ABSTRACT

KLEIN, IAN HARVEY. The Total Chromatic Quasisymmetric Functions. (Under the direction of Dr. Laura Colmenarejo).

In this thesis, we introduce and study two variants of the chromatic quasisymmetric function of a graph: the total chromatic quasisymmetric function via vertex labeling and via acyclic orientations. The original definition of the chromatic quasisymmetric function of a graph by Shareshian and Wachs depends on a labeling of the vertices of the graph, which directly affects the properties of the coefficients appearing in the decomposition of the chromatic quasisymmetric function of a graph into different bases. Motivated by this, we construct the first variant of the chromatic quasisymmetric function of a graph by normalizing it with respect to all the labelings of the vertices. The second variant is motivated by the *Tree Isomorphism Conjecture* and is constructed in terms of acyclic orientations.

We investigate the properties of the coefficients in the expansion in the monomial quasisymmetric basis for both variants and provide a comparative analysis. Furthermore, we derive explicit formulas for the coefficients in the monomial decomposition of the two variants for the star graph. For the labeling-based variant, these coefficients arise from a binomial identity for which we provide a combinatorial proof, and for the orientation-based variant, we provide a deletion-near-contraction identity.

There are several avenues to continue this work. Much of the work in this thesis relates to the star graph, but such results may be able to be replicated for other graph types, such as the path and cycle. Furthermore, some results have the potential to be expanded upon. For instance, the deletion-near-contraction identity on the orientation-based total chromatic quasisymmetric function is currently stated for a special case, but could be generalized.

The Total Chromatic Quasisymmetric Functions

by
Ian Harvey Klein

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APPROVED BY:

Dr. Alonzo Alexander

Dr. Jacob Matherne

Dr. Nathan Reading

Dr. Andrew Sageman-Furnas

Dr. Laura Colmenarejo
Chair of Advisory Committee

DEDICATION

To Oliver.

BIOGRAPHY

Ian Klein was born and raised in Edwardsville, Illinois, a town accross the river from St. Louis. He graduated from Edwardsville High School in 2017 and received his Bachelor of Arts in Mathematics from Carleton College in 2021. That fall, he entered the Mathematics PhD program at North Carolina State University.

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TABLE OF CONTENTS

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

AUTHORSHIP STATEMENT

Chapters 1 and 2 provide the motivation and outline for the work presented in this thesis as well as a comprehensive literature review and background for the research. Chapter 6 outlines future directions to take the work in this thesis. All 3 chapters were written by me with feedback provided by Dr. Laura Colmenarejo.

Chapters 3 through 5 represent collaborative research conducted with my advisor, Dr. Laura Colmenarejo, during my PhD program. The results were submitted to AlCo in February 2026, and the latest version is available in ArXiV.

My primary individual contributions include:

1. The definitions for the total labeling and total orientation chromatic quasisymmetric functions introduced in Chapter 3. I also proposed and led the study of most of the properties of these functions presented in this chapter.

2. The discovery of the combinatorial description of the coefficients detailed in Chapter 4. This involved developing original SAGE code to generate and analyze large data sets, from which I identified the underlying combinatorial patterns and formulated the resulting descriptions.

3. The original combinatorial model, including its various extensions and variants, which forms the core of Chapter 5. While the overarching proof strategies were developed through collaborative discussion, I provided the key technical steps and logical derivations for the majority of the results while Dr. Laura Colmenarejo organized the final version of the argument presented in the thesis.

While the technical derivations and computational models were my primary focus, the development of the manuscript submitted for publication was a deeply collaborative effort with Dr. Laura Colmenarejo. Her feedback was key to improving the writing and ensuring the final presentation was clear and well-organized. Finally, she provided extensive feedback on the several versions of this thesis presented to the committee, ensuring the work met the required academic standards for submission.

Use of generative artificial intelligence: No generative artificial intelligence was used to write this dissertation.

CHAPTER

1 INTRODUCTION

1.1 Context

In 1995, Stanley [Sta95] defined a generalization of the chromatic polynomial in the framework of symmetric functions. Given a (finite) graph $G = (V, E)$, the chromatic symmetric function of G is defined as

$$\chi_G(x) := \sum_{\kappa} x^{\kappa},$$

where the sum runs over all proper colorings of the vertices of the graph and $x^{\kappa} = x_1^{k_1} x_2^{k_2} \cdots$, with k_i being the number of vertices colored i. Since then, the study of the chromatic symmetric function of graphs has been a source of interesting research within algebraic combinatorics and other related areas. Among the most interesting problems, we highlight the *Stanley-Stembridge conjecture*, also known as the *e-positivity conjecture*, which has been recently proved by Hikita [Hik25a].

Theorem 1.1.1 (Stanley-Stembridge conjecture [Hik25a; Hik25b])**.** *Let G be a unit interval graph and consider the expansion of the chromatic symmetric function of G in the e-basis, $\chi_G(x) = \sum_{\lambda \vdash n} a_\lambda e_\lambda(x)$. Then, χ_G is e-positive; that is, $a_\lambda \in \mathbb{Z}_{\geq 0}$.*

It should be noted that the original statement of this conjecture was a priori stronger, required instead that G be the incomparability graph of a $(3+1)$-free poset. Guay-Paquet's work reduced the problem to the case of G being a unit interval graph [GP14]. This conjecture stood for nearly 30 years, during which plenty of progress was made proving special cases [Cho22; Cho02; Fol19; Har19; Sag06], developing combinatorial theory surrounding $(3+1)$-free posets [Atk12; GP14], and developing algebraic and geometric theory related to the conjecture [Ali24; Bro18; Har19; Har22]. Ultimately, in 2024, Hikita proved the Stanley-Stembridge conjecture by relating the coefficients of the e-expansion of the chromatic symmetric function of unit interval order graphs to a probability measure involving partitions, standard Young tableaux, and Maya diagrams, which in particular would require those coefficients to be non-negative [Hik25a]. To do so, he used a (q,t)-analog of the chromatic symmetric function which he outlines in a different paper [Hik25b].

The Stanley-Stembridge conjecture was just one of the prominent open problems related to the chromatic symmetric function when I started my work. Another prominent open problem (that has remained open) is the Tree Isomorphism Conjecture, stated below.

Conjecture 1.1.2 (Tree Isomorphism Conjecture)**.** *[Sta95] Let G and H be non-isomorphic trees. Then, $\chi_G(x) \neq \chi_H(x)$.*

The conjecture has been computationally verified for all trees of up to 29 vertices [Hei19], but the main statement remains open. There has also been work done to verify this conjecture for certain classes of trees. For example, the Tree Isomorphism Conjecture has been verified for caterpillars (the class of trees such that removing the degree-one vertices leaves a path graph) [AP14; Loe19] as well as q-caterpillars, which are graphs which contain fixed-length paths branching out of a central path [Gan24]. It has also been verified for the class of spider graphs (trees with at most one vertex of degree larger than 2) [Mar08], all graphs with diameter 5 or less [Gon26], and all graphs with exactly two vertices with degree 3 or larger [Wan24].

Much of this progress towards the Tree Isomorphism Conjecture takes the form of finding graph invariants which are determined by the chromatic symmetric function. One example is the bivariate subtree polynomial [Cha91], which was used to show that spider graphs are determined by their chromatic symmetric function. Trees with at least one vertex of degree 3 or higher can be decomposed into a trunk T_0 and twigs. Crew has shown that the trunk and lengths of twigs is determined by the tree's bivariate subtree polynomial, and thus its chromatic symmetric function [Cre22].

There are other routes towards progress of this conjecture. For example, Aliste-Prieto, de Mier, Orellana, and Zamora proved the following deletion-near-contraction identity on the chromatic symmetric function.

Theorem 1.1.3. *[AP23] Let G be a simple graph and consider an edge $e \in G$. Then,*

$$\chi_G(x) = \chi_{G\setminus e}(x) - \chi_{(G\odot e)\setminus \ell_e}(x) + \chi_{G\odot e}(x). \tag{1.1}$$

In that paper, the authors use this identity to outline a way to write any chromatic symmetric function in terms of the chromatic symmetric function of a star forest. This framework has been used to show that the chromatic symmetric function contains certain information about its graph [Ore26] and also was used to prove that all graphs with diameter 5 or less can be reconstructed from their chromatic symmetric function [Gon26].

Shifting gears, in 2012, while working on the Stanley-Stembridge conjecture, Shareshian and Wachs [Sha12] introduced a refinement of the chromatic symmetric function of a graph in the framework of quasisymmetric functions. Given a graph $G = (V, E)$ and an ordering of its vertices so that $V = \{1, 2, \ldots, |V|\}$, the chromatic quasisymmetric function of a graph G is defined as

$$\chi_G(x; q) = \sum_{\kappa} q^{\mathrm{asc}(\kappa)} x^{\kappa},$$

where the sum runs over all the proper colorings of the vertices of G and asc(κ) is the number of edges $\{i, j\}$ such that $i < j$ and $\kappa(i) < \kappa(j)$. This refinement was introduced as a way to connect the Stanley-Stembridge conjecture, and more broadly the chromatic symmetric functions framework, to the cohomology of the Hessenberg varieties. Shareshian and Wachs noted that, if G is a unit interval graph, then $\chi_G(q)$ is symmetric. They also made the following conjecture, which was proved by Brosnan and Chow in 2015.

Theorem 1.1.4. *[Bro18; Sha12] Let $G = inc(P)$ be the incomparability graph of a natural unit order interval P. Then,*

$$\sum_{j=0}^{|E(G)|} chH^{2j}(H(P))q^j = \omega\chi_G(q)$$

where $H(P)$ is the regular, semisimple Hessenberg variety of type A associated to P, and ω is the involution on symmetric functions.

Theorem 1.1.4 details a concrete connection between algebraic combinatorics (via the chromatic symmetric function and Stanley-Stembridge conjecture) and geometry (via cohomology of Hessenberg varieties). Shareshian and Wachs also introduced a quasisymmetric version of the Stanley-Stembridge conjecture.

Conjecture 1.1.5. *[Sha12] Let $G = (V, E)$ be a unit interval graph and consider the natural order in V. Then, $\chi_G(x; q)$ is symmetric and e-positive.*

Notably, Hikita's proof of the Stanley-Stembridge conjecture does not imply the Shareshian-Wachs conjecture, leaving the latter still open. However, there has been some progress made towards this conjecture. The Shareshian-Wachs conjecture was shown for a special case of unit order interval graphs, the abelian case. Using the modular relation [Ale22; GP13], Abreu and Nigro provide an e-expansion for the chromatic quasisymmetric function of these graphs using q-hit numbers [Abr21] while Guay-Paquet provided an expansion in terms of q-hit numbers and the chromatic quasisymmetric function of unit order interval graphs associated with rectangular partitions [GP]. Colmenarejo, Morales, and Panova connected these two expansions and provided a recursive relation on q-hit numbers [Col23]. Lee and Soh also showed that the Shareshian-Wachs conjecture holds for certain non-abelian cases [Lee22].

Due to the significance of this refinement of the chromatic symmetric function, a natural question is whether or not the quasisymmetric analogue of the Tree Isomorphism Conjecture holds on labeled trees. This is not the case, however, since two unique labelings of the same graph can have the same chromatic quasisymmetric function (for example, the chromatic quasisymmetric function of the star graph is determined only by the label of its root). Therefore, if we desire a framework within which one can generalize this conjecture, we have to look elsewhere. A second variant of the chromatic quasisymmetric function of a graph is thus defined using the definition of the ascents in terms of orientations. Given a graph $G = (V, E)$, an orientation γ on the edges E is a function that assigns an orientation to each edge $\{u, v\} \in E$; that is $u \to v$ or $v \to u$. Then, we define the ascents of G with respect to γ as the number of edges $u \to v$ such that $\kappa(r) < \kappa(v)$.

With this concept of ascents, which we denote by $\mathrm{asc}^o(q)$, Ellzey [Ell17; Ell18] introduced a variant of the chromatic quasisymmetric function on graphs with respect to an orientation. The definition is exactly the same as for $\chi_G(x;q)$ with this variant of ascents, $\mathrm{asc}^o(q)$, and we denote it by $\chi^o_G(x;q)$. Aval, Djenabou, and McNamara [Ava23] then introduced the following conjecture.

Conjecture 1.1.6. *[Ava23] Let G and H be non-isomorphic trees with an orientation. Then, $\chi^o_G(x;q) \neq \chi^o_H(x;q)$.*

Note that this conjecture is stated in terms of directed graphs, which are essentially graphs with orientations. Additionally, note that it is not clear whether or not one conjecture is weaker than the other between Conjecture 1.1.2 and Conjecture 1.1.6.

1.2 My work

Inspired by the deletion-near-contraction result in Theorem 1.1.3, we explore the chromatic quasisymmetric function of the star graphs as well as if there is any such deletion-near-contraction identity with the chromatic quasisymmetric function. In doing so, we run into trouble. The reliance of the chromatic quasisymmetric function on a standardized labeling makes both avenues difficult. This problem inspires our first variant of the total chromatic quasisymmetric function of a graph, defined below.

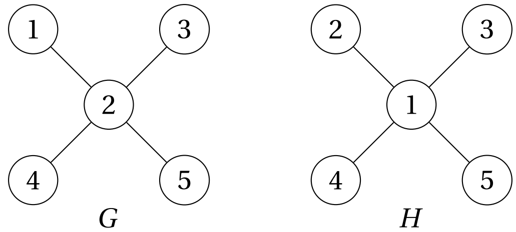
Definition. Let G be a graph. We define the *total labeling chromatic quasisymmetric function of* G as

$$T\chi^L_G(q) := \sum_L \chi_G(x;q),$$

where we sum over all possible labelings L of the vertices of G.

Again, this variant is motivated by the dependency of $\chi_G(x;q)$ on *a natural ordering of the vertices of* G. The ordering can be viewed as a labeling of the vertices, and for many families, including unit interval graphs, there is a natural, canonical labeling. However, that is not the case for all families of graphs. Moreover, the coefficients appearing in $\chi_G(x;q)$, which are polynomials in $\mathbb{Z}[q]$, can be significantly different depending on the labeling. For instance, consider the following example.

Example 1.2.1. Consider the star graph ST_5 with the following two labelings:



Consider the expansion of $\chi_G(x;q)$ and $\chi_H(x;q)$ in the monomial quasisymmetric basis, $\chi_G(q) = \sum_\alpha c_\alpha(q) M_\alpha$ and $\chi_H(q) = \sum_\alpha b_\alpha(q) M_\alpha$, respectively. These coefficients are displayed in Table 1.1, and we notice that the coefficients of $\chi_H(x;q)$ are more interesting from a combinatorial perspective than the coefficients of $\chi_H(x;q)$.

Table 1.1 Coefficients of the M-expansion of the chromatic quasisymmetric function for the star graph ST_5 with two different labelings.

α	$c_\alpha(q)$	$b_\alpha(q)$
$(1,1,1,1,1)$	$6q^4+36q^3+36q^2+36q+6$	$24(q^4+q^3+q^2+q+1)$
$(1,1,1,2)$	$3q^4+18q^3+9q^2+6q$	$12(q^4+q^3+q^2)$
$(1,1,2,1)$	$3q^4+12q^3+9q^2+12q$	$12(q^4+q^3+1)$
$(1,2,1,1)$	$12q^3+9q^2+12q+3$	$12(q^4+q+1)$
$(2,1,1,1)$	$6q^3+9q^2+18q+3$	$12(q^2+q+1)$
$(1,1,3)$	$q^4+4q^3+3q^2$	$4(q^4+q^3)$
$(1,3,1)$	$4q^3+4q$	$4(q^4+1)$
$(3,1,1)$	$3q^2+4q+1$	$4(q+1)$
$(1,2,2)$	$6q^3$	$6q^4$
$(2,1,2)$	$3q^3+3q$	$6q^2$
$(2,2,1)$	$6q$	6
$(1,4)$	q^3	q^4
$(4,1)$	q	1

With this definition in mind, we explore the properties of the total labeling CQF and find some results. The following proposition says that the total labeling CQF behaves well with the disjoint union of graphs.

Proposition. *Let $G=(V,E)$ and $G'=(V',E')$ be two graphs, and consider their disjoint union $H=G\sqcup G'$. Then,*

$$T\chi_H^L(q) = \binom{|V|+|V'|}{|V|} T\chi_G^L(q) T\chi_{G'}^L(q).$$

We also prove that the total labeling CQF yields coefficients in its M-expansion which are palindromic, as well as a partial symmetry result.

Proposition. *Let $G=(V,E)$ be a graph on $n=|V|$ vertices, and consider the M-expansion of its total labeling CQF, $T\chi_G^L(q) = \sum_\alpha c_\alpha^L(q) M_\alpha$. Then, $c_\alpha^L(q)$ is a palindromic polynomial in q with degree $|E|$, i.e.,* *for all* k,

$$[q^k]c^L_\alpha(q) = [q^{|E|-k}]c^L_\alpha(q).$$

Also, for any composition α *of* n, $c^L_\alpha(q) = c^L_{\alpha^{\mathrm{rev}}}(q)$.

Finally, we give the M-expansion of the star graph.

Theorem. *Let* ST_n *be the star graph on* n *vertices, and consider the* M*-expansion of its normalized total labeling CQF,* $\mathrm{Tst}_n(q) = \sum_\alpha b_\alpha(q)M_\alpha$. *Then,*

$$b_\alpha(q) = \sum_i \mathrm{Mult}(\alpha_{i\rightarrow})\mathrm{Mult}(\alpha_{\leftarrow i})\sum_{l=0}^{s}\binom{n}{l}q^l[n-2l]_q,$$

where the first sum runs over all the i *such that* $\alpha_i = 1$, *and* $s = \min\{R_{\alpha_i}, L_{\alpha_i}\}$. *Equivalently,*

$$[q^k]b_\alpha(i;q) = \mathrm{Mult}(\alpha_{i\rightarrow})\mathrm{Mult}(\alpha_{\leftarrow i})\sum_{l=0}^{s_0}\binom{n}{l},$$

where $s_0 = \min\{k, s\}$ *and* $0 \le k \le n-1$.

Wanting a deletion-near-contraction identity with the work by Ellzey and Aval in mind, we define a second variant of the total chromatic quasisymmetric function of a graph constructed from the CQF defined in terms of acyclic orientations.

Definition. Let G be a graph and Γ be the set of acyclic orientations of G. We define the *total orientation chromatic quasisymmetric function of* G as

$$T\chi^o_G(q) := \sum_{\gamma\in\Gamma}\chi^\gamma_G(x;q).$$

Similar to the total labeling CQF, we find that the total orientation CQF behaves well with the disjoint union of graphs.

Proposition. *Let* G *and* G' *be two graphs and consider* $H = G \sqcup G'$. *Then,*

$$T\chi^o_H(q) = T\chi^o_G(q)\cdot T\chi^o_{G'}(q).$$

We also find that the coefficients of the M-expansion of the total orientation CQF are palindromic and get a partial symmetry result, just like the labeling case.

Theorem. *Let* $G = (V,E)$ *be a graph, and consider the* M*-expansion of its total orientation CQF,* $T\chi^o_G(q) = \sum_\alpha c^o_\alpha(q)M_\alpha$. *Then,* $c^o_\alpha(q)$ *is a palindromic polynomial in* q *of degree* $m = |E|$, *and* $c^o_\alpha(q) = c^o_{\alpha^{\mathrm{rev}}}(q)$.

Furthermore, we find a partial deletion-near-contraction identity for the total orientation CQF, which eludes us in the labeling case.

Theorem. *Let G be a graph and let e be an internal edge in G that is not part of a cycle. Then,*

$$T\chi_G^o = T\chi_{G\odot e}^o + (1+q)\Big(T\chi_{G\setminus e}^o - T\chi_{(G\odot e)\setminus \ell_e}^o\Big).$$

Finally, we explore the star graph, which, in the orientation case, ends up being a special case of a general result for trees.

Corollary. *Let $G = \mathrm{ST}_n$. Then,*

$$T\chi_{\mathrm{ST}_n}^o(q) = \sum_{\lambda \vdash n} a_1(\lambda)\cdot \mathrm{Mult}(\tilde{\lambda})(q+1)^{n-1} m_\lambda.$$

1.3 Overview

In Chapter 2, we introduce the background necessary for (quasi)symmetric functions, graphs, and chromatic (quasi)symmetric functions.

In Chapter 3, we introduce and study our two variants of the total chromatic quasisymmetric function of a graph. The first variant is constructed from the chromatic quasisymmetric function of a graph by normalizing it with respect to all the labelings of the vertices of the graph (Definition 3.1.1). We also prove some properties of its coefficients, which are polynomials of q, appearing in the M-expansion of $T\chi_G^L(q)$ for any graph G. For instance, we show that it behaves well with respect to the disjoint union of graphs (Proposition 3.1.3), that the coefficients are symmetric and of maximal degree (Proposition 3.1.5), and that they are invariant under reversing the indexing composition (Theorem 3.1.6). We attempted to find a variant of the deletion-contraction relation on $T\chi_G^L(q)$, but found some empirical evidence that makes us skeptical about the existence of one. In Section 3.2, we introduce the second variant of the total chromatic quasisymmetric function of a graph. This variant is motivated by work by Ellzey, Aval, and others on the CQF defined via directed graphs, as well as a desire to normalze the CQF in a way that illicits a deletion-near-contraction relation. We also prove some properties of its coefficients, which are polynomials of q, appearing in the M-expansion of $T\chi_G^o(q)$ for any graph G. For instance, we show that it behaves well with respect to the disjoint union of graphs (Proposition 3.2.2), that the coefficients are symmetric and of maximal degree (Theorem 3.2.5), and that they are invariant under reversing the indexing composition (Theorem 3.2.6). Moreover, we also show that $T\chi_G^o(q)$ satisfies a *deletion-near-contraction* relation (Theorem 3.2.7), like the one presented by Aliste-Prieto, de Mier, Orellana, and Zamora [AP23]. We also give a formula for $T\chi_G^o(q)$ in terms of χ_G when G is a tree, which also shows that $T\chi_G^o(q)$ is a symmetric function when G is a tree.

