeled $x_{a_1}, \ldots, x_{a_r}$, and to the vertex having r' external edges whose free ends are labeled $x_{b_1}, \ldots, x_{b_{r'}}$, and repeat the procedure above. We obtain

$$\sum_{G \in \mathscr{C}} \alpha^*_G = \sum_{G^* \in \mathscr{A}} \gamma_{G^*} = 1\,.$$

Therefore, according to formula (3), the contribution to $\sum_{G \in \mathscr{C}} \alpha_G$ is $1/m$.

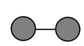
We conclude that every one of the m internal edges of the graph G adds $1/m$ to $\sum_{G \in \mathscr{C}} \alpha_G$. Hence, the overall contribution is exactly 1. This completes the proof. □

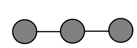
This completes the proof of Theorem 12. □

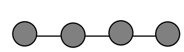
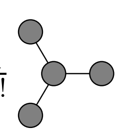
5.2.1 Examples

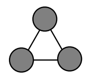
We show the result of computing all mutually non-isomorphic simple connected graphs without external edges as contributions to $\sigma^{n,k,0}$ via formula (3), up to order $n+k \leq 6$. The coefficients in front of graphs are the inverses of the orders of their groups of automorphisms.

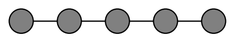
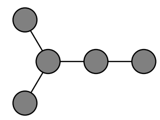
$n = 1, k = 0$ 

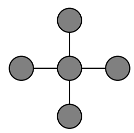
$n = 2\,, k = 0$ $\frac{1}{2}$ 

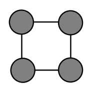
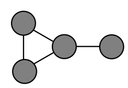
$n = 3\,, k = 0$ $\frac{1}{2}$ 

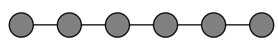
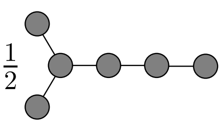
$n = 4\,, k = 0$ $\frac{1}{2}$  $+ \frac{1}{3!}$ 

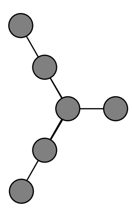
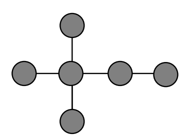
$n = 3\,, k = 1$ $\quad \frac{1}{3!}$ 

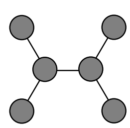
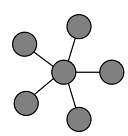
$n = 5\,, k = 0$ $\quad \frac{1}{2}$  $+ \frac{1}{2}$  $+$

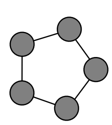
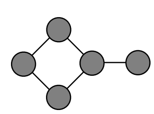
$+ \frac{1}{4!}$ 

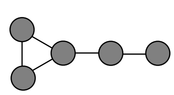
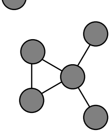
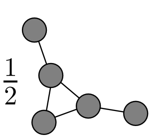
$n = 4\,, k = 1$ $\quad \frac{1}{8}$  $+ \frac{1}{2}$ 

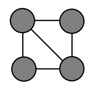
$n = 6\,, k = 0$ $\quad \frac{1}{2}$  $+ \frac{1}{2}$  $+$

$+ \frac{1}{2}$  $+ \frac{1}{3!}$  $+$

$+ \frac{1}{2^3}$  $+ \frac{1}{5!}$ 

$n = 5\,, k = 1$ $\quad \frac{1}{10}$  $+ \frac{1}{2}$  $+$

$+ \frac{1}{2}$  $+ \frac{1}{4}$  $+ \frac{1}{2}$ 

$n = 4\,, k = 2$ $\quad \frac{1}{4}$ 

5.3 Loopless connected graphs

The present section gives two algorithms to generate all loopless connected graphs. The second one is amenable to direct implementation via Hopf algebra in the sense of [5, 6].