Chapter 4 explores the total CQF variants of the star graph in greater detail. In the case of the orientation variant, since the star graph is a tree, we give a formula for the coefficients appearing in the m-decomposition of the total orientation chromatic symmetric function of the star graph, which is a straightforward computation (Theorem 3.2.8). In the case of the labeling variant, we find that the coefficients in its M-expansion take a certain form (Theorem 4.3.4).

The proof of this formula follows from a combinatorial argument in terms of the proper colorings of ST_n and a binomial identity (Theorem 4.3.6).

The proof of this binomial identity turns out to be more challenging than expected. Chapter 5 is dedicated to presenting a combinatorial model and its proof. Essentially, we introduce a combinatorial model and then find an alternative formulation of the model (Proposition 5.2.7). Using this new formulation, we begin to show the independence of our binomial identity with respect to some of its parameters (Proposition 5.3.1 and Corollary 5.5.7). This allows for the elimination of a parameter in a recursive relationship we find (Theorem 5.4.1 and Corollary 5.5.9), which proves the binomial identity.

Finally, in Chapter 6, we present a series of questions outlining future research directions of this work.

CHAPTER

2

BACKGROUND

In this chapter, we introduce some relevant definitions and give the background on symmetric and quasisymmetric functions and the theory of chromatic symmetric and quasisymmetric functions necessary for our study. For more details on the theory of symmetric and quasisymmetric functions, see [Sta99], and for more details on the theory of chromatic symmetric and quasisymmetric functions, see [Sha12].

2.1 Compositions and partitions

A sequence $\alpha = (\alpha_1, \dots, \alpha_\ell)$ is a composition of n, denoted $\alpha \models n$, if $\alpha_i \in \mathbb{Z}_{>0}$ and $|\alpha| := \sum_i \alpha_i = n$. We refer to ℓ as the length of α, $\ell(\alpha)$. If we allow zero entries, $\alpha_i \in \mathbb{Z}_{\geq 0}$, we say that α is a weak composition, and we denote by $\ell(\alpha)$ the number of nonzero entries. Moreover, if the entries in α are nonzero and in weakly decreasing order, that is $\alpha_1 \geq \alpha_2 \geq \dots \geq \alpha_\ell > 0$, we say that α is a partition of n, denoted $\alpha \vdash n$. Note that we usually denote (weak) compositions by α, β, γ, and partitions by λ, μ, ν. Given a (weak) composition $\alpha = (\alpha_1, \dots, \alpha_\ell)$, we denote by $\mathrm{sort}(\alpha)$ the partition obtained by reordering the entries of α in weakly decreasing order and deleting the zero entries if necessary. Suppose that $\alpha = (\alpha_1, \dots, \alpha_\ell)$ is a weak composition such that $\alpha_\ell \neq 0$; that is, α could have zero entries, but we do not consider the zero entries at the end. Then, we define the *reverse composition* as $\alpha^{\mathrm{rev}} = (\alpha_\ell, \alpha_{\ell-1}, \dots, \alpha_1)$.

2.2 Symmetric and quasisymmetric functions

Let $x = \{x_1, x_2, \ldots\}$ be an alphabet with infinitely many variables. A formal power series in x over $\mathbb{Q}[q]$ is a function of the form $f(x;q) = \sum_\alpha c_\alpha(q) x^\alpha$, where the sum runs over all weak compositions α, $c_\alpha \in \mathbb{Q}[x]$, and $x^\alpha = x_1^{\alpha_1} x_2^{\alpha_2} \cdots$. We say that $f(x;q)$ is homogeneous of degree n if $c_\alpha(q) \neq 0$ for some $\alpha \models n$. Moreover, we denote by $[x^\alpha] f(x;q)$ the coefficient of x^α in $f(x;q)$, and for the coefficients $c_\alpha(q) \in \mathbb{Q}[q]$, we denote by $[q^k] c_\alpha(q)$ the coefficient of q^k in $c_\alpha(q)$, for $k \in \mathbb{Z}_{\geq 0}$. Note also that we may omit the alphabet x if it is clear from context, and write simply $f(q)$ or f if the coefficients are in $\mathbb{Q}[q]$ or $\mathbb{Q}$, respectively.

We say that $f(x;q)$ is a symmetric function if it is invariant under the action of permutations; that is, $f(x_1, x_2, \ldots; q) = f(x_{\sigma(1)}, x_{\sigma(2)}, \ldots; q)$ for any permutation σ. We denote by Λ the ring of symmetric functions on x with coefficients in $\mathbb{Q}[q]$, and by Λ^n the ring of homogeneous symmetric functions on x of degree n with coefficients in $\mathbb{Q}[q]$. Then, $\Lambda := \Lambda^0 \oplus \Lambda^1 \oplus \Lambda^2 \oplus \cdots$, where $\Lambda^0 = \mathbb{Q}[q]$. As a vector space, Λ^n has many interesting bases, all of them indexed by partitions of n. We introduce here the three bases that are more relevant for our study. The monomial basis is defined as $m_\lambda = \sum_\alpha x^\alpha$, where the sum runs over all weak compositions α such that $\mathrm{sort}(\alpha) = \lambda$. The elementary basis is defined as

$$e_k = \sum_{i_1 < i_2 < \cdots < i_k} x_{i_1} x_{i_2} \cdots x_{i_k}, \qquad \text{and} \qquad e_\lambda = e_{\lambda_1} e_{\lambda_2} \cdots e_{\lambda_{\ell(\lambda)}}.$$

The power sum basis is defined as

$$p_k = \sum_i x_i^k, \qquad \text{and} \qquad p_\lambda = p_{\lambda_1} p_{\lambda_2} \cdots p_{\lambda_\ell}.$$

Next, we introduce the quasisymmetric functions. We say that a formal power series $f(x;q)$ over $\mathbb{Q}[q]$ is quasisymmetric if for any weak composition $\alpha = (\alpha_1, \ldots, \alpha_\ell)$, the coefficient of x^α equals the coefficient of $x_{i_1}^{\alpha_1} x_{i_2}^{\alpha_2} \cdots x_{i_\ell}^{\alpha_\ell}$ for any set of subindices $0 < i_1 < i_2 < \cdots < i_\ell$. We denote the ring of quasisymmetric functions on x with coefficients in $\mathbb{Q}[q]$ by QSym, and the ring of homogeneous quasisymmetric functions of degree n by QSym^n. As for Λ^n, there are many interesting bases for quasisymmetric functions, all of them indexed by compositions. We introduce the monomial basis as it is the one relevant for our study. The monomial quasisymmetric basis is defined as

$$M_\alpha := \sum_{i_1 < i_2 < \cdots i_\ell} x_{i_1}^{\alpha_1} x_{i_2}^{\alpha_2} \cdots x_{i_\ell}^{\alpha_\ell}.$$

2.3 Graphs

Consider a graph $G = (V(G), E(G))$, where $V(G)$ is the set of vertices and $E(G)$ is the set of edges, which are unordered pairs $e = \{u, v\}$ with $u, v \in V(G)$. We denote the graph as $G = (V, E)$ if G is known by context, and the edges as $e = \{u, v\} = uv$. Note that we only work with finite graphs, and so the sets of vertices and edges are finite. If $e = \{u, v\} \in E(G)$, we say that u and v are *adjacent*. The *degree* of a vertex $v \in V(G)$, $\deg(v)$, is the number of edges $e = \{u, v\} \in E(G)$ for some $u \in V(G)$, and we say that $e = \{u, v\} \in E(G)$ is an internal edge if $\deg(u), \deg(v) \geq 2$.

Our *favorite example* of graphs in this thesis is the *star graph* ST_n defined as the graph with n vertices and such that there is a vertex r called the *root* and all the edges are of the form rv with $v \in V$, $v \neq r$. Note that despite the name for this special vertex, we do not consider ST_n as a rooted tree. Also, we reserve the notation r for the root of the star graph.

We say that a graph $G = (V, E)$ is *simple* if it contains no edges of the form $\{v, v\}$, with $v \in V$, and no repeated edges. Given $G = (V, E)$, we define a *path* as a sequence of distinct vertices $v_1, v_2, \ldots, v_k$ in V such that $\{v_i, v_{i+1}\} \in E$ for $i = 1, \ldots k-1$. A *cycle* is a path such that $v_1 = v_k$. We say that G is connected if there exists a path between any two vertices of the graph. We say that G is a *tree* if it is a connected graph with no cycles, and a forest if we only require the graph not to have cycles.

We define an *orientation* of G as a map γ that assigns a direction to each edge $e \in E$. That is, for every $e = \{u, v\}$, we either assign (u, v) or (v, u). We say that an orientation is *acyclic* if the resulting graph has no cycles of the form $v_1, v_2, \ldots, v_k$ with $v_i \in V$ and $(v_i, v_{i+1}) \in E$ for all $i = 1, \ldots k-1$, and $v_1 = v_k$. We denote by $\Gamma(G)$, or simply Γ, the set of all acyclic orientations of G. Note that a graph with an orientation is also known as a *directed graph*.

We consider two decorations on the vertices of the graph $G = (V, E)$. We define a *labeling* of the vertices of the G as a bijective map $L : V \longrightarrow \{1, 2, \ldots, |V|\}$. That is, a labeling of G is an ordering of the vertices of G. We refer to $L(v)$ as the label of $v \in V$ and we denote by $L(G)$, or simply L, the set of all labelings of G. We also define a *proper coloring* of G as a map $\kappa : V \longrightarrow \mathbb{Z}^+$ such that if u, v are adjacent vertices, then $\kappa(r) \neq \kappa(v)$. We refer to $\kappa(v)$ as the color of the vertex v and we denote by $K(G)$, or simply K, the set of all the proper colorings of G. We associate the proper coloring κ with the weak composition given by the number of vertices colored i, that is $(\#\kappa^{-1}(1), \#\kappa^{-1}(2), \ldots)$. We abuse the notation and denote this weak composition by κ. We say a composition α is the *associated composition* of κ if α is obtained from the weak composition κ by deleting the zero entries in κ.

For the star graph, we may need to keep track of the label of the root, and so we denote by ST_n^r the star graph together with a labeling L such that $L(r) = r$, where we abuse notation and denote by r both the root and its labeling. Note that there are $(n-1)!$ such labelings.

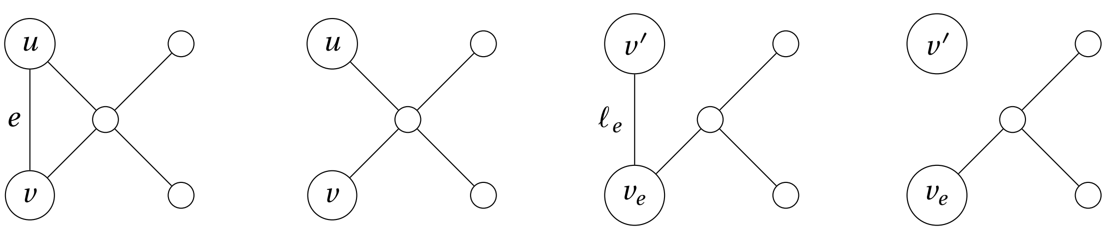
Next, we define a statistic on the graphs related to the proper colorings. Let G be a simple graph, with a labeling L and a proper coloring κ. We say that the edge $e = \{u, v\} \in E$ is an *ascent* if $L(r) < L(v)$ and $\kappa(r) < \kappa(v)$. We denote by $\mathrm{asc}^L(\kappa)$ the number of ascents in G. If G is a simple graph with an orientation, we say that $e = (u, v) \in E$ is an ascent if $\kappa(r) < \kappa(v)$. We denote by $\mathrm{asc}^o(\kappa)$ the number of ascents in G.

Example 2.3.1. In the example below there are two graphs with proper colorings. The color of each vertex is the number inside the vertex. The graph on the left is a labeled graph, with labelings of each vertex adjacent to the vertices, while the graph on the right is a directed graph with arrows near and pointing towards the "incoming" vertex. Each red edge does not contribute an ascent, while each blue edge does. Below each graph is the number of ascents, weak coloring composition, and associated composition.

asc$(\kappa)=2$, $\kappa=(2,1,0,0,2,0,0,\dots)$, $\alpha=(2,1,2)$ asc$(\kappa)=2$, $\kappa=(1,1,0,0,2,0,1,0,\dots)$, $\alpha=(1,1,2,1)$

Finally, we define some operations on graphs. The first operation is the disjoint union of two graphs G and H, written $G \sqcup H$, which is the graph with set of vertices $V(G)\cup V(H)$ and set of edges $E(G)\cup E(H)$. The other operations are defined over a graph $G=(V,E)$, with a vertex $e=\{u,v\}\in E$. We define $G\backslash e$ as the graph obtained from G by deleting the edge e. We define G/e as the graph obtained from G by *contracting the edge* e; that is, deleting e, u, and v, adding a new vertex v_e, and replacing the edges of the form $\{u,w\}\in E$ and $\{v,w\}\in E$ with edges of the form $\{v_e,w\}$. In this case, we say that G/e contracts e into the contracted vertex v_e. Finally, we define $G\odot e$ as the graph obtained by first contracting $e=\{u,v\}$ into the contracted vertex v_e and then attaching a vertex v' to v_e, denoting this edge by $\ell_e=\{v',v_e\}$. Note that v' is only attached to v_e and it is called the *near-contracted edge* of $G\odot e$ and the graph $G\odot e$ is called the *near-contraction of* e. Note that if e is not an internal edge (i.e., $\deg(u)=\deg(v)\geq 2$), $G\odot e=G$. This operation was first introduced by Aliste-Prieto, de Mier, Orellana, and Zamora in 2022 [AP23].

Example 2.3.2. In this example, we present the graph G on the right, with the edge $e=\{u,v\}$, and the graphs $G\setminus e$, $G\odot e$, and $(G\odot e)\setminus \ell_e$ to its left.



G $G\setminus e$ $G\odot e$ $(G\odot e)\setminus \ell_e$

Finally, we define a unit interval order graph. A *unit interval* is a subset of $\mathbb{R}$ containing all numbers between $a-1$ and a for some $a\in\mathbb{R}$ (with $a-1$ being its left endpoint and a its right endpoint). A *unit interval order* is a partial ordering on a set of unit intervals $\{I_1,I_2,\dots,I_n\}$ such that $I_k\leq I_j$ if the right endpoint of I_k is smaller than the left endpoint of I_j. Notably, under this partial ordering, two intervals are incomparable if they intersect. The *unit interval order graph* of a set of unit intervals is the incomparability graph of the resulting poset, meaning if G is a unit interval order graph, $\{k,j\}\in E(G)$

when I_k and I_j intersect.

2.4 Chromatic symmetric functions

In [Sta95], Stanley introduced the chromatic symmetric function of a graph as a generalization of the chromatic polynomial.

Definition 2.4.1. Given a graph $G = (V, E)$, we define the *chromatic symmetric function* (CSF) of G as

$$\chi_G(x) := \sum_{\kappa \in K(G)} x^\kappa, \qquad \text{where } x^\kappa = x_1^{\#\kappa^{-1}(1)} x_2^{\#\kappa^{-1}(2)} \cdots .$$

We note that $\chi_G(x)$ is a symmetric function over $\mathbb{Q}$ since permuting the variables corresponds to permuting the colors, and this does not affect the conditions on proper colorings.

As symmetric functions, the CSF of graphs are very interesting. For instance, the CSF of a disjoint union of graphs equals the product of the CSF of each of the graphs. The CSF of a graph also encodes information about its acyclic orientations and stable vertex partitions [Sta95].

Moreover, chromatic symmetric functions can be used to construct bases for the symmetric functions. To see this, we consider a family of graphs $\{G_k\}_{k\geq 0}$, where G_k is a connected graph in k vertices, and for a partition $\lambda = (\lambda_1, \dots, \lambda_\ell)$, we define G_λ as the forest whose connected components are graphs in this family, $G_\lambda := G_{\lambda_1} \sqcup \dots \sqcup G_{\lambda_\ell}$. Since the disjoint union of graphs corresponds to the product of the corresponding CSF of the graphs, we have that then, $\chi_{G_\lambda}(x) = \prod_k \chi_{G_{\lambda_k}}(x)$.

Theorem 2.4.2. *[Cho16] Let $\{G_k\}_{k\geq 0}$ be a family of connected graphs such that G_k has k vertices. Then, $\{\chi_{G_\lambda}(x)\}_{\lambda\vdash n}$ is a $\mathbb{Q}$-basis for Λ^n. Furthermore, the functions $\chi_{G_k}(x)$ are algebraically independent over $\mathbb{Q}$ and $\Lambda = \mathbb{Q}[\chi_{G_1}, \chi_{G_2}, \dots]$.*

This result tells us that any such family of graphs defines a basis of the symmetric functions. In [Gon26] the authors consider the family of star graphs, $G_k = \mathrm{ST}_k$, so that the set of functions $\{\mathrm{st}_\lambda(x)\}_{\lambda\vdash n}$, defined by $\mathrm{st}_k(x) = \chi_{\mathrm{ST}_{\lambda_k}}(x)$ and $\mathrm{st}_\lambda(x) := \prod_k \mathrm{st}_k(x)$, forms a basis of Λ, called the *star basis*. This is a very interesting basis, and we highlight here the change of basis between the star basis and the power sum basis.

Theorem 2.4.3. *[Gon26]*

$$\mathrm{st}_{n+1}(x) = \sum_{r=0}^{n} (-1)^r \binom{n}{r} p_{(r+1,1^{n-r})}(x) \qquad \textit{and} \qquad p_{n+1}(x) = \sum_{r=0}^{n} (-1)^r \binom{n}{r} \mathrm{st}_{(r+1,1^{n-r})}(x).$$

Remark 2.4.4. *Note that we use uppercase letters to denote the star graph, ST_n, and lowercase letters for the CSF of the star graph, $\mathrm{st}_n = \chi_{\mathrm{ST}_n}(x)$.*

The CSF of a graph does not satisfy the usual deletion/contraction formula that chromatic polynomials do. However, it satisfies a variant of it involving deletion and the near-contraction operation.

Theorem 2.4.5. *[AP23] Let G be a simple graph and consider an edge $e \in G$. Then,*

$$\chi_G(x) = \chi_{G\backslash e}(x) - \chi_{(G\odot e)\backslash \ell_e}(x) + \chi_{G\odot e}(x). \tag{2.1}$$

As mentioned in [AP23], if e is an internal edge, then the graphs represented in the RHS of (2.1) all have one fewer edge than G. Thus, applying this relation to these three graphs, we can compute the chromatic symmetric function of G as the sum of chromatic symmetric functions of graphs with 2 fewer internal edges than G. Since forests of star graphs are the only graphs with no internal edges, eventually this process leads to writing the chromatic symmetric function of any graph G as the sum of products of the chromatic symmetric function of star graphs.

2.5 Chromatic quasisymmetric functions

In 2012, Shareshian and Wachs [Sha12] introduced a refinement of the CSF of a graph within the framework of quasisymmetric functions.

Definition 2.5.1. Let G be a graph with a labeling L. The *labeled chromatic quasisymmetric function* (labeled CQF) of G is defined as

$$\chi_G^L(x;q) := \sum_{\kappa\in K(G)} q^{\mathrm{asc}^L(\kappa)} x^\kappa.$$

Their motivation came from the connection of the CQF of graphs and to the cohomology of the Hessenberg varieties. As stated in the Introduction, it is important to note that the analog of Stanley-Stembridge conjecture, known as *Shareshian-Wachs' conjecture* and stated in Conjecture 1.1.5, remains open. Also, note that although there are other variants of the chromatic quasisymmetric function of a graph, the Shareshian-Wachs chromatic quasisymmetric function of labeled graphs is what we refer to simply as the CQF of a graph since it is the most prevalent variant in the literature.

Since the labeled CQF has such a connection with algebraic geometry and its quasisymmetric analogue to the Stanley-Stembridge conjecture remains open, these functions are of much interest. On top of the direct work done on the Shareshian-Wachs conjecture mentioned in Section 1.1, Gillespie, Pappe, and Salois explore the conditions under which a graph's labeled CQF is symmetric [Gil25], and different variations on the CQF have been defined and explored, such as the chromatic signed quasisymmetric function [Ava25] and the CQF based on orientations introduced by Ellzey [Ell18], which we will next outline.

The ascent statistic is also defined when we consider a graph with an orientation instead of a graph with a labeling (see Section 2.3). Therefore, we also consider the following variant of the CQF of a graph.

Definition 2.5.2. Let $G = (V,E)$ be a simple graph with an orientation γ. The *oriented chromatic quasisymmetric function of G* (oriented CQF) is defined to be

$$\chi_G^\gamma(x;q) := \sum_\kappa q^{\mathrm{asc}^o(\kappa)} x^\kappa.$$

Remark 2.5.3. *To simplify the notation, we drop the alphabet from the symmetric and quasisymmetric functions. For instance,* χ_G *denotes the CSF of the graph* G*,* $\chi_G^L(q)$ *denotes the labeled CQF, and* $\chi_G^\gamma(q)$ *denotes the oriented CQF of the graph* G*.*

CHAPTER

3

THE TOTAL CHROMATIC QUASISYMMETRIC FUNCTIONS

As mentioned in the Introduction, one of the key aspects of the CQF of a graph is its reliance either on the labeling of the vertices or on the acyclic orientation, as in both cases, it directly affects the number of ascents, and consequently, the coefficient of x^α (which is a polynomial in $\mathbb{Q}[q]$).

In this chapter, we introduce two new variants of the CSF of a graph and study their properties in general. In Section 3.1, we define and study the variant with respect to the labelings, while in Section 3.2, we do it for the variant with respect to the acyclic orientations. In Section 3.3, we compare both variants.

3.1 Via labellings

We start defining the variant with respect to the labeling.