5.3.1 Main recursion formula

We generalize Theorem 6 to loopless connected graphs. To this end, we replace the maps t_i by the maps $l^a_{i,j}$ in formula (1).

Theorem 15 *Fix an integer $s \geq 0$. Let $L = \{x_1, \ldots, x_s\}$ be a label set. For all integers $k \geq 0$ and $n \geq 1$, define $\theta^{n,k,s} \in \mathbb{Q}V^{n,k,s}_{loopless}$ by the following recursion relation:*

- *$\theta^{1,0,s}$ is a single vertex with s external edges whose free ends are labeled $x_1, \ldots, x_s$, and unit coefficient;*
- $$\theta^{n,k,s} := \frac{1}{k+n-1}\left(\sum_{i=1}^{n-1} q_i^{(1)}(\theta^{n-1,k,s}) + \sum_{i=1}^{n}\sum_{j=1}^{i-1} l^a_{i,j}(\theta^{n,k-1,s})\right)\,, n > 1\,. \tag{4}$$

Then, for fixed values of n and k, $\theta^{n,k,s} = \sum_{G \in V^{n,k,s}_{loopless}} \alpha_G\, G$; $\alpha_G \in \mathbb{Q}$ and $\alpha_G > 0$ for all $G \in V^{n,k,s}_{loopless}$. Moreover, $\sum_{G \in \mathscr{C}} \alpha_G = 1/S^{\mathscr{C}}$, where $\mathscr{C} \subseteq V^{n,k,s}_{loopless}$ denotes an arbitrary equivalence class of graphs and $S^{\mathscr{C}}$ denotes their symmetry factor.

In the recursion equation above, the $l^a_{i,j}$ summand does not appear when $k = 0$.

Proof: As in the preceding section, every lemma given in Section 4 holds when stated for $\theta^{n,k,s}$. Hence, we restrict the proof of Theorem 15 to the following two lemmas.

Lemma 16 *Fix integers $s, k \geq 0$ and $n \geq 1$. Let $\theta^{n,k,s} = \sum_{G \in V^{n,k,s}_{loopless}} \alpha_G\, G \in \mathbb{Q}V^{n,k,s}_{loopless}$ be defined by formula (4). Then, $\alpha_G > 0$ for all $G \in V^{n,k,s}_{loopless}$.*

Proof: The proof proceeds by induction on the internal edge number m. Clearly, the statement holds for $m = 0$. We assume the statement to hold for a general number of internal edges $m - 1$. Let $G = (V, K, E)$; $E = E_{\text{int}} \cup E_{\text{ext}}$, $m := \text{card}(E_{\text{int}})$, together with the maps φ_{int} and φ_{ext} denote an arbitrary graph in $V^{n,k,s}_{\text{loopless}}$, where $m = k + n - 1$. We now show that the graph G

is generated by applying the maps $q_i^{(1)} := \frac{1}{2} l_{i,n} \circ s_i$ to graphs occurring in $\theta^{n-1,k,s} = \sum_{G' \in V^{n-1,k,s}_{\text{loopless}}} \beta_{G'} G'$; $\beta_{G'} \in \mathbb{Q}$, or the maps $l^a_{i,j} := l_{i,j} \circ \delta_{i,j}$ to graphs occurring in $\theta^{n,k-1,s} = \sum_{G^* \in V^{n,k-1,s}_{\text{loopless}}} \gamma_{G^*} G^*$; $\gamma_{G^*} \in \mathbb{Q}$.

(i) Suppose that the graph G has no multiple edges. By Lemma 7, $\alpha_G > 0$.

(ii) Suppose that the graph G has at least one pair of vertices, say, $v_i, v_j \in V$; $i, j \in \{1, \ldots, n\}$ with $i \neq j$, connected together by multiple edges. Erasing any one of those edges yields a graph ${l_{i,j}}^{-1}(G) \in V^{n,k-1,s}_{\text{loopless}}$. By induction assumption, $\gamma_{{l_{i,j}}^{-1}(G)} > 0$. Hence, applying the map $l^a_{i,j} := l_{i,j} \circ \delta_{i,j}$ to ${l_{i,j}}^{-1}(G)$ produces again the graph G. That is, $\alpha_G > 0$.