Definition 3.1.1. Let $G=(V,E)$ be a graph, and let L and K be the sets of vertex labelings and proper colorings of G, respectively. We define the *total labeling chromatic quasisymmetric function of* G to be

$$T\chi_G^L(q) := \sum_{L\in L} \chi_G^L(q) = \sum_{L\in L}\sum_{\kappa\in K} q^{\mathrm{asc}^L(\kappa)} x^\kappa.$$

For short, we refer to $T\chi_G^L(q)$ as the *total labeling CQF of* G.

We start by noticing that the total labeling CQF of graphs behaves well for unions of graphs. First, however, we must make a quick remark about the potential of vertex labelings using numbers outside of $[n]$.

Remark 3.1.2. *Note that $\chi_G^L(q)$ does not depend on the exact labeling itself, but rather on the relative order of the labeling of the vertices. Therefore, given any subset $S=\{s_1,s_2,\dots,s_{|V(G)|}\}\subseteq\mathbb{Z}_{>0}$ (written in ascending order), any labeling L_S from $V(G)$ to S induces a labeling L from $V(G)$ to $[n]$ by setting $L(v)=i$ if $L_S(v)=s_i$. Notably, this means that $\chi_G^{L_S}(q)=\chi_G^L(q)$. Similarly, one can define $T\chi_G^{L_S}(q)=T\chi_G^L(q)$ where $T\chi_G^{L_S}(q)$ sums over all vertex labelings of G using numbers in S.*

Proposition 3.1.3. *Let $G=(V,E)$ and $G'=(V',E')$ be two graphs, and consider their disjoint union $H=G\sqcup G'$. Then,*

$$T\chi_H^L(q)=\binom{|V|+|V'|}{|V|}T\chi_G^L(q)T\chi_{G'}^L(q).$$

Proof. Let $n=|V|+|V'|$. Consider a partition of $[n]$ into two blocks $A\sqcup A'=[n]$ with $|A|=|V|$ and $|A'|=|V'|$. Take $L\cup L'$ to be a labeling of the vertices of H such that the restrictions to G and G' coincide with the labelings L and L' using the numbers in A and A', respectively. From Remark 3.1.2, we have that

$$\chi_G^L(q)\cdot\chi_{G'}^{L'}(q)=\chi_{G\sqcup G'}^{L\sqcup L'}(q),$$

where $L\sqcup L'$ labels the G subgraph of H in accordance with L and the G' subgraph of H in accordance with L'. Furthermore, every labeling of H can be uniquely determined by a partition of $[n]$ into these subsets A and A', then determining a labeling L of the G subgraph of H using the numbers in A and a labeling L' of the G' subgraph of H using the numbers in A'.

$$\begin{aligned}
T\chi_H^L(q) &= \sum_{L\in L(H)}\chi_H^L(q)\\
&=\sum_{A,A'}\sum_{L\sqcup L'}\chi_H^{L\sqcup L'}(q)\\
&=\sum_{A,A'}\left(\sum_L \chi_G^L(q)\right)\left(\sum_{L'}\chi_{G'}^{L'}(q)\right)\\
&=\sum_{A,A'}T\chi_G^L T\chi_{G'}^L\\
&=\binom{|V|+|V'|}{|V|}T\chi_G^L T\chi_{G'}^L.
\end{aligned}$$

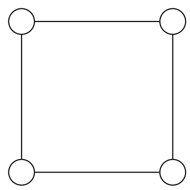
Note that the binomial coefficient comes from the fact that $T\chi_G^L T\chi_{G'}^L$ does not depend on our partition of $[n]$ into $A\sqcup A'$ and there are $\binom{|V|+|V'|}{|V|}$ such set partitions. $\square$

Our study of the total labeling CQS of a graph focuses on its expansion in the monomial quasisymmetric basis. That is, given a graph G, we study the coefficients $c_\alpha^L(q)$ appearing in

$$T\chi_G^L(q)=\sum_\alpha c_\alpha^L(q)M_\alpha,$$

where the sum runs over all compositions α of $n=|V|$. We refer to it as the M-expansion of the total labeling CQF of G. Below is an example, the M-expansion of the total labeling CQF of C_4.

Example 3.1.4. Let G be the cycle with 4 vertices, and write $T\chi_G^L(q)=\sum_\alpha c_\alpha^L(q)M_\alpha$. Then, we have the following coefficients $c_\alpha^L(q)$:



G

α	$c_\alpha^L(q)$
$(1,1,1,1)$	$54q^4+128q^3+208q^2+128q+54$
$(1,1,2)$	$16q^4+16q^3+32q^2+16q+16$
$(1,2,1)$	$8q^4+16q^3+48q^2+16q+8$
$(2,1,1)$	$16q^4+16q^3+32q^2+16q+16$
$(2,2)$	$8q^4+8q^3+16q^2+8q+8$

In this example, one notices that the q-coefficients are palindromic. Indeed, this pattern holds in general.

Proposition 3.1.5. *Let $G=(V,E)$ be a graph on $n=|V|$ vertices, and consider the M-expansion of its total labeling CQF, $T\chi_G^L(q)=\sum_\alpha c_\alpha^L(q)M_\alpha$. Then, $c_\alpha^L(q)$ is a palindromic polynomial in q with degree $|E|$, i.e., for all k,*

$$[q^k]c_\alpha^L(q)=[q^{|E|-k}]c_\alpha^L(q).$$

Proof. Let $J_\alpha(G)\subseteq K\times L$ represent the set of all coloring, labeling ordered pairs of G with associated composition α, and $J_\alpha^k(G)$ be the set of all such ordered pairs yielding k ascents. Then, $[q^k]c_\alpha^L(q)=\#J_\alpha^k(G)$. First, note that for each pair $(\kappa,L)\in J_\alpha$, there can be at most $|E|$ ascents since each edge in G contributes at most one ascent. Therefore, $|E|$ is the largest possible exponent of q for any monomial added in the definition of $T\chi_G^L(q)$.

Next, fix a coloring $\kappa\in K$ with associated composition α such that $\mathrm{comp}(\alpha)=\beta$. Since α is a weak composition, it may have some zero-entries. So, let $\alpha_{i'}$ be the i^{th} entry in α larger than 0, so that $\beta_i=\alpha_{i'}$. We define a labeling $L_0\in L$ in the following way: For each $i\in[\ell(\beta)]$, label the β_i vertices colored i' using the integers $\left(\sum_{j=1}^{i-1}\beta_j\right)+1$ to $\sum_{j=1}^{i}\beta_i$ in any way (if $i=1$, use the integers 1 to β_1). We have that $(\kappa,L)\in J_\alpha(G)$ since κ has associated composition α. Now, for any edge between vertices v_1 and v_2, WLOG if $\kappa(v_1)<\kappa(v_2)$, then $L(v_1)<L(v_2)$, so the edge between v_1 and v_2 contributes an ascent. Thus, this pair (κ_0,L_0) yields $|E|$ ascents, meaning that $c_\alpha^L(q)$ is indeed a polynomial of degree $|E|$.

We now define a map $\phi: J_\alpha^k(G)\to J_\alpha^{|E|-k}$ by $(\kappa,L)\mapsto(\kappa,L^{\text{rev}})$. Here, L^{rev} means that if $L(v)=i$, then $L^{\text{rev}}(v)=n+1-i$. We now claim that an edge $e=\{v_1,v_2\}\in E$ contributes an ascent according to (κ,L) if and only if e does not contribute an ascent according to (κ,L^{rev}).

We prove the forward direction first. If e contributes an ascent according to (κ,L), assume WLOG that $\kappa(v_1)<\kappa(v_2)$. Then, $L(v_1)<L(v_2)$. This means that $L^{\text{rev}}(v_1)>L^{\text{rev}}(v_2)$, so e does not contribute an ascent according to (κ,L^{rev}).

For the reverse direction, if e does not contribute an ascent according to (κ, L), assume WLOG that $\kappa(v_1) < \kappa(v_2)$. Then, $L(v_1) > L(v_2)$, which implies that $L^{\text{rev}}(v_1) < L^{\text{rev}}(v_2)$, and so e does contribute an ascent according to (κ, L^{rev}). This proves our claim, and so ϕ is well-defined.

Next, define $\phi^{-1} : J_\alpha^{|E|-k}(G) \to J_\alpha^k$ by $(\kappa, L) \mapsto (\kappa, L^{\text{rev}})$. From the same if and only if claim as above, ϕ^{-1} is well-defined. Furthermore, for $(\kappa, L) \in J_\alpha^k(G)$ and $(\kappa', L') \in J_\alpha^{|E|-k}(G)$, $\phi(\phi^{-1}(\kappa', L')) = (\kappa', L')$ and $\phi^{-1}(\phi(\kappa, L)) = (\kappa, L)$ because κ has associated composition α. Thus, ϕ^{-1} is the inverse map of ϕ, and so ϕ is a bijection, proving that

$$[q^k]c_\alpha^L(q) = \#J_\alpha^k(G) = \#J_\alpha^{|E|-k}(G) = [q^{|E|-k}]c_\alpha^L(q).$$

This completes the proof of the proposition.

□

We also notice that the q-coefficients are invariant under reversing the composition.

Theorem 3.1.6. *Let $G = (V, E)$ be a graph on $n = |V|$ vertices and consider the M-expansion of its total labeling CQF, $T\chi_G^L(q) = \sum_\alpha c_\alpha^L(q) M_\alpha$. Then, for any composition α of n, $c_\alpha^L(q) = c_{\alpha^{\text{rev}}}^L(q)$.*

Proof. Given k and α, let A_α^k be the set of pairs $(\kappa, L) \in K \times L$ such that $\text{comp}(\kappa) = \alpha$ and $\text{asc}^L(\kappa) = k$. Note that $[q^k]c_\alpha^L(q) = |A_\alpha^k|$.

For each fixed α and k define a map $\phi_{\alpha,k} : J_\alpha^k(G) \to J_{\alpha^{\text{rev}}}^k(G)$ in the following way: Given $(\kappa, L) \in J_\alpha^k(G)$, $\phi_{\alpha,k}(\kappa, L) := (\kappa^{\text{rev}}, L^{\text{rev}})$, where $\kappa^{\text{rev}}(v) = \ell(\alpha) - \kappa(v) + 1$ and $L^{\text{rev}}(v) = n - L(v) + 1$.

First, note that if κ has associated composition α, then κ^{rev} has associated composition α^{rev}. Next, consider an edge $e = \{u, v\} \in E$ that contributes an ascent with respect to (κ, L). Assume without loss of generality that $L(u) < L(v)$ and $\kappa(u) < \kappa(v)$. Then, $L^{\text{rev}}(u) > L^{\text{rev}}(v)$ and $\kappa^{\text{rev}}(u) > \kappa^{\text{rev}}(v)$, and so $\{u, v\}$ contributes an ascent with respect to $(\kappa^{\text{rev}}, L^{\text{rev}})$. Similarly, if $e = \{u, v\} \in E$ does not contribute to the ascents of κ with labeling L, $\{u, v\}$ does not contribute to the ascents of κ^{rev} with labeling L^{rev}. Thus, ϕ preserves the number of ascents, and so $\phi_{\alpha,k}$ is a well-defined map from $J_\alpha^k(G)$ to $J_{\alpha^{\text{rev}}}^k(G)$.

Next, notice that $\phi_{\alpha,k}(\phi_{\alpha^{\text{rev}},k}(\kappa, L)) = (\kappa, L)$ for any $(\kappa, L) \in J_{\alpha^{\text{rev}}}^k(G)$ and $\phi_{\alpha^{\text{rev}},k}(\phi_{\alpha,k}(\kappa, L)) = (\kappa, L)$ for any $(\kappa, L) \in J_\alpha^k(G)$ since $(\kappa^{\text{rev}})^{\text{rev}} = \kappa$ and $(L^{\text{rev}})^{\text{rev}} = L$,. This means that $\phi_{\alpha,k}^{-1} = \phi_{\alpha^{\text{rev}},k}$, so each $\phi_{\alpha,k}$ is a bijection. This proves the claim. □

3.2 Via acyclic orientations

While the total labeling CQF of a graph seems natural to consider, its computation is fairly complex. Here, we consider another variant in terms of acyclic orientations since the set of acyclic orientations of a graph is smaller than the set of labelings.

Recall that we can also consider the statistic of ascents for graphs with orientations, rather than labelings. Moreover, given a simple graph $G = (V, E)$, a labeling L of its vertices induces an acyclic orientation γ_L on G by assigning the edge $\{i, j\} \in E$ the orientation (i, j) if $L(i) < L(j)$, and (j, i) otherwise.

Now, several labelings may yield the same acyclic orientation since γ_L only depends on the relative order of the adjacent vertices. Therefore, $\chi_G^L(q) = \chi_G^{\gamma_L}(q)$. Also, given an orientation γ, $\chi_G^{\gamma}(q) = \chi_G^L(q)$ for any labeling L such that $\gamma_L = \gamma$.

Moreover, we can say that while we can define the CQF of a graph G under any orientation, the acyclic orientations are the ones that reflect the original idea of the CQF as introduced by Shareshian and Wachs. This leads us to the following definition.

Definition 3.2.1. Let G be a graph, and let Γ be the set of acyclic orientations of G. Define the *total orientation chromatic quasisymmetric function* of G as

$$T\chi_G^o(q) := \sum_{\gamma\in\Gamma} \chi_G^{\gamma}(q).$$

We start by noticing that the total orientation CQF of graphs also behaves well for disjoint unions of graphs.

Proposition 3.2.2. *Let G and G' be two graphs and consider $H = G \sqcup G'$. Then,*

$$T\chi_H^o(q) = T\chi_G^o(q) \cdot T\chi_{G'}^o(q).$$

Proof. Given an acyclic orientation γ on G and another acyclic orientation γ' on G', we know that $\chi_G^{\gamma}(q) \cdot \chi_{G'}^{\gamma'}(q) = \chi_{G\sqcup G'}^{\gamma\sqcup\gamma'}(q)$, where $\gamma \sqcup \gamma'$ is the orientation on $G \sqcup G'$ found by placing the γ orientation on the G subgraph of H and the γ' orientation on the G' subgraph of H. Therefore,

$$T\chi_G^o(q) \cdot T\chi_{G'}^o(q) = \left(\sum_{\gamma} \chi_G^{\gamma}(q)\right)\left(\sum_{\gamma'} \chi_{G'}^{\gamma'}(q)\right) = \sum_{(\gamma,\gamma')} \chi_G^{\gamma}(q) \cdot \chi_{G'}^{\gamma'}(q) = \sum_{\gamma,\gamma'} \chi_H^{\gamma\sqcup\gamma'}(q) = T\chi_H^o(q).$$

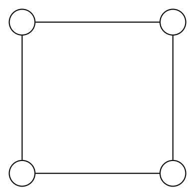
□

As for the labeling variant, our study of the total orientation CQS of a graph focuses on its expansion in the monomial quasisymmetric basis. That is, given a graph G, we study the coefficients $c_\alpha^o(q)$ appearing in

$$T\chi_G^o(q) = \sum_{\alpha} c_\alpha^o(q) M_\alpha,$$

where the sum runs over all compositions α of $n = |V|$. We refer to it as the M-expansion of the total orientation CQF of G. Below is an example of the total orientation CQF, again on C_4.

Example 3.2.3. Let G be the cycle with 4 vertices, and write $T\chi_G^o(q) = \sum_\alpha c_\alpha^o(q) M_\alpha$. Then, the coefficients $c^o_\alpha(q)$ are:



G

α	$c^o_\alpha(q)$
$(1,1,1,1)$	$24q^4+88q^3+112q^2+88q^3+24q^4$
$(1,1,2)$	$4q^4+16q^3+16q^2+16q+4$
$(1,2,1)$	$4q^4+16q^3+16q^2+16q+4$
$(2,1,1)$	$4q^4+16q^3+16q^2+16q+4$
$(2,2)$	$2q^4+8q^3+8q^2+8q+2$

If we compare this to Example 3.1.4, we can see that $T\chi^o_{C_4}(q)$ is symmetric, while $T\chi^L_{C_4}(q)$ is not. Furthermore, each $c^o_\alpha(q)$ is a log-concave polynomial, while that is not true for $c^L_\alpha(q)$ for $\alpha=(1,1,2)$, $(1,2,1)$, $(2,1,1)$, and $(2,2)$.

Now, the chromatic symmetric function of C_4 is

$$\chi_{C_4} = 24m_{(1,1,1,1)} + 4m_{(2,1,1)} + 2m_{(2,2)}.$$

Looking at our example of the total orientation CQF, we can see those coefficients appearing as the coefficients of q^4 and q^0. We formalize this property with the following proposition.

Proposition 3.2.4. *Let $G=(V,E)$ be a graph and consider the M-expansion of its total orientation CQF, $T\chi^o_G(q)=\sum_\alpha c^o_\alpha(q)M_\alpha$. Consider also the m-expansion of the CSF of G, $\chi_G=\sum_\lambda c_\lambda m_\lambda$. Then,*

$$[q^{|E|}]c^o_\alpha(q) = c_{\mathrm{sort}(\alpha)}.$$

Proof. Recall that $c_{\mathrm{sort}(\alpha)}$ counts the number of proper colorings of G with associated composition α, and that $[q^{|E|}]c_\alpha(q)$ is the number of pairs (κ,γ), where κ is a proper coloring of G with associated composition α and γ is an acyclic orientation of G, such that the pair yields $|E|$ ascents.

We first notice that, given a coloring κ, the orientation γ_κ defined by orienting the edge $\{u,v\}$ as (u,v) whenever $\kappa(r)<\kappa(v)$ yields to exactly $|E|$ ascents. Moreover, we claim this orientation is acyclic. Suppose by contradiction that there exists a cycle $v_1v_2\dots v_\ell v_1$ with $(v_i,v_{i+1})\in E$ for $1\le i<\ell$ and $(v_\ell,v_1)\in E$. Then, looking at the proper coloring κ, we have that by definition of the orientation γ_κ, $\kappa(v_1)<\kappa(v_2)\le\cdots\le\kappa(v_\ell)\le\kappa(v_1)$, which is a contradiction and our claim is proven. We also notice that any other orientation $\gamma\neq\gamma_\kappa$ has at least one edge that does not yield an ascent, and so it does not contribute to $[q^{|E|}]c^o_\alpha(q)$.

Thus, for each proper coloring κ, there is a unique acyclic orientation γ_κ that contributes to the coefficient $[q^{|E|}]c^o_\alpha(q)$, meaning that $[q^{|E|}]c^o_\alpha(q)=c_{\mathrm{sort}(\alpha)}$ as stated in the result. □

We now notice that the q-coefficients are symmetric.

Theorem 3.2.5. *Let $G=(V,E)$ be a graph, and consider the M-expansion of its total orientation CQF, $T\chi^o_G(q)=\sum_\alpha c^o_\alpha(q)M_\alpha$. Then, $c^o_\alpha(q)$ is a symmetric polynomial in q of degree $m=|E|$.*

Proof. Let $Q_\alpha^k(G)$ be the set of ordered pairs (κ,γ) with $\kappa\in K$, $\gamma\in\Gamma$ such that the associated composition of κ is α, and κ yields k ascents with respect to γ. We know then that $[q^k]c_\alpha^o(q)=\#Q_\alpha^k(G)$.

For each α,k, define $\phi_{\alpha,k}:Q_\alpha^k(G)\to Q_\alpha^{|E|-k}(G)$ by $(\kappa,\gamma)\mapsto(\kappa,\gamma^{\text{rev}})$ where γ^{rev} is the acyclic orientation with $uv\in E(G)$ oriented (u,v) if and only if uv is oriented (v,u) according to γ.

Fix $(\kappa,\gamma)\in Q_\alpha^k(G)$. Note that γ^{rev} is acyclic if and only if γ is acyclic. Furthermore, take edge $e=uv\in E(G)$ and assume WLOG that $\kappa(u)<\kappa(v)$. If e contributes an ascent according to γ, then $(u,v)\in\gamma$, which means $(v,u)\in\gamma^{\text{rev}}$, and so e does not contribute an ascent according to γ^{rev}. Similarly, if e does not contribute an ascent according to γ, then $(v,u)\in\gamma$, meaning $(u,v)\in\gamma^{\text{rev}}$, so e does contribute an ascent with respect to γ^{rev}. This means that e contributes an ascent with respect to γ^{rev} if and only if e does not contribute an ascent to γ, and so κ has $|E|-k$ ascents with respect to γ^{rev}. This means that $\phi_{\alpha,k}(\kappa,\gamma)\in Q_\alpha^{|E|-k}(G)$, so the map $\phi_{\alpha,k}$ is well-defined.

Next, notice that $\phi_{\alpha,k}(\phi_{\alpha,|E|-k}(\kappa,\gamma))=(\kappa,L)$ for any $(\kappa,\gamma)\in Q_\alpha^{|E|-k}(G)$ and $\phi_{\alpha,|E|-k}(\phi_{\alpha,k}(\kappa,\gamma))=(\kappa,\gamma)$ for any $(\kappa,\gamma)\in Q_\alpha^k(G)$ since $(\gamma^{\text{rev}})^{\text{rev}}=\gamma$. This means that $\phi_{\alpha,k}^{-1}=\phi_{\alpha,|E|-k}$, so each $\phi_{\alpha,k}$ is a bijection. This proves the claim.

□

Next, we notice that, as for the total labeling CQF, the q-coefficients are invariant under reversing the composition.

Theorem 3.2.6. *Let $G=(V,E)$ be a graph, and consider the M-expansion of its total orientation CQF, $T\chi_G^o(q)=\sum_\alpha c_\alpha^o(q)M_\alpha$. Then, $c_\alpha^o(q)=c_{\alpha^{\text{rev}}}^o(q)$.*

Proof. Let $Q_\alpha^k(G)$ be the set of ordered pairs (κ,γ) with $\kappa\in K$, $\gamma\in\Gamma$ such that the associated composition of κ is α, and κ yields k ascents with respect to γ. We know then that $[q^k]c_\alpha^o(q)=\#Q_\alpha^k(G)$.

For each α,k, define $\phi_{\alpha,k}:Q_\alpha^k(G)\to Q_{\alpha^{\text{rev}}}^{|E|-k}(G)$ by $(\kappa,\gamma)\mapsto(\kappa^{\text{rev}},\gamma)$.

Fix $(\kappa,\gamma)\in Q_\alpha^k(G)$. Note that the associated composition to κ^{rev} is α^{rev}. Furthermore, take edge $e=uv\in E(G)$ and assume WLOG that $(u,v)\in\gamma$. Clearly, e contributes an ascent according to κ if and only if it does not contribute an ascent according to κ^{rev}, and so κ^{rev} has $|E|-k$ ascents with respect to γ. This means that $\phi_{\alpha,k}(\kappa,\gamma)\in Q_{\alpha^{\text{rev}}}^{|E|-k}(G)$, so the map $\phi_{\alpha,k}$ is well-defined.

Next, notice that $\phi_{\alpha,k}(\phi_{\alpha^{\text{rev}},|E|-k}(\kappa,\gamma))=(\kappa,L)$ for any $(\kappa,\gamma)\in Q_{\alpha^{\text{rev}}}^{|E|-k}(G)$ and $\phi_{\alpha^{\text{rev}},|E|-k}(\phi_{\alpha,k}(\kappa,\gamma))=(\kappa,\gamma)$ for any $(\kappa,\gamma)\in Q_\alpha^k(G)$ since $(\kappa^{\text{rev}})^{\text{rev}}=\kappa$. This means that $\phi_{\alpha,k}^{-1}=\phi_{\alpha^{\text{rev}},|E|-k}$, so each $\phi_{\alpha,k}$ is a bijection. This proves that $[q^k]c_\alpha^o(q)=[q^{|E|-k}]c_{\alpha^{\text{rev}}}^o(q)$. Now, by Theorem 3.2.5,

$$[q^k]c_\alpha^o(q)=[q^{|E|-k}]c_{\alpha^{\text{rev}}}^o(q)=[q^k]c_{\alpha^{\text{rev}}}^o(q).$$

□

The following result presents a *deletion-near-contraction* property for the total orientation CQF, for which we have not found an analog in the total labeling CQF case.

Theorem 3.2.7. *Let G be a graph and let e be an internal edge in G that is not part of a cycle. Then,*

$$T\chi_G^o = T\chi_{G\odot e}^o + (1+q)\Big(T\chi_{G\backslash e}^o - T\chi_{(G\odot e)\backslash \ell_e}^o\Big).$$

Proof. First, we rewrite the identity in the statement as

$$(1+q)T\chi_{G\backslash e}^o - T\chi_G^o = +(1+q)T\chi_{(G\odot e)\backslash \ell_e}^o - T\chi_{G\odot e}^o. \tag{3.1}$$

Next, we observe the following. Let H be a graph and h be an edge in H that is not part of a cycle. Then, we have that an acyclic orientation of $H\backslash h$ induces two acyclic orientations in H, one for each possible orientation of h. Moreover, a proper coloring of $H\backslash h$ corresponds to a proper coloring of H as long as the vertices corresponding to h have different colors. Moreover, we note that for the two orientations, the coloring either keeps the same number of ascents or increases it by one. This observation applies to both G, with the edge e, and $G\odot e$, with the edge ℓ_e. It implies that the remaining terms on each side of (3.1) are those corresponding to colorings with the vertices of e and ℓ_e, respectively, having the same color in $G\backslash e$ and $(G\odot e)\backslash \ell_e$, respectively, with the $(1+q)$ factor. That is, if $e=\{u,v\}$ and $\ell_e=\{v',v_e\}$, we have that

$$(1+q)T\chi_{G\backslash e}^o - T\chi_G^o = (1+q)\sum_{\gamma\in\Gamma(G\backslash e)}\sum_{\substack{\kappa\in K(G\backslash e)\\ \kappa(r)=\kappa(v)}} q^{\mathrm{asc}^o(\kappa)}x^\kappa, \qquad \text{and}$$

$$(1+q)T\chi_{(G\odot e)\backslash \ell_e}^o - T\chi_{G\odot e}^o = (1+q)\sum_{\gamma\in\Gamma((G\odot e)\backslash \ell_e)}\sum_{\substack{\kappa\in K((G\odot e)\backslash \ell_e)\\ \kappa(v')=\kappa(v_e)}} q^{\mathrm{asc}^o(\kappa)}x^\kappa,$$

and so Equation (3.1) follows if we can show that

$$\sum_{\gamma\in\Gamma(G\backslash e)}\sum_{\substack{\kappa\in K(G\backslash e)\\ \kappa(r)=\kappa(v)}} q^{\mathrm{asc}^o(\kappa)}x^\kappa = \sum_{\gamma\in\Gamma((G\odot e)\backslash \ell_e)}\sum_{\substack{\kappa\in K((G\odot e)\backslash \ell_e)\\ \kappa(r)=\kappa(v)}} q^{\mathrm{asc}^o(\kappa)}x^\kappa.$$

Let $H=G\setminus e$ and $H'=(G\odot e)\setminus \ell_e$. Let H be the set of pairs (γ,κ) with $\gamma\in\Gamma(H)$ and $\kappa\in K(H)$ such that $\kappa(u)=\kappa(v)$ and define H' to be the set of (κ',γ') pairs with $\gamma'\in\Gamma(H'$ and $\kappa'\in K(H')$ such that $\kappa'(v')=\kappa'(v_e)$. Now, define the map $\varphi: H\to H'$ mapping (κ,γ) to $\varphi(\kappa,\gamma)=(\kappa',\gamma')$, with κ' and γ' defined in the following way.

- γ' is defined from γ by keeping the same orientation on those edges not involving u and v in $G\backslash e$, and orienting the edges $\{v_e,w\}$ in γ' with the same orientation as the corresponding edge $\{u,w\}$ or $\{v,w\}$ in γ (so, for example if $\{u,w\}$ is oriented (w,u) in γ, then $\{v_e,w\}$ is oriented (w,v_e) in γ'). Note that it is never the case that $\{u,w\}$ and $\{v,w\}$ are both edges in $G\setminus e$, otherwise $\{u,v,w\}$ would form a 3-cycle in G, but we assume that e is not part of a cycle.

- $\kappa'(w)=\kappa(w)$ for all $w\notin\{v_e,v'\}$ and $\kappa'(v')=\kappa'(v_e):=\kappa(u)=\kappa(v)$.

We now claim that the map φ is a well-defined bijection such that $\mathrm{asc}^o(\kappa)=\mathrm{asc}^o(\kappa')$ and $x^\kappa=x^{\kappa'}$. The result follows then if we show that φ is a well-defined bijection.

First, note that γ' is an acyclic orientation of H'. Next, note that if $\{v_1, v_2\}$ is an edge in H', then either $\{v_1, v_2\}$ is an edge in H (i.e. $v_1, v_2 \notin \{v_e, v'\}$), or $\{v_1, v_2\}$ is an edge in H (i.e. $v_1 = v_e$ WLOG since v' is degree 0). In the former case, $\kappa'(v_1) \neq \kappa'(v_2)$ since κ is a proper coloring of H. In the latter case, it must be that either $\{u, v_2\}$ or $\{v, v_2\}$ is an edge in H. We know that $\kappa'(v_e) \neq \kappa'(v_2)$ since $\kappa'(v_e) = \kappa(u) = \kappa(v) \neq \kappa(v_2)$, so κ' is a valid proper coloring of H'. This means that φ is well-defined.

Furthermore, one can see that $x^\kappa = x^{\kappa'}$ since κ and κ' color u, v, v_e, v' the same color. Now, we want to show that $\mathrm{asc}^o(\kappa) = \mathrm{asc}^o(\kappa')$. Take an edge $\{v_1, v_2\} \in E(H')$. Again, in our first case, if $v_1, v_2 \notin \{v_e, v'\}$, then $\{v_1, v_2\} \in E(H)$, $\kappa(v_1) = \kappa'(v_1)$, $\kappa(v_2) = \kappa'(v_2)$, and γ and γ' orient $\{v_1, v_2\}$ the same way, so clearly $\{v_1, v_2\}$ yields an ascent in H if and only if it yields an ascent in H'.

In the latter case, WLOG assume $v_1 = v_e$. Also WLOG, assume that $\{u, v_2\} \in E(H)$. We know that $\kappa'(v_e) = \kappa(u)$ and $\kappa(v_2) = \kappa'(v_2)$. Since γ and γ' also orient this edge the same way, we have that in this case, $\{v_e, v_2\}$ contributes an ascent in H' if and only if the corresponding edge $\{u, v_2\}$ contributes an ascent in H. Thus, $\mathrm{asc}^o(\kappa') = \mathrm{asc}^o(\kappa)$.

Now, define the map $\varphi^{-1} : H' \to H$ as $(\kappa', \gamma') \mapsto (\kappa, \gamma)$ with (κ, γ) defined in the following way.

- γ is defined from γ' by keeping the same orientation on those edges not involving v_e in H. For each edge $\{v_e, w\} \in E(H')$, vertex w is adjacent to either u or v (but not both, since we assume $e = \{u, v\}$ is not part of a cycle). WLOG, say $\{u, w\} \in E(H)$. Orient $\{u, w\}$ in accordance with $\{v_e, w\}$, that is to say if $(v_e, w) \in \gamma'$, $(u, w) \in \gamma$ and if $(w, v_e) \in \gamma'$, $(w, u) \in \gamma$.

- $\kappa(w) = \kappa'(w)$ for all $w \notin \{u, v\}$ and $\kappa(u) = \kappa(v) := \kappa'(v_e) = \kappa'(v')$.

We can see that γ in this definition is an acyclic orientation of H, and κ is a proper coloring, so φ^{-1} is well-defined.

Look at $\varphi(\varphi^{-1}(\kappa', \gamma')) = (\kappa_2, \gamma_2)$. If we take a vertex $w \in V(H')$, if $w \notin \{v_e, v'\}$, then clearly $\kappa'(w) = \kappa_2(w)$. If $w \in \{v_e, v'\}$ then $\kappa'(w) = c = \kappa(w) = \kappa_2(w)$. Now, if we take an edge $\{v_1, v_2\} \in E(H')$. Its orientation according to γ' is the same as its orientation according to γ, so $\varphi(\varphi^{-1}(\kappa', \gamma')) = (\kappa', \gamma')$.

Similarly, $\varphi^{-1}(\varphi(\kappa, \gamma)) = (\kappa, \gamma)$. Thus, φ is a well-defined bijection, which proves the claim. □

We finish this section by analyzing a particular case in which $T\chi^o_G$ is symmetric and conjecturing a more general result.

Theorem 3.2.8. *Let $G = (V, E)$ be a tree with $m = |E|$. Then,*

$$T\chi^o_G(q) = \left(q+1\right)^m \chi_G.$$

Where χ_G is the chromatic symmetric function of G. In particular, $T\chi^o_G(q)$ is symmetric.

Proof. We start comparing the monomial expansions of χ_G and $T\chi^o_G(q)$ in the monomial basis for symmetric and quasisymmetric functions, respectively. Let $\chi_G = \sum_\lambda c_\lambda m_\lambda$ and $T\chi^o_G(q) = \sum_\alpha c^o_\alpha(q) M_\alpha$.

Then, $T\chi^o_G(q) = (q+1)^m \chi_G$ if and only if

$$[q^k]c^o_\alpha(q) = c_\lambda \binom{m}{k}, \qquad \text{for any } \alpha \text{ such that } \mathrm{sort}(\alpha) = \lambda.$$

On one hand, the LHS counts the number of colorings κ and acyclic orientations γ such that $x^\kappa = x^\alpha$ and $\mathrm{asc}^o(\kappa) = k$. On the other hand, in the RHS, c_λ counts the number of colorings κ' such that $x^\kappa = x^\beta$ for any composition β with $\mathrm{sort}(\beta) = \lambda$, and in particular we can take $\beta = \alpha$. Moreover, $\binom{m}{k}$ counts the number of ways of choosing k edges among $m = |E(G)|$. Since any orientation in a tree is an acyclic orientation, any k-subset of $E(G)$ gives us an acyclic orientation so that $\mathrm{asc}^o(\kappa) = k$. Thus, the result follows.

□

We finish this section with a conjecture generalizing the previous result for trees.

Conjecture 3.2.9. *If G is a graph for which no two cycles share an edge, then $T\chi^o_G(q)$ is symmetric.*

3.3 Comparison: Labelings vs acyclic orientations

These functions do share several similar properties. For instance, as shown in Proposition 3.1.5 and Theorem 3.2.5, both functions yield palindromic coefficients in their monomial expansions. Similarly, as in Theorems 3.1.6 and 3.2.6, we achieve some partial symmetry of $T\chi^L_G(q)$ and $T\chi^o_G(q)$ in general.

One immediate difference between these two interpretations of "normalizing" the chromatic quasisymmetric function is the behavior of the function on trees. In particular, note that if $G = \mathrm{ST}^r_n$, then $T\chi^L_G(q)$ is not symmetric in general (e.g. Example 4.3.2), while Theorem 3.2.8 shows that $T\chi^o_G(q)$ is always symmetric. On the contrary, $T\chi^o_G$ admits a deletion-near-contraction formula that can be applied to graphs with cycles, while no such deletion-near-contraction formula has been found for $T\chi^L_G(q)$.

Another big difference between these two functions is in the size of the coefficients. Since there are, in general, many more potential labelings of a graph than there are acyclic orientations, $T\chi^L_G$ often has much larger coefficients than $T\chi^o_G$, as shown in the following example.

Example 3.3.1. Let $G = C_4$. Let $T\chi^L_G(q) = \sum_{\alpha\vDash 4} c^L_\alpha(q) M_\alpha$ and $T\chi^o_G(q) = \sum_{\alpha\vDash 4} c^o_\alpha(q) M_\alpha$. The following table compares $c^L_\alpha(q)$ and $c^o_\alpha(q)$ for each α for which they are nonzero.

α	$c^L_\alpha(q)$	$c^o_\alpha(q)$
$(1,1,1,1)$	$56q^4+128q^3+208q^2+128q+56$	$24q^4+88q^3+112q^2+88q+24$
$(1,1,2)$	$16q^4+16q^3+32q^2+16q+16$	$4q^4+16q^3+16q^2+16q+4$
$(1,2,1)$	$8q^4+16q^3+48q^2+16q+8$	$4q^4+16q^3+16q^2+16q+4$
$(2,1,1)$	$16q^4+16q^3+32q^2+16q+16$	$4q^4+16q^3+16q^2+16q+4$
$(2,2)$	$8q^4+8q^3+16q^2+8q+8$	$2q^4+8q^3+8q^2+8q+2$

Note also that this is another example that shows their discrepancy in terms of symmetry since $T\chi^o_{C_4}(q)$ is a symmetric function, while $T\chi^L_{C_4}(q)$ is not.

CHAPTER

4

THE STAR GRAPH

In this chapter, we focus our study on the star graph and examine its chromatic quasisymmetric function, as well as its total chromatic quasisymmetric functions, both with respect to labelings and orientations. Our study focuses on the expansion in the monomial bases for the corresponding framework, symmetric functions or quasisymmetric functions. The computation for the CQF and for the total orientation CQF is relatively straightforward. However, for the total labeling CQF of the star graph, the formula is more interesting and relies on proving a binomial identity, which we do in Chapter 5.

4.1 The chromatic quasisymmetric function

In this section, we include the expansion of the CQF of the star graph in the monomial quasisymmetric basis.

Recall that we denote the star graph in n vertices by ST_n, and the root by r. We also denote by ST_n^r the star graph together with a labeling L for which $L(r) = r$. Moreover, we denote by st_n the CSF of the star graph ST_n and by $\mathrm{st}_n(q)$ its CQF. When referring to ST_n^r, we denote by st_n^r and by $\mathrm{st}_n^r(q)$ its CSF and its CQF, respectively. Note that $\mathrm{st}_n^r(q)$ is independent of the choice of labeling as long as $L(r) = r$. Throughout this section, when we write ST_n^r, we assume that the root vertex is denoted by r and that there is a labeling L of the vertices of G such that $L(r) = r$.

We need to introduce some notation related to the weak compositions α. Let $\alpha = (\alpha_1, \dots, \alpha_\ell)$ be the weak composition of n encoding the coloring κ; that is, α_i counts the number of vertices with color i in κ. We define $\alpha_{\leftarrow i}$ and $\alpha_{i\rightarrow}$ as the weak compositions obtained by looking at the entries strictly to the left and right of α_i, respectively; that is, $\alpha_{\leftarrow i} = (\alpha_1, \alpha_2, \dots, \alpha_{i-1})$ and $\alpha_{i\rightarrow} = (\alpha_{i+1}, \alpha_{i+2}, \dots, \alpha_\ell)$. We also denote its sizes, respectively, by $L_{\alpha_i} = |\alpha_{\leftarrow i}|$ for $i > 1$, with $L_{\alpha_1} = 0$, and by $R_{\alpha_i} = |\alpha_{i\rightarrow}|$ for $i < \ell$, with $R_{\alpha_\ell} = 0$. Similarly, $L^m_{\alpha_i} = \min\{m, L_{\alpha_i}\}$ and $R^m_{\alpha_i} = \min\{m, R_{\alpha_i}\}$. Finally, we denote by $\mathrm{Mult}(\alpha)$ the multinomial coefficient $\mathrm{Mult}(\alpha) = \binom{|\alpha|}{\alpha_1, \ldots, \alpha_\ell}$, where $0! = 1$ and $\mathrm{Mult}(\emptyset) = \mathrm{Mult}(0) = 1$.

Remark 4.1.1. *We use L and $L(v)$ to refer to vertex labelings, while L_{α_i} are used to refer to statistics about compositions.*

The following result summarizes all the possible values for the number of ascents of κ in terms of the label and the coloring of the root, $L(r)$ and $\kappa(r)$.

Lemma 4.1.2. *Consider the star graph ST^r_n and a proper coloring κ such that $\kappa(r) = i$. Then,*

$$\mathrm{asc}^L(\kappa) = \left|n - r - L_{\alpha_i}\right| + 2j \quad \textit{for some} \quad 0 \le j \le \min\left\{L^{n-r}_{\alpha_i}, R^{r-1}_{\alpha_i}\right\}.$$

Proof. We start by observing that since the root r has color i and is connected to all the other vertices, there are no other vertices with color i. That is, $\alpha_i = 1$.

We split the argument into two cases depending on whether $n - r - L_{\alpha_i}$ is positive or negative.

- Case 1: $L_{\alpha_i} \le n - r$. In this case, $L^{n-r}_{\alpha_i} = L_{\alpha_i}$, and $R_{\alpha_i} = n - 1 - L_{\alpha_i} \ge n - 1 - (n - r) = r - 1$, so that $R^{r-1}_{\alpha_i} = r - 1$.

  Let j be the number of vertices v such that $L(v) < r$ and $\kappa(v) < i$. We want to count how many vertices v there are with $L(v) > r$ and $\kappa(v) > i$, since these are the ones contributing to the number of ascents. We know that there are $L_{\alpha_i} - j$ vertices v such that $L(v) > r$ and $\kappa(v) < i$. Consequently, there are $n - 1 - L_{\alpha_i}$ vertices with $\kappa(v) > i$, and of those, $r - 1 - j$ have $L(v) < r$. Therefore, there are exactly $n - 1 - L_{\alpha_i} - (r - 1 - j) = n - r - L_{\alpha_i} + j$ vertices v such that $L(v) > r$ and $\kappa(v) > i$. Thus, κ has $\left|n - r - L_{\alpha_i}\right| + 2j$ ascents.

  Now, because there cannot be more than $r - 1$ vertices with $L(v) < r$, we have that $j \le r - 1 = R^{r-1}_{\alpha_i}$. We also know that there are most L_{α_i} vertices with $\kappa(v) < i$, and so $j \le L^{n-r}_{\alpha_i}$. Thus, $j \le \min\left\{L^{n-r}_{\alpha_i}, R^{r-1}_{\alpha_i}\right\}$.

- Case 2: $L_{\alpha_i} > n - r$. In this case, $L^{n-r}_{\alpha_i} = n - r$, and $R^{r-1}_{\alpha_i} = R_{\alpha_i}$, since $R_{\alpha_i} = n - 1 - L_{\alpha)i} < n - 1 - (n - r) = r - 1$.

  Let j be the number of vertices v such that $L(v) > r$ and $\kappa(v) > i$. We want to count how many vertices v there are with $L(v) < r$ and $\kappa(v) < i$, since we know they also contribute to the number of ascents. We know that there are $R_{\alpha_i} - j$ vertices v such that $L(v) < r$ and $\kappa(v) > i$. Consequently, there are $n - 1 - R_{\alpha_i}$ vertices with $\kappa(v) < i$, and of those, $n - r - 1 - j$ have $L(v) > r$. Therefore, there are exactly $n - 1 - R_{\alpha_i} - (n - r - 1 - j) = r + R_{\alpha_i} + j$ vertices v such that $L(v) > r$ and $\kappa(v) > i$. Recalling that $R_{\alpha_i} = n - 1 - L_{\alpha_i}$, we get that κ has $\left|n - r - L_{\alpha_i}\right| + 2j$ ascents.

  Now, because there cannot be more than R_{α_i} vertices with $\kappa(v) > i$, we have that $j \le R_{\alpha_i} = R^{r-1}_{\alpha_i}$. We also know that there are most $n - r$ vertices with $L(v) > r$, and so $j \le n - r = L^{n-r}_{\alpha_i}$. Thus, $j \le \min\left\{L^{n-r}_{\alpha_i}, R^{r-1}_{\alpha_i}\right\}$. □

With this lemma, we are now ready to describe the coefficients in the monomial expansion of the CQF of the star graph.