□

Lemma 17 *Fix integers $k \geq 0$, $n \geq 1$ and $s \geq n$. Let $\mathscr{C} \subseteq V^{n,k,s}_{\text{loopless}}$ denote an equivalence class. Let $G = (V, K, E)$; $E = E_{int} \cup E_{ext}$, together with the maps φ_{int} and φ_{ext} denote a graph in $\mathscr{C}$. Assume that $V \cap \varphi_{ext}(E_{ext}) = V$. Let $\theta^{n,k,s} = \sum_{G \in V^{n,k,s}_{\text{loopless}}} \alpha_G\, G \in V^{n,k,s}_{\text{loopless}}$ be defined by formula (4). Then, $\sum_{G \in \mathscr{C}} \alpha_G = 1/S^{\mathscr{C}}$, where $S^{\mathscr{C}}$ denotes the symmetry factor of every graph in $\mathscr{C}$.*

Proof: The proof proceeds by induction on the internal edge number m. Clearly, the statement holds for $m = 0$. We assume the statement to hold for a general number of internal edges $m-1$. Consider the graph $G = (V, K, E) \in \mathscr{C}$; $E = E_{\text{int}} \cup E_{\text{ext}}$, $m := \text{card}(E_{\text{int}}) = k + n - 1$, together with the maps φ_{int} and φ_{ext}. By Lemma 16, the coefficient of the graph G in $\theta^{n,k,s}$ is positive: $\alpha_G > 0$. Moreover, $S^{\mathscr{C}} = S^{\mathscr{C}}_{\text{edge}}$ for the graph $G \in \mathscr{C}$ has no non-trivial vertex symmetries. We proceed to show that $\sum_{G \in \mathscr{C}} \alpha_G = 1/S^{\mathscr{C}}$. To this end, choose any one of the m internal edges of the graph $G \in \mathscr{C}$.

(i) If that internal edge is the only one connecting a given pair of vertices together, by Lemma 8, it adds $1/(m \cdot S^{\mathscr{C}})$ to $\sum_{G \in \mathscr{C}} \alpha_G$.

(ii) If that internal edge is one of the, say, $1 < \rho \leq k+1$, multiple edges connecting together the vertices $v_i, v_j \in V$; $i, j \in \{1, \ldots, n\}$ with $i \neq j$, assume that v_i has $r \geq 1$ external edges whose free ends are labeled $x_{a_1}, \ldots, x_{a_r}$, with $1 \leq a_1 < \cdots < a_r \leq s$, while v_j has $r' \geq 1$ external edges whose free ends are labeled $x_{b_1}, \ldots, x_{b_{r'}}$, with $1 \leq b_1 < \cdots < b_{r'} \leq s$ and $a_z \neq b_{z'}$ for all $z \in \{1, \ldots, r\}, z' \in \{1, \ldots, r'\}$. Erasing any one of the given internal edges yields a graph ${l_{i,j}}^{-1}(G) \in V^{n,k-1,s}_{\text{loopless}}$ whose symmetry factor is related to that of the graph $G \in \mathscr{C}$ via $S^{{l_{i,j}}^{-1}(G)} = S^{\mathscr{C}}/\rho$. Let $\theta^{n,k-1,s} = \sum_{G^* \in V^{n,k-1,s}_{\text{loopless}}} \gamma_{G^*} G^*$; $\gamma_{G^*} \in \mathbb{Q}$. Also, let $\mathscr{A} \subseteq V^{n,k-1,s}_{\text{loopless}}$ denote the equivalence class containing ${l_{i,j}}^{-1}(G)$. The map $l^a_{i,j} := l_{i,j} \circ \delta_{i,j}$ produces the graph G from the graph ${l_{i,j}}^{-1}(G)$ with coefficient $\alpha^*_G = \gamma_{{l_{i,j}}^{-1}(G)} \in \mathbb{Q}$. Each vertex of the graph ${l_{i,j}}^{-1}(G)$ has at least one labeled external edge. Therefore, by induction assumption, $\sum_{G^* \in \mathscr{A}} \gamma_{G^*} = 1/S^{{l_{i,j}}^{-1}(G)} = 1/S^{\mathscr{A}}$.