Proposition 4.1.3. *Consider* ST_n^r *and the* M*-expansion of its CQF,* $\mathrm{st}_n^r(q) = \sum_{\alpha \models n} c_\alpha^r(q) M_\alpha$. *Then,*

$$c_\alpha^r(q) = \sum_i \mathrm{Mult}(\alpha_{i\rightarrow})\mathrm{Mult}(\alpha_{\leftarrow i}) \sum_{j=0}^{\min\{L_{\alpha_i}^{n-r}, R_{\alpha_i}^{r-1}\}} \binom{n-r}{L_{\alpha_i}^{n-r}-j}\binom{r-1}{R_{\alpha_i}^{r-1}-j} q^{2j+|n-r-L_{\alpha_i}|},$$

where the first summation runs over the i *such that* $\alpha_i = 1$.

Proof. First, note that fixing i such that $\alpha_i = 1$ is essentially fixing the color of the root. That is, we want to describe the polynomial given by looking at the proper colorings κ such that its associated weak composition is α and $\kappa(r) = i$. We count these proper colorings by first choosing those vertices that are colored less than or greater than i, and then choosing the specific colors afterwards.

By Lemma 4.1.2, we know that $\mathrm{asc}^L(\kappa) = \left|n - r - L_{\alpha_i}\right| + 2j$, where j denotes the number of vertices v such that $L(v) < r$ and $\kappa(v) < i$, or $L(v) > r$ and $\kappa(v) > i$, and we also know that $0 \le j \le \min\left\{L_{\alpha_i}^{n-r}, R_{\alpha_i}^{r-1}\right\}$. The argument now splits into two cases, one where $n - r \ge L_{\alpha_i}$ and one where $n - r < L_{\alpha_i}$.

Case 1: $n - r \ge L_{\alpha_i}$. Following a similar process to the one outlined in the proof of Lemma 4.1.2, we choose j vertices such that $L(v) < r$ to be colored such that $\kappa(v) < i$. There are $r - 1$ of these vertices, so there are $\binom{r-1}{j}$ ways to do this. Note that since $r - 1 = R_{\alpha_i}^{r-1}$ in this case, $\binom{r-1}{j} = \binom{r-1}{R_{\alpha_i}^{r-1}-j}$. We still need to choose the remaining $L_{\alpha_i} - j$ vertices that must be colored less than i. Since $L_{\alpha_i} = L_{\alpha_i}^{n-r}$ in this case, we choose $L_{\alpha_i}^{n-r} - j$ vertices from the $n - r$ vertices such that $L(v) > r$ and there are $\binom{n-r}{L_{\alpha_i}^{n-r}-j}$ ways to do it. Thus, in this case, there are $\binom{n-r}{L_{\alpha_i}^{n-r}-j}\binom{r-1}{R_{\alpha_i}^{r-1}-j}$ ways to assign L_{α_i} vertices to be colored less than i and R_{α_i} vertices to be colored greater than i.

Case 2: $n - r < L_{\alpha_i}$. In this case, we choose j vertices such that $L(v) > r$ and $\kappa(v) > i$. There are $n - r$ vertices such that $L(v) > r$, and so we have $\binom{n-r}{j}$ ways of doing this. We must then choose $R_{\alpha_i} - j$ remaining vertices to be colored greater than i. These must be pulled from the $r - 1$ vertices such that $L(v) < r$, so there are $\binom{r-1}{R_{\alpha_i}-j}$ ways to do this. Now, in this case, $L_{\alpha_i}^{n-r} = n - r$ and $R_{\alpha_i}^{r-1} = R_{\alpha_i}$, we have that $\binom{n-r}{j} = \binom{n-r}{L_{\alpha_i}^{n-r}-j}$ and $\binom{r-1}{R_{\alpha_i}-j} = \binom{r-1}{R_{\alpha_i}^{r-1}-j}$. Thus, in this case, there are $\binom{n-r}{L_{\alpha_i}^{n-r}-j}\binom{r-1}{R_{\alpha_i}^{r-1}-j}$ ways to assign L_{α_i} vertices to be colored less than i and R_{α_i} vertices to be colored greater than i.

Now, once we have determined exactly which vertices are colored greater than i and which are colored less than i, the factor $\mathrm{Mult}(\alpha_{i\rightarrow})\mathrm{Mult}(\alpha_{\leftarrow i})$ comes from choosing the precise color for every vertex. This gives, in total, $\mathrm{Mult}(\alpha_{i\rightarrow})\mathrm{Mult}(\alpha_{\leftarrow i})\binom{n-r}{L_{\alpha_i}^{n-r}-j}\binom{r-1}{R_{\alpha_i}^{r-1}-j}$ ways to choose one of these proper colorings, and this proves the claim. $\square$

We also have the following property, which will be useful later in the paper.

Lemma 4.1.4. *Let* ST_n^r *be the star graph on* n *vertices, and consider the* M*-expansion of its CQF,* $\mathrm{st}_n^r(q) = \sum_\alpha c_\alpha^r(q) M_\alpha$. *Then,*

$$[q^k]c_\alpha^r(q) = [q^{n-1-k}]c_\alpha^{n-1-r}(q) \quad \textit{and} \quad [q^k]c_\alpha^r(q) = [q^{n-1-k}]c_{\alpha^{\mathrm{rev}}}^r,$$

where α^{rev} is the reverse of α.

Proof. We first prove that $[q^k]c^r_\alpha(q) = [q^{n-1-k}]c^{n-1-r}_\alpha(q)$. Let L be a labeling of ST^r_n such that $L(r) = r$, and define L^{rev} as the labeling defined by $L^{\text{rev}}(v) = n-1-i$ if $L(v) = i$. Then, the root is labeled $L^{\text{rev}}(r) = n-1-r$ and L^{rev} is a labeling of ST^{n-1-k}_n. Now, $[q^k]c^r_\alpha(q)$ counts the number of colorings κ of ST^r_n with associated composition α and that has k ascents with respect to L. These are exactly the colorings of ST^{n-1-r}_n with associated composition α and that have $n-1-k$ ascents with respect to L^{rev}. Thus, $[q^k]c^r_\alpha(q) = [q^{n-1-k}]c^{n-1-r}_\alpha(q)$.

Next, we prove that $[q^k]c^r_\alpha(q) = [q^{n-1-k}]c^r_{\alpha^{\text{rev}}}$ similarly. Let L be a labeling of ST^r_n such that $L(r) = r$, and consider a coloring κ of ST^r_n with associated composition α and that has k ascents with respect to L. We define the coloring κ^{rev} by setting $\kappa^{\text{rev}}(v) = n-1-i$ if $\kappa(v) = i$. Therefore, κ^{rev} is a coloring of ST^r_n with associated composition α^{rev} and that has $n-1-k$ ascents. Thus, $[q^k]c^r_\alpha(q) = [q^{n-1-k}]c^r_{\alpha^{\text{rev}}}$. □

4.2 Total CQF via acyclic orientations

In this section, we compute the expansion of the total orientation CQF of ST_n, which is a direct consequence of the m-expansion of the CSF of ST_n. Before stating the results, we introduce some notation. Given a partition $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_\ell)$, we can rewrite it in terms of its repeated parts, $\lambda = \langle 1^{a_1} \ldots k^{a_k} \rangle$, where a_i denotes the number of entries in λ equal to i. We write $a_i(\lambda)$ whenever we need to specify the partition λ. We also denote $\tilde{\lambda} = (\lambda_1, \lambda_2, \ldots, \lambda_{\ell-1})$.

Theorem 4.2.1. *Consider ST_n and the m-expansion of its CSF, $\mathrm{st}_n = \sum_{\lambda \vdash n} c_\lambda m_\lambda$. Then,*

$$c_\lambda = a_1(\lambda) \cdot \mathrm{Mult}(\tilde{\lambda}).$$

Proof. Recall that c_λ counts the number of proper colorings of ST_n with associated weak composition λ. We can count these colorings by choosing first a color for the root, and then choosing colors for all other vertices. We start noticing that $a_1(\lambda) \geq 1$ since for any proper coloring of ST_n, the color of the root is never repeated. Now, the root r can be colored any color i such that $\lambda_i = 1$, and so there are $a_1(\lambda)$ ways to color the root. Suppose that the root is colored i. Then, we have that $\lambda_i = \lambda_{i+1} = \ldots = \lambda_\ell = 1$, and so $(\lambda_1, \ldots, \lambda_{i-1}, \lambda_{i+1}, \ldots, \lambda_\ell) = \tilde{\lambda}$. Thus, there are $\mathrm{Mult}(\tilde{\lambda})$ ways to color the remaining vertices, and the result follows. □

Recall now that Theorem 3.2.8 tells us that

$$T\chi^o_{\mathrm{ST}_n}(q) = \big(q+1\big)^{n-1} \chi_{\mathrm{ST}_n}.$$

We then have the following corollary.

Corollary 4.2.2. *Let $G = \mathrm{ST}_n$. Then,*

$$T\chi^o_{\mathrm{ST}_n}(q) = \sum_{\lambda \vdash n} a_1(\lambda) \cdot \mathrm{Mult}(\tilde{\lambda})(q+1)^{n-1} m_\lambda.$$

4.3 Total CQF via labelings

Notice that Proposition 4.1.3 tells us that, as mentioned before, the labeling CQF of the star graph depends only on the label of the root, which allows us to focus on the following normalization for the total labeling CQF.

Definition 4.3.1. We define the *normalized total labeling CQF of* ST_n as

$$\mathrm{Tst}_n(q) := \sum_{\text{labelings of the root}} \chi_{\mathrm{st}_n^r}(q) = \frac{1}{(n-1)!} T\chi^L_{\mathrm{ST}_n}(q).$$

We want to analyze the M-expansion of $\mathrm{Tst}_n(q)$, and we start by looking at an example. Note that in this section, we denote the coefficients with the letter b, so that it is more explicit that these are not the same as the coefficients for the total labeling CQF of the star graph.

Example 4.3.2. Consider ST_n and consider the M-expansion of $\mathrm{Tst}_4(q) = \sum_\alpha b_\alpha(q) M_\alpha$. In Table 4.1, we show the coefficients $b_\alpha(q)$.

Table 4.1 Coefficients in the M-expansion of $\mathrm{Tst}_4(q)$.

α	$b_\alpha(q)$
[1,1,1,1]	$16q^3+32q^2+32q+16$
[1,1,2]	$4q^3+8q^2+8q+4$
[1,2,1]	$6q^3+6q^2+6q+6$
[1,3]	q^3+q^2+q+1
[2,1,1]	$4q^3+8q^2+8q+4$
[3,1]	q^3+q^2+q+1

For comparison, in Table 4.2, we show the coefficients $c^r_\alpha(q)$ in the M-expansion of $\mathrm{st}^r_n(q)$, where we recall that r corresponds to the color of the root.

Table 4.2 Coefficients in the M-expansion of $\mathrm{st}_4^r(q)$ for $1 \le r \le 4$.

α	$c_\alpha^1(q)$	$c_\alpha^2(q)$	$c_\alpha^3(q)$	$c_\alpha^4(q)$
$[1,1,1,1]$	$6q^3+6q^2+6q+6$	$2q^3+10q^2+10q+2$	$2q^3+10q^2+10q+2$	$6q^3+6q^2+6q+6$
$[1,1,2]$	$3q^3+3q^2$	q^3+3q^2+2q	$2q^2+3q+1$	$3q+3$
$[1,2,1]$	$3q^3+3$	$3q^2+3q$	$3q^2+3q$	$3q^3+3$
$[1,3]$	q^3	q^2	q	1
$[2,1,1]$	$3q+3$	$2q^2+3q+1$	q^3+3q^2+2q	$3q^3+3q^2$
$[3,1]$	1	q	q^2	q^3

Before continuing, we introduce more notation associated with ST_n^r and the normalized total labeling CQF, $\mathrm{Tst}_n(q)$. Firstly, for each possible labeling of the root, $1 \le r \le \lfloor n/2 \rfloor$, we fix a *representative labeling* such that the label of the root is r, and we denote that labeling by L_r. For the other possible values of the labeling of the root, $\lfloor n/2 \rfloor < r' \le n$, we write $r' = n+1-r$ and define $L_{r'}$ as the labeling $L_{r'}(v) = n+1-L_r(v)$, for any $v \in V(\mathrm{ST}_n)$. We refer to $L_{r'}$ as the *complementary labeling*. We denote by K_α^r the set of colorings of ST_n^r with associated composition α and by $K_\alpha^r(i)$ the subset of colorings of K_α^r such that $\kappa(r) = i$. Now, consider the M-expansion of $\mathrm{Tst}_n(q)$, $\mathrm{Tst}_n(q) = \sum_\alpha b_\alpha(q) M_\alpha$. Then, we have that

$$b_\alpha(q) = \sum_{r=1}^{n} c_\alpha^r(q) = \sum_i b_\alpha(i;q) = \sum_{i,r} b_\alpha^r(i;q),$$

where the first sum runs over the possible labelings of the root and we recall that $c_\alpha^r(q)$ is independent of the concrete labeling L as long as $L(r) = r$; the second sum runs over the i such that $\alpha_i = 1$, which corresponds to the color of the root $\kappa(r)$; and the third sum runs over the possible labelings and colorings of the root. That is,

$$c_\alpha^r(q) = \sum_{\kappa \in K_\alpha^r} q^{\mathrm{asc}^L(\kappa)} \qquad \text{and} \qquad b_\alpha^r(i;q) = \sum_{\kappa \in K_\alpha^r(i)} q^{\mathrm{asc}^L(\kappa)},$$

where the labeling L is fixed.

Lemma 4.3.3. *Let* ST_n *be the star graph in* n *vertices, and consider the* M*-expansion of its normalized total labeling CQF:* $\mathrm{Tst}_n(q) = \sum_\alpha b_\alpha(q) M_\alpha$*, where* $b_\alpha(q) = \sum_{i,r} b_\alpha^r(i;q)$*. Then,*

$$[q^k] b_\alpha^r(i;q) = [q^k] b_{\alpha^{\mathrm{rev}}}^{n+1-r}(\ell - i + 1; q), \qquad \text{where} \qquad \ell = \ell(\alpha).$$

That is, $b_\alpha(i;q) = b_{\alpha^{\mathrm{rev}}}(\ell - i + 1; q)$.

Proof. Note that $[q^k] b_\alpha^r(i;q)$ counts the number of colorings $\kappa \in K_\alpha^r(i)$ such that $\mathrm{asc}^L(\kappa) = k$ and that $[q^k] b_{\alpha^{\mathrm{rev}}}^{n+1-r}(\ell - i + 1; q)$ counts the number of colorings $\kappa' \in K_{\alpha^{\mathrm{rev}}}^{n+1-r}(\ell - i + 1)$ such that $\mathrm{asc}^L(\kappa') = k$.

Consider the following map:

$$\begin{array}{rccc}\varphi: & \left\{\kappa \in K_{\alpha}^{r}(i) \mid \operatorname{asc}^{L}(\kappa)=k\right\} & \longrightarrow & \left\{\kappa' \in K_{\alpha^{\mathrm{rev}}}^{n+1-r}(\ell+1-i) \mid \operatorname{asc}^{L}(\kappa')=k\right\} \\ & \kappa & \longmapsto & \varphi(\kappa):=\kappa',\end{array}$$

where κ' is the coloring $\kappa'(v)=\ell+1-\kappa(v)$, for all $v\in \mathrm{ST}_n$.

By definition of φ, κ' is a coloring in $K_{\alpha^{\mathrm{rev}}}^{n+1-r}(\ell+1-i)$. Moreover, the number of ascents is preserved since φ flips the relative label order and relative color order between each vertex. Thus, φ is a well-defined map. φ^{-1} is defined as

$$\begin{array}{rccc}\varphi^{-1}: & \left\{\kappa' \in K_{\alpha^{\mathrm{rev}}}^{n+1-r}(\ell+1-i) \mid \operatorname{asc}^{L}(\kappa')=k\right\} & \longrightarrow & \left\{\kappa \in K_{\alpha}^{r}(i) \mid \operatorname{asc}^{L}(\kappa)=k\right\} \\ & \kappa' & \longmapsto & \varphi^{-1}(\kappa):=\kappa,\end{array}$$

where κ is the coloring $\kappa(v)=\ell+1-\kappa'(v)$. Since $\ell+1-(\ell+1-\kappa(v))=\kappa(v)$. Moreover, $\varphi^{-1}(\varphi(\kappa))=\varphi(\varphi^{-1}(\kappa))=\kappa$. Thus, φ is a bijection. □

Now we are ready to state the formula for the M-expansion of the normalized total labeling CQF of ST_n.

Theorem 4.3.4. *Let* ST_n *be the star graph on n vertices, and consider the M-expansion of its normalized total labeling CQF,* $\mathrm{Tst}_n(q)=\sum_\alpha b_\alpha(q)M_\alpha$. *Then,*

$$b_\alpha(q)=\sum_i \mathrm{Mult}(\alpha_{i\rightarrow})\mathrm{Mult}(\alpha_{\leftarrow i})\sum_{l=0}^{s}\binom{n}{l}q^l[n-2l]_q,$$

where the first sum runs over all the i such that $\alpha_i=1$, and $s=\min\{R_{\alpha_i},L_{\alpha_i}\}$. Equivalently,

$$[q^k]b_\alpha(i;q)=\mathrm{Mult}(\alpha_{i\rightarrow})\mathrm{Mult}(\alpha_{\leftarrow i})\sum_{l=0}^{s_0}\binom{n}{l},$$

where $s_0=\min\{k,s\}$ and $0\le k\le n-1$.

This result is a consequence of the two results we state below. The first result is another interpretation of the coefficients $b_\alpha(q)$, which is proved in Section 4.4.

Theorem 4.3.5. *Let* ST_n *be the star graph on n vertices, and consider the M-expansion of its normalized total labeling CQF,* $\mathrm{Tst}_n(q)=\sum_\alpha b_\alpha(q)M_\alpha$. *For $k\le\lfloor\frac{n-1}{2}\rfloor$,*

$$[q^k]b_\alpha(q)=\sum_i \mathrm{Mult}(\alpha_{i\rightarrow})\mathrm{Mult}(\alpha_{\leftarrow i})\sum_{j=0}^{s_0}\binom{s+k-2j}{s-j}\binom{n-1-s-k+2j}{j},$$

where the first sum runs over all the i *such that* $\alpha_i = 1$, $s = \min\{R_{\alpha_i}, L_{\alpha_i}\}$, *and* $s_0 = \min\{s, k\}$. *Equivalently,*

$$[q^k]b_\alpha(i;q) = \mathrm{Mult}(\alpha_{i\rightarrow})\mathrm{Mult}(\alpha_{\leftarrow i})\sum_{j=0}^{s_0}\binom{s+k-2j}{s-j}\binom{n-1-s-k+2j}{j}.$$

The second result is a binomial identity, which is more challenging to prove than we expected. In Chapter 5 we present a combinatorial model for it together with its proof.

Theorem 4.3.6. *Let* n, k, *and* s *be non-negative integers with* $k, s \le \lfloor \frac{n-1}{2} \rfloor$, *and* $s_0 = \min\{s, k\}$. *Then,*

$$\sum_{j=0}^{s_0}\binom{s+k-2j}{s-j}\binom{n-1-s-k+2j}{n-1-s-k+j} = \sum_{l=0}^{s_0}\binom{n}{l}.$$

Remark 4.3.7. *Note that by Proposition 3.1.5, we know that the coefficients* $b_\alpha(q)$ *are symmetric, and so in Theorems 4.3.5 and 4.3.6 we only need to consider* $0 \le k \le \lfloor \frac{n-1}{2} \rfloor$. *Moreover,* s *is exactly the minimum between the number of entries to the left and right of the entry* $\alpha_i = 1$ *that we consider, and so, in Theorem 4.3.6, we also have that* $s \le \lfloor \frac{n-1}{2} \rfloor$.

4.4 Proof of Theorem 4.3.5

Proof. By Proposition 4.1.3 and Definition 4.3.1, we have that

$$\begin{aligned}
b_\alpha(q) &= \sum_{r=1}^{n} c_\alpha^r(q)\\
&= \sum_{r=1}^{n}\sum_{i:\alpha_i=1}\sum_{p=0}^{\min\{L_{\alpha_i}^{n-r}, R_{\alpha_i}^{r-1}\}} \mathrm{Mult}(\alpha_{i\rightarrow})\mathrm{Mult}(\alpha_{\leftarrow i})\binom{n-r}{L_{\alpha_i}^{n-r}-p}\binom{r-1}{R_{\alpha_i}^{r-1}-p} q^{2p+|n-r-L_{\alpha_i}|}\\
&= \sum_{i:\alpha_i=1}\sum_{r=1}^{n}\sum_{p=0}^{\min\{L_{\alpha_i}^{n-r}, R_{\alpha_i}^{r-1}\}} \mathrm{Mult}(\alpha_{i\rightarrow})\mathrm{Mult}(\alpha_{\leftarrow i})\binom{n-r}{L_{\alpha_i}^{n-r}-p}\binom{j-1}{R_{\alpha_i}^{r-1}-p} q^{2p+|n-r-L_{\alpha_i}|}. \qquad (4.1)
\end{aligned}$$

Let us fix i such that $\alpha_i = 1$, that is, let us fix the color of the root $\kappa(r) = i$, for $1 \le r \le n$. By Lemma 4.3.3, we can assume that $L_{\alpha_i} \le R_{\alpha_i}$, so that $s = \min\{R_{\alpha_i}, L_{\alpha_i}\} = L_{\alpha_i}$.

Suppose we fix $k \le \lfloor \frac{n-1}{2} \rfloor$, the exponent of q on the LHS of the statement of theorem 4.3.4. Then, we have that $k = 2p + |n-r-L_{\alpha_i}|$ for the different values of r and p. We claim that the smallest labeling of the root of ST_n, that is r, that contributes a nonzero amount to the coefficient of q^k corresponds to taking $p = 0$ and $r_0 = R_{\alpha_i} - k + 1$. To see this, we first assume that $p = 0$. Then, recall that $n = R_{\alpha_i} + L_{\alpha_i} + 1$, and so $k = |R_{\alpha_i} + L_{\alpha_i} + 1 - r - L_{\alpha_i}| = |R_{\alpha_i} + 1 - r|$. Thus, $r_0 = \min_r\{R_{\alpha_i} - k + 1, R_{\alpha_i} + k - 1\} = R_{\alpha_i} - k + 1$ as desired. Now, assume that $p > 0$ and suppose that there exists some $r_1 = r_0 - \varepsilon$, with $\varepsilon > 0$. Then, we have that

$$k = 2p + |n - r - L_{\alpha_i}| = k = 2p + |R_{\alpha_i} - r_1 + 1| = 2p + |k + \varepsilon| > k,$$

which is a contradiction.

In fact, we can write $r = r_0 + 2j$, with $0 \le j \le \lfloor \frac{n-r_0}{2} \rfloor$. To see that, we note that the parity of $k = 2p + |R_{\alpha_i} + 1 - r|$ depends on the parity of r, and so the only nonzero contributions correspond to the labeling of the form $r = r_0 + 2j$, with $0 \le j \le \lfloor \frac{n-r_0}{2} \rfloor$ where r_0 and k have the same parity.

Therefore, in Equation (4.1), we have that the coefficient of q^k in $b_\alpha(q)$ is

$$[q^k]\left(\sum_{i:\alpha_i=1}\sum_{j=0}^{\lfloor \frac{n-r_0}{2}\rfloor}\sum_{p=0}^{\min\{L_{\alpha_i}^{n-r_0-2j},R_{\alpha_i}^{r_0+2j-1}\}}\mathrm{Mult}(\alpha_{i\rightarrow})\mathrm{Mult}(\alpha_{\leftarrow i})\binom{n-r_0-2j}{L_{\alpha_i}^{n-r_0-2j}-p}\binom{r_0+2j-1}{R_{\alpha_i}^{r_0+2j-1}-p}q^{2p+|k-2j|}\right), \quad (4.2)$$

where in the exponent of q we use that $|n-r_0-2j-L_{\alpha_i}| = |R_{\alpha_i}-r_0-2j+1| = |k-2j|$.

Our next step is to calculate the coefficient for the labels r_0+2j of the root. Now, we first want to show that this contribution is nonzero exactly when $0 \le j \le s_0 = \min\{s,k\}$. Note that the condition $j \le k$ comes from the exponent of q while the condition $j \le s$ comes from the binomial coefficients.

Suppose that $j > k$. Then $|k-2j| > k$ and so, the exponent of q is $2p+|k-2j| > k$. That is, it does not contribute to the coefficient of q^k that we are looking at. Thus, we have to $j \le k$. Moreover, note that if j is fixed, then $2p+|k-2j| = k$ has only one solution in terms of p. In fact, p takes the following values:

(a) If $2j \le k$, then $p = j$. This follows since $2p+|k-2j| = 2p+k-2j$, and so $2p+k-2j = k$ implies that $p = j$.

(b) If $2j \ge k$, then $p = k-j$. This follows since $2p+|k-2j| = 2p-k+2j$, and so $2p-k+2j = k$ implies that $p = k-j$.

Now we want to show the following claim:

$$p \le \min\{L_{\alpha_i}^{n-r_0-2j}, R_{\alpha_i}^{r_0+2j-1}\} \qquad \text{if and only if} \qquad j \le s.$$

Firstly, we analyze $\min\{L_{\alpha_i}^{n-r_0-2j}, R_{\alpha_i}^{r_0+2j-1}\}$ depending on the values of p. Note that, since $L_{\alpha_i} \le R_{\alpha_i}$ and $L_{\alpha_i} = n-r_0-k$, we have that

$$\min\{L_{\alpha_i}^{n-r_0-2j}, R_{\alpha_i}^{r_0+2j-1}\} = \min\{n-r_0-2j, n-r_0-k, r_0+2j-1\}.$$

Then,

(1) $\min\{L_{\alpha_i}^{n-r_0-2j}, R_{\alpha_i}^{r_0+2j-1}\} = n-r_0-2j$ implies that $p = k-j$;

(2) $\min\{L_{\alpha_i}^{n-r_0-2j}, R_{\alpha_i}^{r_0+2j-1}\} = n-r_0-k$ implies that $p = j$; and

(3) $\min\{L_{\alpha_i}^{n-r_0-2j}, R_{\alpha_i}^{r_0+2j-1}\} = r_0+2j-1$ implies that $p = j$;

Assume $p \le \min\{L_{\alpha_i}^{n-r_0-2j}, R_{\alpha_i}^{r_0+2j-1}\}$. Then, we prove both directions of our claim by analyzing each case.

We start with the forward direction. Suppose that $p \le \min\{L_{\alpha_i}^{n-r_0-2j}, R_{\alpha_i}^{r_0+2j-1}\}$. Then, Case 1 follows since $p = k - j \le n - r_0 - 2j$ implies that $j \le n - r_0 - k = s$; and Cases 2 and 3 follow from the minimum condition since $j = p \le n - r_0 - k = s$ and $j = p \le r_0 + 2j - 1 \le n - r_0 - k = s$, respectively.

For the other direction, suppose that $j \le s$. Then, Case 1 follows since $l \le n - r_0 - k$ implies that $j + k \le n - r_0$, and subtracting $2j$ from both sides yields $p = k - j \le n - r_0 - 2j = \min\{L_{\alpha_i}^{n-r_0-2j}, R_{\alpha_i}^{r_0+2j-1}\}$. Case 2 follows since $j = p \le s = n - r_0 - k = \min\{L_{\alpha_i}^{n-r_0-2j}, R_{\alpha_i}^{r_0+2j-1}\}$ by the assumption. Case 3 follows since $r_0 - 1 + l \ge 0$ implies that $p = j \le r_0 + 2j - 1 = \min\{L_{\alpha_i}^{n-r_0-2j}, R_{\alpha_i}^{r_0+2j-1}\}$. This proves our claim.

Thus, continuing from Equation (4.2), we have that the coefficient of q^k in $b_\alpha(q)$ is

$$[q^k]\left(\sum_{i:\alpha_i=1}\sum_{j=0}^{s_0}\sum_{p=0}^{\min\{L_{\alpha_i}^{n-r_0-2j}, R_{\alpha_i}^{r_0+2j-1}\}} \mathrm{Mult}(\alpha_{i\to})\mathrm{Mult}(\alpha_{\leftarrow i})\binom{n-r_0-2l}{L_{\alpha_i}^{n-r_0-2j}-p}\binom{r_0+2j-1}{R_{\alpha_i}^{r_0+2j-1}-p} q^{2p+|k-2j|}\right), \quad (4.3)$$

Finally, we are ready to look at the coefficients and rewrite them in terms of our parameters. First, we notice the following:

$$\begin{aligned} L_{\alpha_i}^{n-r_0-2j} &= \min\left\{L_{\alpha_i}, n-r_0-2j\right\} = \min\left\{L_{\alpha_i}, L_{\alpha_i}-k+2j\right\} = \min\left\{s, s-k+2j\right\}, \\ R_{\alpha_i}^{r_0+2j-1} &= \min\left\{R_{\alpha_i}, r_0+2j-1\right\} = \min\left\{n-s-1, n-s-1-k+2j\right\}, \end{aligned}$$

where we use that $r_0 = R_{\alpha_i} - k + 1$, $L_{\alpha_i} + k = n - r_0$, $L_{\alpha_i} + R_{\alpha_i} + 1 = n$, and our assumption that $L_{\alpha_i} \le R_{\alpha_i}$ and so $s = \min\{L_{\alpha_i}, R_{\alpha_i}\} = L_{\alpha_i}$. Then, following the possible values of p, we have that

(a) If $2j \le k$, then $p = j$, and we have that

$$\binom{n-r_0-2j}{L_{\alpha_i}^{n-r_0-2j}-p}\binom{r_0+2j-1}{R_{\alpha_i}^{r_0+2j-1}-p} = \binom{s+k-2j}{s-j}\binom{n-s-k+2j-1}{n-s-1-k+2j-j}.$$

(b) If $2j \ge k$, then $p = k - j$, and we have that

$$\binom{n-r_0-2j}{L_{\alpha_i}^{n-r_0-2j}-p}\binom{r_0+2j-1}{R_{\alpha_i}^{r_0+2j-1}-p} = \binom{s+k-2j}{s+k-2j-(k-j)}\binom{n-s-k+2j-1}{n-s-1-(k-j)}.$$

In both cases, we have the simplification

$$\binom{n-r_0-2j}{L_{\alpha_i}^{n-r_0-2j}-p}\binom{r_0+2j-1}{R_{\alpha_i}^{r_0+2j-1}-p} = \binom{s+k-2j}{s-j}\binom{n-s-k+2j-1}{j},$$

and the result follows. □

CHAPTER

5

THE BINOMIAL IDENTITY

In the previous chapter, we found the coefficients of the quasisymmetric monomial basis expansion of the total labeling CQF of the star graph in Theorem 4.3.4. We also stated Theorem 4.3.6 as a way to clean up those coefficients. In this chapter, we slightly reframe Theorem 4.3.6 and provide a combinatorial proof of it.

Theorem 5.0.1. *Let n, k, and s be nonnegative integers with $s \leq k \leq \lfloor \frac{n-1}{2} \rfloor$. Then,*

$$\sum_{j=0}^{s} \binom{s+k-2j}{s-j} \binom{n-1-s-k+2j}{j} = \sum_{l=0}^{s} \binom{n}{l}. \tag{5.1}$$

Remark 5.0.2. *Theorem 5.0.1 is slightly different than the statement in Theorem 4.3.6 since we assume that $s \leq k \leq \lfloor \frac{n-1}{2} \rfloor$. Now, looking at the formula in Theorem 4.3.6, we note that the LHS is symmetric in s and k, and the RHS does not depend on s and k other than the minimum $s_0 = \min\{s, k\}$. Thus, we can assume that $s \leq k$, and so $s_0 = s$.*

In the following example, we observe that the terms on each side do not match directly. Also, in Equation (5.1), the LHS depends on k while the RHS does not.

Example 5.0.3. Let $s = k = 2$ and $n = 6$. Then, the LHS of Equation (5.1) gives

$$\binom{4}{2}\binom{1}{1} + \binom{2}{1}\binom{3}{2} + \binom{0}{0}\binom{5}{3} = 6 + 6 + 10 = 22,$$

while the RHS gives

$$\binom{6}{0}+\binom{6}{1}+\binom{6}{2}=1+6+15=22.$$

We prove this binomial identity combinatorially using a model for which the computation on the LHS of Equation (5.1) is direct, and we work our way to the RHS.

5.1 Combinatorial model

Consider a row of n boxes. We say that a box decorated with $\blacksquare$ is a *barrier* and that a box decorated with $\boxtimes$ is a *marked box*. We define a *configuration* as a row of n boxes with s marked boxes. We encode this information as an increasing sequence of positive integers, $\gamma=(\gamma_1,\dots,\gamma_s)$, where $\gamma_i\in[n]$ indicates the position of the i^{th} marked box labeled from left to right. We say that a configuration satisfies the j*-condition* if the box at position $s+k+1-2j$ can be decorated as a barrier and the configuration contains $s-j$ marked boxes to the left of the barrier, no marked boxes at the barrier, and j marked boxes to the right of the barrier.

Example 5.1.1. In Figure 5.1, we include all 15 configurations that we are considering.

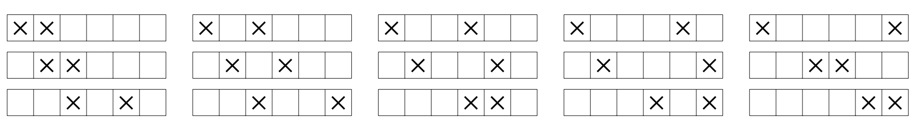


Figure 5.1 All the configurations for $n=6$ and $s=k=2$.

Now, we fix n and s, and we look at the configurations of a row of n boxes with s marked ones. For $0\le j\le s$, we denote by B_j the number of these configurations that satisfy the j-condition. For $1\le l\le s+1$, we denote by K_l the number of these configurations that satisfy at least l of the i-conditions, with $0\le i\le s$. The binomial identity in Equation (5.1) then represents a counting problem regarding this combinatorial model. More concretely, the LHS of Equation (5.1) counts the total number of j-configurations, for $0\le j\le s$. That is, we count the configurations with repetitions (for the j-conditions) via B_j.

Example 5.1.2. In Figure 5.2, we illustrate the corresponding list of configurations for our example according to the j-condition they satisfy, for $0\le j\le 2$. Moreover, we highlight in red one of the configurations to point out that the same configuration can be counted more than once.

The following lemma connects this combinatorial model with the coefficients we find in Theorem 4.3.4.

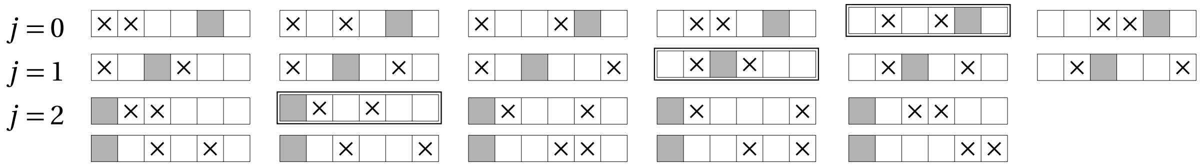


Figure 5.2 Configurations for $n=6$ and $s=k=2$ satisfying the j-condition.

Lemma 5.1.3. *For* $0 \le j \le s$, $B_j = \binom{s+k-2j}{s-j}\binom{n-1-s-k+2j}{j}$.

Proof. If we fix j and want to construct a configuration that satisfies the j-condition, there are $s+k-2j$ boxes to the right of the barrier, from which we choose j of them to be marked boxes, and there are $n-1-s-k+2j$ boxes to the left of the barrier, from which we choose $s-j$ of them to be marked boxes. This proves the claim. □

For the RHS of Equation (5.1), we count the same set of configurations (with repetitions) but grouped by the minimum number of i-conditions they satisfy, with $0 \le i \le s$.

Example 5.1.4. In Figure 5.3, we list all the configurations for our example according to the number t of the i-conditions, with $0 \le i \le 2$, that they satisfy, for $1 \le t \le 3$. Then, we have that K_3 counts the configurations in row $t=3$, $\binom{6}{0}=1$; K_2 counts the configurations in rows $t=2$ and 3, $\binom{6}{1}=6$; and K_1 the configurations in rows $t=1,2$, and 3, $\binom{6}{2}=15$.

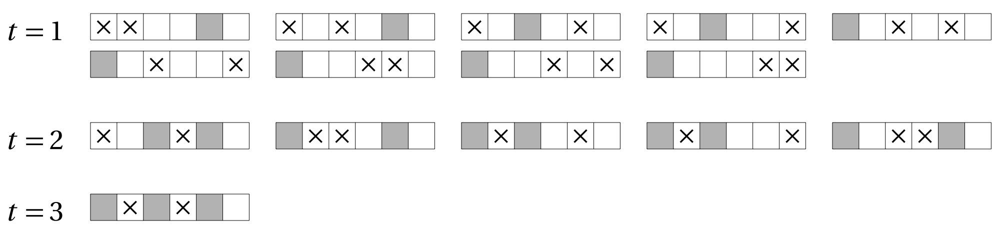


Figure 5.3 Configurations for $n=6$ and $s=k=2$ satisfying t of the i-conditions.

Since we count the same set of configurations, we have the following result.

Lemma 5.1.5. $\sum_{j=0}^{s} B_j = \sum_{l=0}^{s} K_{s+1-l} = \sum_{l=1}^{s+1} K_l$.

Thus, the binomial identity in Equation (5.1) is equivalent to the following result.

Theorem 5.1.6. *For* $0 \le l \le s \le \lfloor \frac{n-1}{2} \rfloor$, $K_{s+1-l} = \binom{n}{l}$.

We dedicate the rest of this chapter to proving this identity.

5.2 Conditions and the nat-statistic

Our first step is to further develop the combinatorial model and find an alternative interpretation for K_{s+1-l}. Recall that K_{s+1-l} counts the number of configurations that satisfy at least $s+1-l$ of the i-conditions, with $0 \le i \le s$, and that for the i-condition, the box at position $s+k+1-2i$ is a barrier. Now, given a configuration, we want to look at all the i-conditions at once. For that, we decorate all the configurations with s marked boxes and $s+1$ barriers in positions $s+k+1-2i$, for $0 \le i \le s$. We need to keep track of the position of the first barrier, and so let $b_0 := k+1-s$. Note that since s and k are fixed parameters of our model and b_0 is determined by s and k, then b_0 is fixed in our model too, and we will assume that it is part of the initial input data.

Example 5.2.1. In Figure 5.4, we illustrate the configurations of our running example, for which $b_0 = 1$.

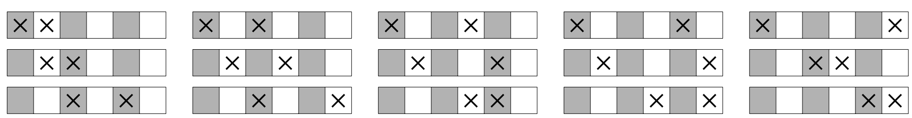


Figure 5.4 Set of configurations for $n = 6$ and $s = k = 2$ together with the 3 barriers starting at $b_0 = 1$.

Since a marked box can be in the same box as a barrier, we introduce the following definition. Given a configuration $\gamma = (\gamma_1, \dots, \gamma_s)$ and b_0, we say that the j^{th} marked box, for $1 \le j \le s$, is *at home (with respect to b_0)* if $\gamma_j = b_0 + 2j - 1$. That is if we label the barriers from left to right from 1^{st} to $(s+1)^{\text{th}}$, the j^{th} marked box is at home if it is between the j^{th} and $(j+1)^{\text{th}}$ barriers and we refer to this particular position as the *j^{th} home*. Otherwise, we say that the j^{th} marked box is *not at home (with respect to b_0)*. Given a configuration γ and b_0, we denote by $\text{nat}(\gamma, b_0)$ the number of marked boxes *not* at home in γ with respect to b_0. We illustrate the relation between the homes, the barriers, and the conditions in Figure 5.5. We denote by $T(n, s, i, b_0)$ the set of all configurations γ with n boxes in total and s marked ones and such that $\text{nat}(\gamma) = i$ with respect to b_0, and by $T(n, s, i, b_0)$ the number of configurations in $T(n, s, i, b_0)$. Since b_0 is fixed in our model, we omit the part of "with respect to b_0" when referring to at home or not at home marked boxes, but we keep b_0 in the notation as it plays an important role later on.

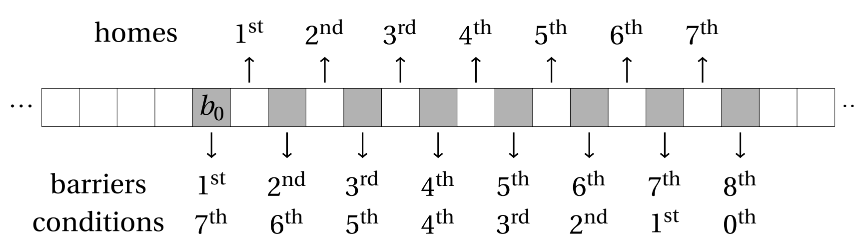


Figure 5.5 The relation of the barriers and conditions.

The next two results provide some technical information regarding the marked boxes, barriers, and conditions given a configuration. The first result gives us some cases in which a configuration satisfies a particular condition.

Lemma 5.2.2. *Consider a configuration γ and suppose that, for some $i \leq s$, the i^{th} marked box is at home. Then, we have that:*

- *if the i^{th} barrier is empty, then γ satisfies the $(s-i+1)$-condition; and*
- *if the $(i+1)^{th}$ barrier is empty, then γ satisfies the $(s-i)$-condition.*

Proof. The $(s-i+1)$-condition requires that there are $i-1$ marks to the left of the i^{th} barrier and $(s-i+1)$ to its right, while the $(s-i)$-condition requires that there are i marks to the left of the $(i+1)^{\text{th}}$ barrier and $(s-i)$ marks to its right.

The i^{th} mark being at home means that it is to the right of the i^{th} barrier and to the left of the $(i+1)^{\text{th}}$ barrier with $i-1$ marks to its left and $s-i$ marks to its right. So, if the i^{th} barrier is empty, then there has to be $i-1$ marks to its left and $s-i+1$ to its right. Similarly, if the $(i+1)^{\text{th}}$ barrier is empty, then there has to be i marks to its left and $s-i$ to its right. This means that in the case of the first statement, γ satisfies the $(s-i+1)$-condition, and in the case of the second statement, γ satisfies the $(s-i)$-condition. ☐

Note that if both barriers are empty, then γ satisfies both the $(s-i)$ and $(s-i-1)$-conditions. The idea of the lemma is sketched in Figure 5.6.

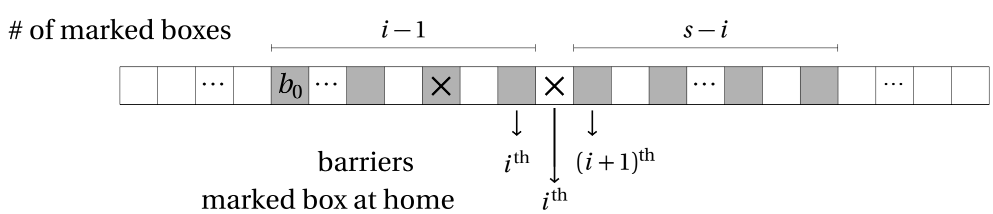


Figure 5.6 Sketch of a configuration γ illustrating the statements in Lemma 5.2.2.

The second result gives us sufficient conditions for a configuration not to satisfy a particular condition.