Now, take one graph (distinct from G) in $\mathscr{C}$ in turn, choose any one of the ρ internal edges connecting together the pair of vertices so that one vertex has r external edges whose free ends are labeled $x_{a_1}, \ldots, x_{a_r}$, while the other has r' external edges whose free ends are labeled $x_{b_1}, \ldots, x_{b_{r'}}$, and repeat the procedure above. We obtain

$$\sum_{G \in \mathscr{C}} \alpha^*_G = \sum_{G \in \mathscr{A}} \gamma_{G^*} = \frac{1}{S^{\mathscr{A}}} = \frac{\rho}{S^{\mathscr{C}}} .$$

Hence, according to formula (4), the contribution to $\sum_{G \in \mathscr{C}} \alpha_G$ is $\rho/(m \cdot S^{\mathscr{C}})$. Distributing this factor between the ρ internal edges considered yields $1/(m \cdot S^{\mathscr{C}})$ for each internal edge.

We conclude that every one of the m internal edges of the graph G adds $1/(m \cdot S^{\mathscr{C}})$ to $\sum_{G \in \mathscr{C}} \alpha_G$. Therefore, the overall contribution is exactly $1/S^{\mathscr{C}}$. This completes the proof. □

This completes the proof of Theorem 15. □

5.3.2 Alternative recursion formula

We give an alternative recursion formula for loopless connected graphs. The underlying algorithm is amenable to direct implementation using the algebraic representation of graphs defined in [5, 6].

Theorem 18 *Fix an integer $s \geq 0$. Let $L = \{x_1, \ldots, x_s\}$ be a label set. For all integers $k \geq 0$ and $n \geq 1$, define $\hat{\theta}^{n,k,s} \in \mathbb{Q}V^{n,k,s}_{\scriptscriptstyle loopless}$ by the following recursion relation:*

- *$\hat{\theta}^{1,0,s}$ is a single vertex with s external edges whose free ends are labeled $x_1, \ldots, x_s$, and unit coefficient;*
- *$\hat{\theta}^{1,k,s} := 0$, $k > 0$;*
-
$$\hat{\theta}^{n,k,s} := \frac{1}{k+n-1} \sum_{\rho=1}^{k+1} \sum_{i=1}^{n-1} q_i^{(\rho)}(\hat{\theta}^{n-1,k+1-\rho,s}) \, , n > 1 \, . \qquad (5)$$

Then, for fixed values of n and k, $\hat{\theta}^{n,k,s} = \sum_{G \in V^{n,k,s}_{loopless}} \alpha_G \, G$; $\alpha_G \in \mathbb{Q}$ and $\alpha_G > 0$ for all $G \in V^{n,k,s}_{loopless}$. Moreover, $\sum_{G \in \mathscr{C}} \alpha_G = 1/S^{\mathscr{C}}$, where $\mathscr{C} \subseteq V^{n,k,s}_{loopless}$ denotes an arbitrary equivalence of graphs class of graphs and $S^{\mathscr{C}}$ denotes their symmetry factor.

Proof: As in the previous sections, every lemma given in Section 4 holds for $\hat{\theta}^{n,k,s}$. Here, details are only given for the following two lemmas.

Lemma 19 *Fix integers $s, k \geq 0$ and $n \geq 1$. Let $\hat{\theta}^{n,k,s} = \sum_{G \in V^{n,k,s}_{loopless}} \alpha_G\, G \in \mathbb{Q}V^{n,k,s}_{loopless}$ be defined by formula (5). Then, $\alpha_G > 0$ for all $G \in V^{n,k,s}_{loopless}$.*

Proof: The proof proceeds by induction on the internal edge number m. Clearly, the statement holds for $m = 0$. We assume the statement to hold for any internal edge number smaller than a fixed $m \geq 1$. Let $G = (V, K, E)$; $E = E_{\text{int}} \cup E_{\text{ext}}$, $m := \text{card}(E_{\text{int}})$, together with the maps φ_{int} and φ_{ext} denote an arbitrary graph in $V^{n,k,s}_{\text{loopless}}$, where $m = k+n-1$. We now show that the graph G is generated by applying the maps $q_i^{(\rho)} := \frac{1}{2(\rho-1)!} {l_{i,n}}^{\rho} \circ s_i$ to graphs occurring in $\hat{\theta}^{n-1,k+1-\rho,s} = \sum_{G' \in V^{n-1,k+1-\rho,s}_{\text{loopless}}} \beta_{G'} G'$; $\beta_{G'} \in \mathbb{Q}$. There exists $i \in \{1, \ldots, n-1\}$ so that $\{v_i, v_n\} \in \varphi_{\text{int}}(E_{\text{int}})$. Assume that the two vertices are connected together with $1 \leq \rho \leq k+1$ internal edges. Erasing $\rho - 1$ of these edges and contracting the final one yields a graph $G' := (c_{i,n} \circ {l_{i,n}}^{1-\rho})(G) \in V^{n-1,k-\rho+1,s}_{\text{loopless}}$, where ${l_{i,n}}^{1-\rho}$ denotes the $(\rho-1)$th iterate of ${l_{i,n}}^{-1}$ with ${l_{i,n}}^{0} := \text{id}$. By induction assumption, $\beta_{G'} > 0$. Hence, applying the map $q_i^{(\rho)}$ to the graph G', produces a linear combination of graphs, one of which is the graph G. That is, $\alpha_G > 0$. This completes the proof. $\square$

Lemma 20 *Fix integers $k \geq 0$, $n \geq 1$ and $s \geq n$. Let $\mathscr{C} \subseteq V^{n,k,s}_{loopless}$ denote an equivalence class. Let $G = (V, K, E)$; $E = E_{int} \cup E_{ext}$, together with the maps φ_{int} and φ_{ext} denote a graph in $\mathscr{C}$. Assume that $V \cap \varphi_{ext}(E_{ext}) = V$. Let $\hat{\theta}^{n,k,s} = \sum_{G \in V^{n,k,s}_{loopless}} \alpha_G\, G \in \mathbb{Q}V^{n,k,s}_{loopless}$ be defined by formula (5). Then, $\sum_{G \in \mathscr{C}} \alpha_G = 1/S^{\mathscr{C}}$, where $S^{\mathscr{C}}$ denotes the symmetry factor of every graph in $\mathscr{C}$.*