Lemma 5.2.3. *Consider a configuration γ. Then, we have that:*

- *if the i^{th} barrier has a marked box, then γ does not satisfy the $(s-i+1)$-condition; and*
- *if the j^{th} marked box is in the i^{th} home and $j \neq i$, then γ satisfies neither condition associated with the barriers adjacent to that marked box.*

Proof. The first statement follows from the fact that the (s-i+1)-condition is the condition associated with the i^{th} barrier, which contains a mark.

For the second statement, if either barrier is not empty, then their associated conditions are not satisfied. Assuming they are both empty, there are $j-1 \neq i-1$ marks to the left of the i^{th} barrier, adn $s-j \neq s-i$ marks to the right of the $(i+1)^{\text{th}}$ barrier. Since there needs to be $i-1$ marks to the left of the i^{th} barrier and $s-(i+1)+1 = s-i$ marks to the right of the $(i+1)^{\text{th}}$ barrier in order for their respective conditions to be satisfied, neither condition is satisfied. This proves the claim. □

Remark 5.2.4. *$T(n,s,0,b_0) = 1$, and this special configuration is the unique configuration with all marks at home. Note that this configuration satisfies all $s+1$ conditions.*

Lemmas 5.2.2 and 5.2.3 provide the relation between the j-conditions and the not at home marked boxes. We now introduce the idea of a "relative order preserving move" which is necessary in stating our desired result.

Definition 5.2.5. Let $\gamma \in T(n,s,i,b_0)$ be a configuration. A *relative order preserving move* is the movement of a mark in γ to an empty box either one place to its right or one place to its left, resulting in a new configuration γ'. We say this preserves relative order since if the i^{th} mark is moved, it remains the i^{th} mark after the move.

We state the following lemma detailing the effect an order preserving move has on the nat statistic and j-conditions.

Lemma 5.2.6. *Let $\gamma \in T(n,s,i,b_0)$, and let γ' be a configuration achieved by performing one relative order preserving move on γ. Then,*

1. *If a mark at home was moved out of its home,* $\text{nat}(\gamma') = i+1$ *and γ' satisfies one fewer j-condition than γ.*
2. *If a mark was moved into its home,* $\text{nat}(\gamma') = i-1$ *and γ' satisfies one more j-condition than γ.*
3. *Otherwise,* $\text{nat}(\gamma') = i$ *and γ' satisfies the same number of j-conditions as γ.*

Proof. We prove the three claims individually.

1. Moving an at home mark increases the number of not at home marks by 1 and decreases the number of j-conditions it satisfies by 1.

   Without loss of generality, Suppose we move the m^{th} mark into the m^{th} barrier. Before the move, it is between the m^{th} and the $(m+1)^{\text{th}}$ barriers, and, since the m^{th} barrier is empty, γ satisfies the $(s-m+1)$-condition by Lemma 5.2.2. After the move, γ' does not satisfy the $(s-m+1)$-condition according to Lemma 5.2.3. Furthermore, the moved mark is no longer at home. The satisfaction of all the other conditions is the same in γ and γ', as the moved mark does not change its relative order with any other barriers. Therefore, γ' satisfies one fewer condition than γ and γ' has one more mark not at home than γ.

2. Moving a not at home mark into its home decreases the number of not at home marked boxes by 1 and increases the number of j-conditions satisfied by 1.

   Suppose we move the m^{th} mark. It starts in either the m^{th} barrier or the $(m+1)^{\text{th}}$ barrier. Either way, the starting configuration γ does not satisfy the condition associated with the barrier the mark starts in by Lemma 5.2.3. After the move, the m^{th} mark is in its home, and the barrier starting location of the mark is empty. So, γ' satisfies the condition associated with the barrier the mark starts in by Lemma 5.2.2. The satisfaction of all other conditions is unchanged, since the moved mark's relative order with respect to all other barriers does not change. Thus, $\text{nat}(\gamma') = i-1$, and γ' satisfies one more condition than γ.

3. Moving a not at home mark in a way that continues to be not at home keeps the number of j-conditions and the number of not at home marked boxes the same.

   There are several different to move a not at home mark in a manner which preserves that status, so we split this case into subcases.

   (a) If the m^{th} mark moves from a barrier into the k^{th} home, then γ does not satisfy the condition associated with the original barrier by Lemma 5.2.3. Furthermore, after the move, γ' still does not satisfy that condition by Lemma 5.2.3 since the original barrier is now empty and $m \neq k$. The satisfaction of all other conditions is unchanged since the move does not change any mark's order relative to any other barriers.

   (b) If the m^{th} mark is moved from the k^{th} home to a barrier, then γ does not satisfy the condition associated with that barrier by Lemma 5.2.3 since $m \neq k$ and the barrier is empty in γ. After the move, γ' still does not satisfy that condition by Lemma 5.2.3 since the barrier has a mark in it. The satisfaction of all other conditions is unchanged since the move does not change any mark's order relative to any other barriers.

   (c) If the m^{th} mark moves from a spot right of all the homes to a spot right of all the homes, then its relative order with respect to any barriers doesn't change (except if it moves into or from the rightmost barrier). In all of these cases, the satisfaction of all conditions is the same in γ' as it is in γ. The same argument can be applied to the subcase where the m^{th} mark moves from a spot left of all the homes to a spot left of all the homes.

   In all three subcases, the nat statistic remains the same, and the number of conditions satisfied remains the same. These subcases handle all possible situations in claim 3, since a not at home mark must start either in an internal barrier (neither the first nor last barrier), a home that isn't its own, or a box to the left or right of all homes. In this third case, such a mark in an internal barrier must move into a home that isn't its own. Such a mark in a home that isn't its own must move into a barrier (internal or external). Such a mark in an external barrier must move either to a home that isn't its own or to a box to the right or left of all homes. Finally, such a mark in a non-barrier box to the left or right of all homes must move into another box to the left or right of all homes. All of these situations are covered in our three subcases. This concludes the proof.

□

Proposition 5.2.7. *For $s \le k \le \lfloor \frac{n-1}{2} \rfloor$ and $b_0 = k - s + 1$, $T(n,s,i,b_0)$ also counts the number of configurations γ with n boxes in total and s marked ones that satisfy exactly $s+1-i$ conditions.*

Proof. Let γ be the unique configuration in $T(n,s,0,b_0)$. Then, all the marked boxes are at home, and γ satisfies all the j-conditions, with $0 \le j \le s$, and the statement is true.

Now, suppose that $i > 0$. A configuration $\beta \in T(n,s,i,b_0)$ can be obtained from the configuration $\gamma \in T(n,s,0,b_0)$ via the following algorithm: Move the first mark to the first box. Then, move the second mark to the second box. Follow this process until the m^{th} mark is in the m^{th} box for each m. Since we started with the leftmost mark, we have used relative order preserving moves and changed γ into the configuration with all marks in a row at the beginning of the configuration. Next, we will start with the rightmost mark (the s^{th} mark) and move it to the β_s box. Then, move the $(s-1)^{\text{th}}$ mark to the β_{s-1} box, and so forth. The resulting configuration will be β, which was achieved by starting with γ and performing relative order preserving moves.

□

Therefore, we have the following interpretation of K_{s+1-l}.

Corollary 5.2.8. *For $s \le k \le \lfloor \frac{n-1}{2} \rfloor$, $0 \le l \le s$, and $b_0 = k - s + 1$,*

$$K_{s+1-l} = \sum_{i=0}^{l} T(n,s,i,b_0).$$

Our next goal is to prove the following closed formula for $T(n,s,i,b_0)$.

Theorem 5.2.9. *Let $s \le \lfloor \frac{n}{2} \rfloor$. For $i = 0$, $T(n,s,0,b_0) = 1$, and for $0 < i \le s$,*

$$T(n,s,i,b_0) = \binom{n}{i} - \binom{n}{i-1}.$$

Remark 5.2.10. *For n odd, we note that $s = \lfloor \frac{n}{2} \rfloor$ implies that $s = \lfloor \frac{n-1}{2} \rfloor$. For n even, $s = \lfloor \frac{n}{2} \rfloor$ implies that $b_0 = 1$ and so exactly half of the boxes are marked, and the barriers are located in alternating positions starting at the 1^{st} position. Thus, we consider the $(s+1)^{th}$ home to be the last box in the configuration, so that the combinatorial model makes sense and we can count the number of configurations in this particular scenario, which will be relevant later.*

Before proving Theorem 5.2.9, we finish the proof of Equation (5.1) in Theorem 5.0.1, which we have reduced to Theorem 5.1.6. We recall the statement below.

Theorem. *For $0 \le l \le s \le \lfloor \frac{n-1}{2} \rfloor$, $K_{s+1-l} = \binom{n}{l}$.*

Proof of Theorem 5.1.6. We have that

$$K_{s+1-l} = \sum_{i=0}^{l} T(n,s,i,b_0) = 1 + \sum_{i=1}^{l} T(n,s,i,b_0) = 1 + \sum_{i=1}^{l}\left[\binom{n}{i} - \binom{n}{i-1}\right] = \binom{n}{l},$$

where we use that we have a telescopic summation and all the terms except one cancel. □

5.3 Independency of b_0

In this subsection, we first show that, for computing $T(n,s,i,b_0)$, we can assume that the barriers start at $b_0 = 1$. We start with some definitions.

Given a configuration $\gamma = (\gamma_1,\dots,\gamma_s)$ and $1 \le j \le s$, let d_j be the number of boxes from the position of the j^{th} marked box to the end, $d_j := n - \gamma_j$, and let $a_j := 2(s-j)$. Moreover, let j_0 be the rightmost marked box such that $d_j > a_j$, with $j_0 = 0$ if no such box exists. Then, we define the *flipped block* of γ, $\mathrm{FB}(\gamma)$, as the set of boxes to the right of the $(j_0+1)^{\text{th}}$ marked box (including that marked box), that is $\mathrm{FB}(\gamma) = (\gamma_{j_0+1},\dots,\gamma_s)$, of length $n - \gamma_{j_0+1} + 1$. Denote by $m := s - j_0$ the number of marked boxes on it. Finally, we denote by γ^0 the marked boxes not in the flipped block, that is $\gamma = \gamma^0 \cdot \mathrm{FB}(\gamma)$, where the union of sentences is defined as the concatenation of the two sentences. Note that if $j_0 = 0$, then $\mathrm{FB}(\gamma) = \gamma$, and that if $j_0 = s$, then $\mathrm{FB}(\gamma) = \emptyset$.

Similarly, we can define the *reverse flipped block* of γ, $\mathrm{FB}'(\gamma)$ in the following way. Define d'_j to be the index of the j^{th} marked box, i.e. $d'_j := \gamma_j - 1$, and let $a'_j := 2(j-1)$. Now, we define j'_0 to be the leftmost marked box such that $d'_j > a'_j$. If no such box exists, then $j'_0 = n+1$. We then define $\mathrm{FB}'(\gamma)$ as the set of boxes to the left of the $(j'_0-1)^{\text{th}}$ marked box, including that marked box. Denote by $m' := j'_0 - 1$ the number of marked boxes in the reverse flipped block, and denote by γ'^0 the boxes in γ' not in the reverse flipped block. Thus, $\gamma = \mathrm{FB}'(\gamma)\cdot\gamma'^0$. Note that if $j'_0 = 1$, then $\mathrm{FB}'(\gamma) = \emptyset$, and that if $j'_0 = n+1$, then $\mathrm{FB}'(\gamma) = \gamma$.

The following result provides a bijection between configurations with the barriers starting at b_0 and configurations with the barriers starting at $b_0 + 1$.

Proposition 5.3.1. *For $0 \le i \le s \le \lfloor \frac{n-1}{2} \rfloor$, we have that $T(n,s,i,b_0) = T(n,s,i,b_0+1)$. In particular, $T(n,s,i,b_0) = T(n,s,i,1)$.*

Proof. Since the parameters n, s, and i are fixed, we simplify the notation in this proof and denote by $T(b_0)$ the set of all configurations γ with s marked boxes and length n and such that $\mathrm{nat}(\gamma) = i$ with respect to b_0. We show that $T(n,s,i,b_0) = T(n,s,i,b_0+1)$ by giving a bijection:

$$\begin{array}{rccc} \phi: & T(b_0) & \longrightarrow & T(b_0+1) \\ & \gamma & \longmapsto & \gamma' := \phi(\gamma). \end{array}$$

Intuitively, ϕ reflects the pattern of marked boxes in the flipped block at the beginning of the configuration and moves the rest of the marked boxes to the right by $2m+1$ spots. For $\gamma = (\gamma_1,\dots,\gamma_s)$, we define

$$\phi(\gamma_j) := \begin{cases} 1 + d_j = 1 + (n - \gamma_j), & \text{if } \gamma_j \in \mathrm{FB}(\gamma), \\ \gamma_j + 2m + 1, & \text{if } \gamma_j \notin \mathrm{FB}(\gamma), \end{cases}$$

so that γ' is the sequence obtained by reordering in increasing order the entries $\phi(\gamma_j)$.

Let us start by showing that ϕ is well-defined. That is, we show that γ' is a configuration and that it has the same number of market boxes not at home as γ. If $\mathrm{FB}(\gamma) = \gamma$, then $d(\gamma) = (d_1, \ldots, d_s)$ is a strictly decreasing sequence of integers, and so $\gamma' = (d_s + 1, \ldots, d_1 + 1)$ is also a strictly increasing sequence of integers. If $\mathrm{FB}(\gamma) \neq \gamma$, then $\gamma = \gamma^0 \cdot \mathrm{FB}(\gamma)$, with $\gamma^0 = \left(\gamma_1, \ldots, \gamma_{j_0}\right)$ and $\mathrm{FB}(\gamma)$ nonempty sets. Then, $\phi(\gamma) = \phi(\mathrm{FB}(\gamma)) \cdot \phi(\gamma^0)$, where $\phi(\mathrm{FB}(\gamma))$ corresponds to the marked boxes in the first $2m+1$ boxes of γ' and $\phi(\gamma^0)$ corresponds to the marked boxes in the last $n - (2m+1)$ boxes of γ'. Thus, the values of $\phi(\gamma^0)$ and $\phi(\mathrm{FB}(\gamma))$ do not overlap and γ' is a configuration with s marked boxes and length n.

Next, we show that the number of marked boxes not at home is preserved under ϕ. That is, if $\mathrm{nat}(\gamma) = i$ with respect to b_0, then $\mathrm{nat}(\gamma') = i$ with respect to $b_0 + 1$. Note that in γ the j^{th} home corresponds to the box in position $b_0 + 2j - 1$ while in γ' the j^{th} home corresponds to the box in position $b_0 + 2j$.

Consider the i^{th} marked box in γ. Then, we have two cases:

- <u>Case 1:</u> $\gamma_i \in \mathrm{FB}(\gamma)$.
  In this case, γ_i is a marked box not at home in γ and $\phi(\gamma_i)$ is also a marked box not at home in γ'. By construction, the marked boxes in the flipped block satisfy that $d_i \leq a_i = 2(s-i)$, and the i^{th} home corresponds to the position $b_0 + 2i - 1$, for which $d_{b_0+2i-1} = n - b_0 - 2i + 1$. However, we have that $b_0 \leq n - 2s$ since there needs to be enough space to the right of b_0 to have s barriers. Therefore, we have

  $$d_{b_0+2i-1} = n - b_0 - 2i + 1 \geq n - (n-2s) - 2i + 1 = 2(s-i) + 1 > 2(s-i) \geq d_i.$$

  This means that the i^{th} home is strictly to the left of the i^{th} marked box, which implies that the i^{th} marked box cannot be at home. Similarly, for $\phi(\gamma_i) = \gamma'_{s-i+1}$ we have that

  $$b_0 + 1 + 2(s-i+1) = b_0 + 2(s-i) + 3 \geq b_0 + 3 + d_i > d_i + 1 = \phi(\gamma_i) = \gamma'_{s-i+1}.$$

  Thus, the position of the $(s-i+1)^{\text{th}}$ home is strictly to the right of the γ'_{s-i+1} marked box, which corresponds to the image of γ_i. Therefore, $\phi(\gamma_i)$ is also not at home in γ'.

- <u>Case 2:</u> $\gamma_i \notin \mathrm{FB}(\gamma)$.
  In this case, $\phi(\gamma_j) = \gamma'_{j+m}$ and γ_j is at home if and only if γ'_{j+m} is at home.

  Note that $\gamma'_{j+m} = \gamma_j + 2m + 1$. Moreover, γ_j is at home if and only if $\gamma_j = b_0 + 2j - 1$. Similarly, γ'_{j+m} is at home if and only if $\gamma'_{j+m} = b_0 + 2(j+m)$. Putting these three observations together, we have that

$$\begin{aligned}\gamma_j \text{ is at home} \quad &\Longleftrightarrow \quad \gamma_j = b_0 + 2j - 1 \quad \Longleftrightarrow \quad \gamma_j + 2m + 1 = b_0 + 2j - 1 + 2m + 1 \\ &\Longleftrightarrow \quad \gamma'_{j+m} = b_0 + 2(j+m) \quad \Longleftrightarrow \quad \gamma'_{j+m} \text{ is at home.}\end{aligned}$$

We now outline the inverse map:

$$\begin{aligned}\phi^{-1}: \quad T(b_0+1) \quad &\longrightarrow \quad T(b_0) \\ \beta \quad &\longmapsto \quad \beta' := \phi^{-1}(\beta).\end{aligned}$$

Intuitively, ϕ^{-1} reflects the pattern of marked boxes in the reverse flipped block at the end of the configuration and moves the rest of the marked boxes to the left by $2m+1$ spots. For $\beta = (\beta_1, \ldots, \beta_s)$, we define

$$\phi^{-1}(\beta_j) := \begin{cases} n - \beta_j + 1, & \text{if } \beta_j \in \mathrm{FB}'(\beta), \\ \beta_j - (2m+1), & \text{if } \beta_j \notin \mathrm{FB}'(\beta), \end{cases}$$

Based on the definition of FB and FB$'$, note that for any configuration $\gamma \in T(b_0)$, $\gamma_j \in \mathrm{FB}(\gamma)$ if and only if $\phi(\gamma_j) \in \mathrm{FB}'(\phi(\gamma))$. Similarly, for any configuration $\beta \in T(b_0+1)$, $\beta_j \in \mathrm{FB}'(\beta)$ if and only if $\phi^{-1}(\beta_j) \in \mathrm{FB}(\phi^{-1}(\beta))$. With this in mind, if $\gamma_j \in \mathrm{FB}(\gamma)$, then

$$\phi^{-1}(\phi(\gamma_j)) = n - \phi(\gamma_j) + 1 = n - (1 + d_j) + 1 = n - d_j = \gamma_j.$$

If $\gamma_j \notin \mathrm{FB}(\gamma)$, then

$$\phi^{-1}(\phi(\gamma_j)) = \phi(\gamma_j) - (2m+1) = \gamma_j + 2m + 1 - (2m+1) = \gamma_j.$$

If $\beta_j \in \mathrm{FB}'(\beta)$, then

$$\phi(\phi^{-1}(\beta_j)) = 1 + (n - \phi^{-1}(\beta_j)) = 1 + (n - (n - \beta_j + 1)) = \beta_j.$$

If $\beta_j \notin \mathrm{FB}'(\beta)$, then

$$\phi(\phi^{-1}(\beta_j)) = \phi^{-1}(\beta_j) + 2m + 1 = \beta_j - (2m+1) + 2m + 1 = \beta_j.$$

Therefore, ϕ^{-1} is indeed the inverse to ϕ, and so ϕ is a bjiection. □

Remark 5.3.2. *For the rest of this section, we assume that $b_0 = 1$, and so we abbreviate $T(n,s,i,b_0)$ to $T(n,s,i)$ and $T(n,s,i,b_0)$ to $T(n,s,i)$.*

5.4 Recursive relations

In this subsection, we study some recursive relations. We start with the general case.

Proposition 5.4.1. *For* $0 < i \le s \le \lfloor \frac{n-1}{2} \rfloor$,

$$T(n,s,i) = T(n-1,s,i) + T(n-1,s-1,i-1). \tag{5.2}$$

Proof. The recursive formula in Equation (5.2) follows from the following counting argument. Given $\gamma \in T(n,s,i)$, let γ' be the configuration obtained by deleting the last box in γ. Then, either:

- the last box of γ is a marked box, and so $\gamma' \in T(n-1,s-1,i-1)$; or
- the last box of γ is not a marked box, and so $\gamma' \in T(n-1,s,i)$.

□

It is important to note that Proposition 5.4.1 does not apply to the case $T(2s,s,s)$ as $s > \lfloor \frac{n-1}{2} \rfloor$. Thus, we need to explore this case separately. We begin with a technical lemma that states that for configurations in $T(2i,i,i)$, the first marked box has to be in the first position.

Lemma 5.4.2. *For* $\gamma = (\gamma_1, \dots, \gamma_i) \in T(2i,i,i)$, *with* $i \ge 1$, $\gamma_1 = 1$.

Proof. We proceed by induction on i. For $i = 1$, the statement is true since $T(2,1,1)$ only contains the configuration $\gamma = (1)$.

Next, assume the statement is true for all configurations in $T(2i-2,i-1,i-1)$. By contradiction, suppose there exists $\gamma = (\gamma_1, \dots, \gamma_i) \in T(2i,i,i)$ such that $\gamma_1 > 1$. In fact, $\gamma_1 > 2$ since otherwise the first marked box will be in the first home, and there cannot be any at home marked box. Now, let $\gamma' \in T(2i-2,i-1,i-1)$ be the configuration $\gamma' = (\gamma_2 - 2, \dots, \gamma_i - 2)$, obtained from γ by ignoring the first two boxes of γ and deleting the first marked box. For any $k \ge 2$, we know that the k^{th} marked box of γ is not in the $(2k)^{\text{th}}$ box. This implies that the $(k-1)^{\text{th}}$ marked box of γ' is not in the $(2k-2)^{\text{th}}$ box of γ', and so every marked box of γ' is not at home. Since γ' is a configuration in $T(2i-2,i-1,i-1)$, by induction hypothesis, γ' has a marked box in its first box. However, by construction, the first marked box of γ' must be in its second box or later. Thus, we get a contradiction, and the result follows. □

Next, we prove the recursive relation from Proposition 5.4.1 for $T(2i,i,i)$.