Proof: The proof proceeds by induction on the internal edge number m. Clearly, the statement holds for $m = 0$. We assume the statement to hold for any internal edge number smaller than a fixed $m \geq 1$. Consider the graph $G = (V, K, E) \in \mathscr{C}$; $E = E_{\text{int}} \cup E_{\text{ext}}$; $m := \text{card}(E_{\text{int}}) = k + n - 1$, together with the maps φ_{int} and φ_{ext}. By Lemma 19, the coefficient of the graph G in $\hat{\theta}^{n,k,s}$ is positive: $\alpha_G > 0$. Moreover, $S^{\mathscr{C}} = S^{\mathscr{C}}_{\text{edge}}$ for the graph $G \in \mathscr{C}$ has no non-trivial vertex symmetries. We proceed to show that $\sum_{G \in \mathscr{C}} \alpha_G = 1/S^{\mathscr{C}}$. To this end, choose any one of the m internal edges of the graph $G \in \mathscr{C}$. Let this edge be connected to the vertices $v_i, v_j \in V$; $i, j \in \{1, \ldots, n\}$ with $i < j$, for instance. Also, assume that v_i has $r \geq 1$ external edges whose free ends are labeled $x_{a_1}, \ldots, x_{a_r}$, with $1 \leq a_1 < \cdots < a_r \leq s$, while v_j has $r' \geq 1$ external edges whose free ends are labeled $x_{b_1}, \ldots, x_{b_{r'}}$, with $1 \leq b_1 < \cdots < b_{r'} \leq s$ and $a_z \neq b_{z'}$ for all $z \in \{1, \ldots, r\}, z' \in \{1, \ldots, r'\}$. Finally, assume that there are $1 \leq \rho \leq k+1$ internal edges connecting the vertices v_i and v_j together. Erasing $\rho - 1$ of these edges and contracting the final one yields a graph $G' := (c_{i,j} \circ {l_{i,j}}^{1-\rho})(G) \in V^{n-1,k-\rho+1,s}_{\text{loopless}}$ whose symmetry factor is related to that of the graph $G \in \mathscr{C}$ via $S^{G'} = \frac{1}{\rho!} S^{\mathscr{C}}$. Let $\hat{\theta}^{n-1,k+1-\rho,s} = \sum_{G' \in V^{n-1,k+1-\rho,s}_{\text{loopless}}} \beta_{G'} G'\,; \beta_{G'} \in \mathbb{Q}$. Let $\mathscr{B} \subseteq V^{n-1,k+1-\rho,s}_{\text{loopless}}$ denote the equivalence class containing G'. Applying the map $q_i^{(\rho)} := \frac{1}{2(\rho-1)!} {l_{i,n}}^{\rho} \circ s_i$ to the graph G' yields a linear combination of graphs, two of which are isomorphic to the graph G. Clearly, the coefficient of each of these two graphs in that linear combination, is $\alpha'_G = \frac{\beta_{G'}}{2(\rho-1)!} \in \mathbb{Q}$. Each vertex of the graph G' has at least one labeled external edge. Hence, by induction assumption, $\sum_{G' \in \mathscr{B}} \beta_{G'} = 1/S^{G'} = 1/S^{\mathscr{B}}$. Now, take one graph (distinct from G) in $\mathscr{C}$ in turn, choose any one of the ρ internal edges connected to the vertex having r external edges whose free ends are labeled $x_{a_1}, \ldots, x_{a_r}$, and to the vertex having r' external edges whose free ends are labeled $x_{b_1}, \ldots, x_{b_{r'}}$, and repeat the procedure above. We obtain

$$\sum_{G \in \mathscr{C}} \alpha'_G = 2 \cdot \frac{1}{2(\rho-1)!} \sum_{G' \in \mathscr{B}} \beta_{G'} = \frac{1}{(\rho-1)! S^{\mathscr{B}}} = \frac{\rho}{S^{\mathscr{C}}} \, ,$$

where the factor 2 on the right hand side of the first equality, is due to the fact that each graph in the equivalence class $\mathscr{B}$ generates two graphs in $\mathscr{C}$. Therefore, according to formula (5), the contribution to $\sum_{G \in \mathscr{C}} \alpha_G$ is $\rho/(m \cdot S^{\mathscr{C}})$. Distributing this factor between the ρ internal edges considered yields $1/(m \cdot S^{\mathscr{C}})$ for each edge.