Theorem 5.4.3. *For* $i \ge 1$, $T(2i,i,i) = T(2i-1,i-1,i-1)$.

Proof. We show that there is a bijection ϕ between $T(2i,i,i)$ and $T(2i-1,i-1,i-1)$. Consider $\gamma = (\gamma_1, \dots, \gamma_i) \in T(2i,i,i)$. We split γ into two configurations, γ_c and γ_r, so that $\gamma_c = (\gamma_1, \dots, \gamma_j)$ is the smallest subsequence such that the configuration has length $2j$ and j marked boxes. We denote by γ_r the rest of γ, $\gamma_r = (\gamma_{j+1}, \dots, \gamma_i)$, with $\gamma_{k+1} > 2j$, and refer to it as the *reflected block*.

Now, we are ready to define the bijection. For $\gamma = (\gamma_1, \dots, \gamma_i) \in T(2i,i,i)$, the configuration $\phi(\gamma) = \beta = (\beta_1, \dots, \beta_{i-1})$ is defined by the following algorithm:

- The marks in γ_c do not move.
- The marks in γ_r are reflected so that the $(j+k)^{\text{th}}$ mark moves from the $(2j+m)^{\text{th}}$ box to the $(2i-m+1)^{\text{th}}$ box.
- Delete the first marked box of γ, which is in the first box.
- The resulting configuration is β.

We need to show that β is in fact a configuration in $T(2i-1,i-1,i-1)$. By construction, it is clear that β is a configuration of length $2i-1$ with $i-1$ marked boxes. Thus, we only need to see the number of not at home marked boxes in β.

For γ_c, we notice that the marked boxes in this part of the configuration are not at home as marked boxes in γ since the k^{th} marked box is in a position before the $(2k-1)^{\text{th}}$ box, and so in β, the $(k-1)^{\text{th}}$ marked box is in a position before the $(2k-2)^{\text{th}}$ box. For γ_r, we want to show that the number of not at home is preserved. Let $(j+k)^{\text{th}}$ be a marked box in γ_r in the $(2j+m)^{\text{th}}$ box. If it is not at home, then it is not in the $(2j+2k)^{\text{th}}$, and so $m \neq 2k$. When we apply ϕ, that box is now the $(i-k)^{\text{th}}$ marked box in β and it is in the $(2i-m)^{\text{th}}$ box, which is not the $(2i-2k)^{\text{th}}$ box since $m \neq 2k$. Thus, ϕ does preserve the nat statistic, and it is well-defined.

We now define the inverse map, ϕ^{-1}. Given a configuration $\beta \in T(2i-1,i-1,i-1)$, employ the following process.

- Add a marked box to the beginning of β, creating β'.
- Split β' into β'_c and β'_r, where β'_c is the smallest subconfiguration of β' such that the configuration has length $2j$ and contains j marked boxes, and $\beta' = \beta'_c \cdot \beta'_r$.
- The marks in β'_c do not move.
- The marks in β'_r are reflected so that the $(j+k)^{\text{th}}$ mark moves from the $(2j+m)^{\text{th}}$ box to the $(2i-m+1)^{\text{th}}$ box.
- The resulting configuration is $\phi^{-1}(\gamma)$.

One can now see that consecutively applying ϕ and ϕ^{-1} in either order reflects the reflected component twice while keeping the constant component still twice. This means that $\phi^{-1}(\phi(\gamma)) = \gamma$ and $\phi(\phi^{-1}(\beta)) = \beta$, and so ϕ is indeed a bijection.

□

5.5 Independency of s

In this subsection, we show that, for computing $T(n,s,i)$, we can assume that $s = \lfloor \frac{n}{2} \rfloor$. We start looking at the special case. Next result tells us how to compute $T(2l,l,l-1)$ in terms of the configurations of smaller size, depending on the position of the last marked box.

Theorem 5.5.1. *Given l and $i < l$, the number of configurations in $T(2l, l, l-1)$ with last marked box in the $(l+i+1)^{th}$ box is equal to $T(l+i, i, i)$.*

Proof. We start by noticing that for $l > 1$, any configuration $\gamma = (\gamma_1, \dots, \gamma_l) \in T(2l, l, l-1)$ has $\gamma_l \geq l+1$ since γ has at least one marked box at home and the configuration with all the marked boxes in the first l boxes has no marked boxes at home.

We proceed by strong induction on l. For $l = 1$, $T(2,1,0)$ there is only one configuration $\gamma = (2)$, for which $i = 0$, and $T(1,0,0) = 1$ since we have the configuration of length 1 and no marked boxes. For the induction step, we split into two cases:

- Suppose $i = l-1$. We want to count the number of configurations in $T(2l, l, l-1)$ with the last marked box in the last box. Note that in such a configuration, the last marked box is in the $(2l)^{\text{th}}$ box and so at home. Thus, deleting the last box of γ decreases the length of the configuration by 1 and does not change the number of not at home marked boxes, and we obtain a configuration of length $2l-1$ with $l-1$ marked boxes and $l-1$ of those not at home. This process can be reversed in a bijective way, and so there are $T(2l-1, l-1, l-1)$ of such configurations.

- Suppose $i < l-1$. In this case, we define γ' to be the configuration obtained by deleting the last mark and the last two boxes of γ. Note that we always delete two boxes in total and one mark in total.

  Now, we need to look at the second-to-last marked box in γ, which we assume is in the j^{th} position. and is also the last marked box in γ'. Then, $\gamma' \in T(2(l-1), l-1, l-2)$ with last marked box in the $((l-1)+1+j)^{\text{th}}$ box, for some $j \geq 0$. By our inductive hypothesis, there are $T(l-1+j, j, j)$ of those configurations. Note that j can range from 0 to i.

  Therefore, the number of configurations in $T(2l, l, l-1)$ with last marked box in the $(l+i+1)^{\text{th}}$ box by its second-to-last marked box is equal to

  $$\sum_{j=0}^{i} T(l-1+j, j, j).$$

  By Proposition 5.4.1, we have that

  $$\begin{aligned}\sum_{j=0}^{i} T(l-1+j, j, j) &= T(l-1,0,0) + \sum_{j=1}^{i} T(l+j-1, j, j) \\ &= T(l-1,0,0) + \sum_{j=1}^{i} \left[T(l+j, j, j) - T(l-1+j, j-1, j-1) \right].\end{aligned}$$

Note that this sum looks like

$$
\begin{aligned}
&T(l-1,0,0)+\sum_{j=1}^{i}\left[T(l+j,j,j)-T(l-1+j,j-1,j-1)\right]= \\
&= T(l-1,0,0)+[T(l+1,1,1)-T(l,0,0)]+[T(l+2,2,2)-T(l+1,1,1)]+\cdots+ \\
&\quad +[T(l+i,i,i)-T(l+i-1,i-1,i-1)].
\end{aligned}
$$

Since $T(l-1,0,0)=T(l,0,0)=1$, this sum telescopes into $T(l+i,i,i)$. Thus, the result follows for this case too.

□

We can now state the following corollary, with which we get the independence of the second parameter in the special case.

Corollary 5.5.2. *For $l>0$, $T(2l,l,l-1)=T(2l,l-1,l-1)$.*

Proof. Using Theorem 5.5.1 and the recursive formula from Proposition 5.4.1 we can get and simplify the following telescopic sum:

$$
\begin{aligned}
T(2l,l,l-1) &= \sum_{i=0}^{l-1} T(l+i,i,i) = T(l+1,0,0)+\sum_{i=1}^{l-1}[T(l+i+1,i,i)-T(l+i,i-1,i-1)] \\
&= T(2l,l-1,l-1).
\end{aligned}
$$

□

Remark 5.5.3. *For the rest of this section, when $s=\left\lfloor \frac{n}{2}\right\rfloor$, we assume that $i=\left\lfloor \frac{n}{2}\right\rfloor$ and write $T\left(n,\left\lfloor \frac{n}{2}\right\rfloor\right)$ and $T\left(n,\left\lfloor \frac{n}{2}\right\rfloor\right)$ instead.*

For the general case, we start with one more definition regarding the concatenation of two configurations and a technical result.

Given $\gamma\in T(2s,s,i)$ and $\beta\in T(n',s',i')$, we define $\gamma\cdot\beta$ as the configuration obtained by concatenating the boxes of β after the boxes of γ. The resulting configuration has length $n+n'$ and $s+s'$ marked boxes in total. Moreover, we know that the at home marked boxes of γ continue to be at home in $\gamma\cdot\beta$. In general, we can not know what marked boxes of γ continue to be at home in $\gamma\cdot\beta$. However, the following result studies the particular case we need.

Example 5.5.4. In Figure 5.7, we illustrate how to concatenate a configuration $\gamma\in T(4,2,1)$ and $\beta\in T(7,2,1)$, so that $\gamma\cdot\beta\in T(11,4,2)$.

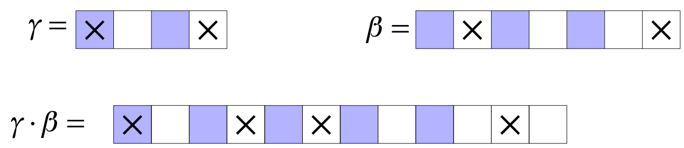


Figure 5.7 Illustration of the concatenation operation for certain configurations.

Lemma 5.5.5. *Let $\gamma \in T(2s,s,i)$ and $\beta \in T(n,s',i')$, with $0 \le i \le s$, $0 \le i' \le s'$ and $s' \le \lfloor \frac{n}{2} \rfloor$. Then, $\gamma \cdot \beta \in T(n+2s, s+s', i+i')$.*

Proof. By definition, a marked box in γ is at home if and only if it is at home in $\gamma \cdot \beta$. We want to show that the same statement is true for β. That is, a marked box in β is at home if and only if it is at home in $\gamma \cdot \beta$. Suppose that the m^{th} marked box in β is at home, and so $\beta_m = 2m$. Then, this marked box corresponds to the $(s+m)^{\text{th}}$ marked box in $\gamma \cdot \beta$ and so $(\gamma \cdot \beta)_{s+m} = 2s + 2m$. Thus, it is also at home in $\gamma \cdot \beta$. For the other direction, suppose that the m^{th} marked box in $\gamma \cdot \beta$ is at home, with $m = s + m'$ for some $m' \ge 1$ (so that it's in the β area). Then, $(\gamma \cdot \beta)_m = 2m = 2s + 2m'$. Now, ignoring the part corresponding to γ, this is the $(m')^{\text{th}}$ marked box in β, and it is in the $(2m')^{\text{th}}$ box, meaning that it is an at home marked box in β. This shows that the nat statistic is preserved in this case. □

Now we are ready to prove the independence of s in the general case.

Theorem 5.5.6. *For n, s, and i such that $i < s < \lfloor \frac{n}{2} \rfloor$,*

$$T(n,s,i) = T(n,s+1,i) \qquad \textit{and} \qquad T(n,s,s) = T(n,s+1,s).$$

Proof. We start by noticing that in Corollary 5.5.2 we prove that $T(n,s,s) = T(n,s+1,s)$ for n is even and $s = \frac{n}{2} - 1$. We prove the claim holds in general by induction on n.

For $n = 2$, we have that $T(2,0,0) = T(2,1,0) = 1$ and the statement follows. Note also that for $i = 0$, $T(n,s',0) = 1$ for any $s' \le \lfloor \frac{n}{2} \rfloor$, as there is always only one possible configuration with all marks at home. For the inductive step, assume that the statement is true for all $l < n$. Applying Proposition 5.4.1 twice, we have that

$$T(n,s,s) = T(n-1,s,s) + T(n-1,s-1,s-1) = T(n-1,s+1,s) + T(n-1,s,s-1) = T(n,s+1,s),$$

where the middle equality follows from the inductive hypothesis, and the base case result follows.

Now, we proceed by strong induction, and so we assume that $T(k,s',s') = T(k,s'+1,s')$ for all $k < n$ and $s' < \lfloor \frac{k}{2} \rfloor$. This implies that there exists a bijection from $T(k,s',s')$ to $T(k,s'+1,s')$. For each pair (k,s'), we fix one such bijection and denote it by $\varphi_{k,s'}$. We construct ϕ from $T(n,s,i)$ to $T(n,s+1,i)$ in terms of these $\varphi_{k,s'}$ maps. Given $\gamma \in T(n,s,i)$, we split it into two configurations γ_l and γ_r, where γ_l is the configuration containing every box in γ up until the block that contains the last marked box at home and γ_r is the remaining of the configuration. Then, if the last marked box at home is the j^{th}

marked box, we have that $\gamma_l \in T(2j, j, j-s+i)$ and $\gamma_r \in T(n-2j, s-j, s-j)$. Then, we define γ'_r as the image of γ_r by its bijection φ, $\gamma'_r = \varphi_{n-2j,s-j}(\gamma_r)$, so that $\gamma'_r \in T(n-2j, s-j+1, s-j)$. Finally, we define $\phi(\gamma) = \gamma_l \cdot \gamma'_r$. By Lemma 5.5.5, $\phi(\gamma) \in T(n, s+1, i)$.

We will now define ϕ^{-1}. Fix $\gamma \in T(n, s+1, i)$. Similarly, define γ_l to be the configuration containing every box and mark in γ up until the second to last marked box at home in γ. Note that there must be at least two marks at home in γ since $s > i$ so $s+1-i \geq 2$. If we have $\gamma = \gamma_l \cdot \gamma_r$, then $\gamma_l \in T(2j, j, j-s+i)$ and $\gamma_r \in T(n-2j, s+1-j, s-j)$. We then set $\gamma'_r = \varphi^{-1}_{n-2j,s-j}(\gamma_r)$, and define $\phi^{-1}(\gamma) = \gamma_l \cdot \gamma'_r$.

Since $\phi^{-1}(\phi(\gamma)) = \gamma$ and $\phi(\phi^{-1}(\gamma)) = \gamma$, ϕ is invertible and thus a bijection. □

Thus, we have the following consequence.

Corollary 5.5.7. *For* $1 \leq i \leq s \leq \lfloor \frac{n-1}{2} \rfloor$, $T(n, s, i) = T(n, i, i)$.

Remark 5.5.8. *For the rest of this section, we assume that* $s = i$, *and so we abbreviate* $T(n, s, i)$ *and* $T(n, s, i)$ *to* $T(n, i)$ *and* $T(n, i)$, *respectively.*

We finish this subsection by rewriting the recursive formula using the abbreviated notation.

Corollary 5.5.9. *For* $1 \leq i \leq \lfloor \frac{n-1}{2} \rfloor$,

$$T(n, i) = T(n-1, i) + T(n-1, i-1) \qquad \textit{with} \qquad T(n, 0) = T(n-1, 0) = 1.$$

Proof. The case when $i = 0$ follows by definition. For $1 \leq i \leq \lfloor \frac{n-1}{2} \rfloor$, we have that

$$T(n, i) = T(n, i, i) = T(n-1, i, i) + T(n-1, i-1, i-1) = T(n-1, i) + T(n-1, i-1).$$

□

5.6 Proof of Theorem 5.1.6

Let's start by recalling the statement of Theorem 5.2.9.

Theorem. *Let* $s \leq \lfloor \frac{n}{2} \rfloor$. *For* $i = 0$, $T(n, s, 0, b_0) = 1$, *and for* $0 < i \leq s$,

$$T(n, s, i, b_0) = \binom{n}{i} - \binom{n}{i-1}.$$

Using the results from Sections 5.3 and 5.5, Theorem 5.2.9 is equivalent to the following result.

Theorem 5.6.1. *For* $1 \leq i \leq \lfloor \frac{n}{2} \rfloor$,

$$T(n, i) = \binom{n}{i} - \binom{n}{i-1} \qquad \textit{and} \qquad T(n, 0) = 1.$$

Proof. For $i=0$, $T(n,0)$ has exactly one configuration, the one with every marked box at home.

For $0<i\leq\left\lfloor\frac{n}{2}\right\rfloor$ and $n\neq 2i$, we proceed by induction on n. The base case is $n=3$, for which we have that $T(3,1)=2=\binom{3}{1}-\binom{3}{0}$.

Now, assume the statement is true for all $\ell<n$. By Proposition 5.4.1, we have that

$$T(n,i)=T(n-1,i-1)+T(n-1,i)=\binom{n-1}{i-1}-\binom{n-1}{i-2}+\binom{n-1}{i}-\binom{n-1}{i-1}.$$

Reordering these terms according to their sign and using the recursive formula for binomial coefficients, we have that

$$T(n,i)=\left[\binom{n-1}{i}+\binom{n-1}{i-1}\right]-\left[\binom{n-1}{i-1}+\binom{n-1}{i-1}\right]=\binom{n}{i}-\binom{n}{i-1}.$$

For $n=2i$, we know that $T(2i,i)=T(2i-1,i-1)$ by Theorem 5.4.3, and so by inductive hypothesis, we get that

$$T(2i,i)=T(2i-1,i-1)=\binom{2i-1}{i-1}-\binom{2i-1}{i-2}.$$

Applying the symmetry of the binomial coefficients and the recursive formula for binomial coefficients, we have that

$$\begin{aligned}T(2i,i)&=\binom{2i-1}{i-1}+\binom{2i-1}{i}-\binom{2i-1}{i}-\binom{2i-1}{i-2}\\&=\binom{2i-1}{i}+\binom{2i-1}{i-1}-\left[\binom{2i-1}{i-1}+\binom{2i-1}{i-2}\right]=\binom{2i}{i}-\binom{2i}{i-1}.\end{aligned}$$

Thus, the result follows. $\square$

CHAPTER

6

CONCLUSION

There are several paths to continue exploring the two variants of the CQF of the graph introduced in this thesis. As part of this project, I implemented the total labeling CQF and the total orientation CQF (in general) in Sagemath This has allowed me to test some of the ideas for future projects presented below, so while we know a lot about the total chromatic quasisymmetric functions, there is still plenty that remains to be investigated. In Section 6.1, we articulate questions about the expansion of the total CQF variants in various bases for various graphs. In Section 6.2 we explore potential future work related to the deletion-near-contraction formula for the total orientation CQF, and in Section 6.3 we outline where this work may fit in to the current landscape and what future work linking this thesis to pre-existing literature might look like.

6.1 Questions about coefficients

There are patterns we noticed about the coefficients of both total CQF variants that we were unable to prove, but suspect may hold in general. One such pattern is listed below.

Conjecture 6.1.1. *Let G be a graph, and let $T\chi_G^L(q) = \sum_\alpha c_\alpha(q) M_\alpha$ and $T\chi_G^o(q) = \sum_\alpha b_\alpha(q)$. Then, both $c_\alpha(q)$ and $b_\alpha(q)$ are unimodal polynomials in q, and $b_\alpha(q)$ is log-concave.*

We also question for which graphs the total chromatic quasisymmetric functions are actually symmetric. We know that $T\chi_G^o(q)$ is symmetric for any tree, unlike $T\chi_G^L(q)$. We have the following conjecture for the orientation CQF.

Conjecture 6.1.2. *Let G be a graph for which no two cycles share an edge. Then, $T\chi_G^o(q)$ is symmetric.*

This is a conjecture about a sufficient condition for symmetry. It is definitely not a necessary condition, as the total orientation CQF is symmetric for all complete graphs, for example.

We also would like to find expansions of the total labeling CQF for non-star graphs. For instance, we have investigated the path and cycle graphs but have not found a conjectured expression for the coefficients which appear. Similarly, for the total orientation CQF of non-tree graphs like the cycle, we have investigated their expansions into various bases but again have not found a conjectured expression for the coefficients which appear.

6.2 Questions about deletion/contraction formulas

Although we only proved a partial deletion-near-contraction relation (requiring that the deleted/near-contracted edge be not part of a cycle), there is reason to believe that the deletion-near-contraction relation on the total orientation CQF, with some extra terms, can be extended to cases where internal edges in cycles are deleted and near-contracted. We do not believe that such a deletion-near-contraction relation holds for the total labeling CQF, however. Even analyzing simple examples like P_4 or C_3 yielded unwieldy results.

Using the code previously mentioned, we investigated the total CQF (labeling and orientation) for other graphs, namely the path graph and the cycle graph. While the total orientation CQF for the path graph is known since it is a tree, we were unable to find an explicit formula for the total labeling CQF of either graph and the total orientation CQF of the cycle.

6.3 Questions about connections

The CQF of a graph appears in algebraic geometry via the following result, which we previously stated in the introduction.

Theorem. *[Bro18; Sha12] Let $G = \mathrm{inc}(P)$ be the incomparability graph of a natural unit order interval P. Then,*

$$\sum_{j=0}^{|E(G)|} \mathrm{ch}\, H^{2j}(H(P))q^j = \omega\chi_G(q)$$

where $H(P)$ is the regular, semisimple Hessenberg variety of type A associated to P, and ω is the involution on symmetric functions.

This result details a concrete connection between algebraic combinatorics (via the chromatic symmetric function and Shareshian-Wachs conjecture) and geometry (via cohomology of Hessenberg varieties). It is possible that there is a similar geometric connection with the total chromatic quasisymmetric functions, a possibility that has not yet been explored but may be of interest for the broader community.

Finally, we believe that $T\chi_G^o(q)$ could provide a link between the quasisymmetric and symmetric formulations of the Tree Isomorphism Conjecture. The quasisymmetric analogous conjecture that $\chi_G(q)$ distinguishes directed (or labeled) trees was posed by Aval et al [Ava23]. $T\chi_G^o(q)$ is well-understood for trees, and by Theorem 3.2.8, we in fact have the following result.

Theorem 6.3.1. *$T\chi_G^o(q)$ distinguishes trees if and only if χ_G distinguishes trees.*

Since $T\chi_G^o(q)$ is created from adding together $\chi_G^o(q)$ of directed trees, this total CQF may provide some link between conjecures 1.1.2 and 1.1.6.

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