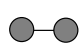
We conclude that every one of the m internal edges of the graph G adds $1/(m \cdot S^{\mathscr{C}})$ to $\sum_{G \in \mathscr{C}} \alpha_G$. Hence, the overall contribution is exactly $1/S^{\mathscr{C}}$. This completes the proof. □

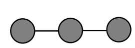
This completes the proof of Theorem 18. □

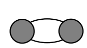
5.3.3 Examples

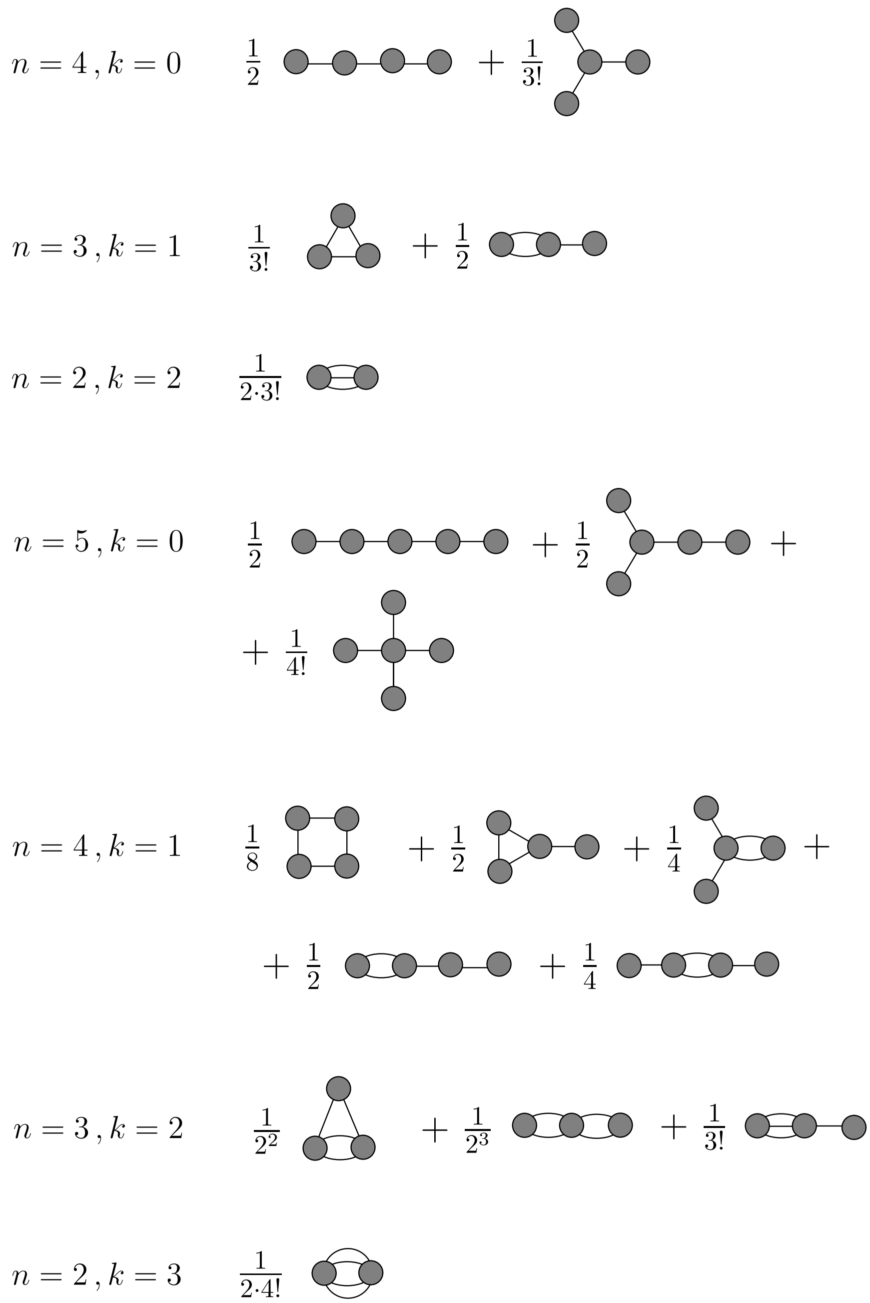
We show the result of computing all mutually non-isomorphic loopless connected graphs without external edges as contributions to $\theta^{n,k,0}$ or $\hat{\theta}^{n,k,0}$ via formulas (4) and (5), respectively, up to order $n + k \leq 5$. The coefficients in front of graphs are the inverses of the orders of their groups of automorphisms.

$n = 1, k = 0$ 

$n = 2\,, k = 0$ $\frac{1}{2}$ 

$n = 3\,, k = 0$ $\frac{1}{2}$ 

$n = 2\,, k = 1$ $\frac{1}{2^2}$ 



5.3.4 Algorithmic considerations

The two algorithms underlying the recursive definitions (1) and (5) given in Sections 4 and 5.3.2, respectively, are amenable to direct implementation using the Hopf algebraic representation of graphs given in [5, 6]. This representation can be used directly and efficiently in implementing concrete calculations of graphs. For a discussion of some algorithmic aspects of the recursive structure of formula (1) we refer the reader to Section IV of [6], and to Section VI C of [5] if only trees are considered. In the present section, we extend the results of those papers to loopless connected graphs.

An important aspect for the efficiency of concrete calculations is to discard graphs that do not contribute. For instance, assume that one is only interested in calculating loopless connected graphs so that all vertices have a minimum degree, say, $\nu > 1$. In particular, in the recursive definition (5), the number of ends of edges assigned to a vertex changes after applying the maps $q_i^{(\rho)}$. The only graphs with degree $1 \leq \rho \leq k+1$ vertices are those produced by the maps s_i when one of the new vertices receives no ends of edges at all. This, thus, acquires degree ρ after being connected to the other vertex with ρ internal edges. Hence, to eliminate the irrelevant graphs with degree $\nu' < \nu$ vertices, replace the maps $q_i^{(\rho)}$ by ${q_i^{(\rho)}}_{\geq\nu} := \frac{1}{2(\rho-1)!}{l_{i,n}}^{\rho} \circ s_{i_{\geq \nu-\rho}}$ if $1 \leq \rho < \nu$, in formula (5), where the maps $s_{i_{\geq \nu-\rho}}$ are defined as the maps s_i except that the former are required to partition the set $\mathcal{E}_i$ of ends of edges assigned to the vertex v_i of a graph G, into two sets, each of cardinality equal or greater than $\nu - \rho$ and, $s_{i_{\geq \nu-\rho}}(G) = 0$ if $0 \leq \mathrm{card}(\mathcal{E}_i) < 2(\nu - \rho)$. Moreover, by Lemma 9, one can even impose independent lower bounds on the numbers of internal and external edges assigned to every vertex of a loopless connected graph with $n > 1$ vertices. In this context, suppose that one is interested in calculating all loopless connected graphs (up to a maximal cyclomatic number) with $n > 1$ vertices and s external edges, so that every vertex has minimum degree $\nu_{\mathrm{int}} + \nu_{\mathrm{ext}}$, where $\nu_{\mathrm{int}} > 1$ and $\nu_{\mathrm{ext}} \geq 0$ are the minimum numbers of internal and external edges, respectively, assigned to every vertex of a graph. To this end, first, use the maps ${q_i^{(\rho)}}_{\geq\nu_{\mathrm{int}}}$ in formula (5) to calculate all loopless graphs with $n > 1$ vertices and no external edges, so that every vertex has minimum degree ν_{int}. Then, use the map $\xi_{E_{\mathrm{ext}},V_{\geq\nu_{\mathrm{ext}}}}$, where $\mathrm{card}(V) = n$ and $\mathrm{card}(E_{\mathrm{ext}}) = s \geq n\nu_{\mathrm{ext}}$, to distribute s external edges between the vertices of each graph in all possible ways so that every vertex is assigned with at least ν_{ext} external edges. Accordingly, the map $\xi_{E_{\mathrm{ext}},V_{\geq\nu_{\mathrm{ext}}}}$ is defined as $\xi_{E_{\mathrm{ext}},V}$ except that the former is required to partition the set E_{ext} into n sets, each of cardinality equal or great than ν_{ext}.

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