What makes a D_0 graph Schur positive?

Jonah Blasiak

Abstract We define a D_0 graph to be a graph whose vertex set is a subset of permutations of n, with edges of the form \( \cdots bac \cdots \equiv \cdots bca \cdots \) or \( \cdots acb \cdots \equiv \cdots abc \cdots \equiv \cdots \) (Knuth transformations), or \( \cdots bac \cdots \equiv \cdots acb \cdots \equiv \cdots bca \cdots \equiv \cdots \) (rotation transformations), such that whenever the Knuth and rotation transformations at positions \( i-1, i, i+1 \) are available at a vertex, exactly one of these is an edge. The generating function of such a graph is the sum of the quasisymmetric functions associated to the descent sets of its vertices. Assaf studied D_0 graphs in (Dual equivalence and Schur positivity, http://www-bcf.usc.edu/~shassaf/degs.pdf, 2014) and showed that they provide a rich source of examples of the D graphs of (Dual equivalence graphs and a combinatorial proof of LLT and Macdonald positivity, http://www-bcf.usc.edu/~shassaf/positivity.pdf, 2014). A key construction of Assaf expresses the coefficient of \( q^k \) in an LLT polynomial as the generating function of a certain D_0 graph. LLT polynomials are known to be Schur positive by work of Grojnowski-Haiman, and experimentation shows that many D_0 graphs have Schur positive generating functions, which suggests a vast generalization of LLT positivity in this setting. As part of a series of papers, we study D_0 graphs using the Fomin-Greene theory of noncommutative Schur functions. We construct a D_0 graph whose generating function is not Schur positive by solving a linear program related to a certain noncommutative Schur function. We go on to construct a D graph on the same vertex set as this D_0 graph.

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Jonah Blasiak
jblasiak@gmail.com

1 Department of Mathematics, Drexel University, Philadelphia, PA 19104, USA
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1 Introduction

In the 1990s, Fomin and Greene [8] developed a theory of noncommutative Schur functions and used it to give positive combinatorial formulæ for the Schur expansions of a large class of symmetric functions that includes the Stanley symmetric functions and stable Grothendieck polynomials. Lam [14] later showed how this theory can be adapted to study LLT polynomials. This paper is part of a series of papers [4,5] which further develop this theory and connect it to the D graphs of Assaf [3].

LLT polynomials are a family of symmetric functions defined by Lascoux, Leclerc, and Thibon [15]. They play an important role in Macdonald theory and have intriguing connections to Kazhdan–Lusztig theory, k-Schur functions, and plethysm. LLT polynomials were proven to be Schur positive [10,17] using deep geometric results from Kazhdan–Lusztig theory, but a fundamental problem remains open:

Find a positive combinatorial formula, in terms of simple tableau-like objects, for the coefficients in the Schur expansion of LLT polynomials.

This problem is particularly important because the Haglund–Haiman–Loehr formula [12] expresses the transformed Macdonald polynomials \( \tilde{H}_\mu(x; q, t) \) as a positive sum of LLT polynomials. Hence a solution to this problem would yield an explicit formula for the Schur expansions of transformed Macdonald polynomials.

To attack this problem, Lam [14] showed that expanding LLT polynomials in terms of Schur functions is equivalent to writing certain noncommutative versions of Schur functions \( J_\lambda(u) \) as positive sums of monomials in an algebra he called the algebra of ribbon Schur operators. Unfortunately, this mostly translates the difficulty of computing the Schur expansions to another language but does not make the problem much easier. This setup does produce some new results, however. Lam obtains the coefficient of \( s_\lambda(x) \) in an LLT polynomial for \( \lambda \) of the form \( (a, 1^b) \), \( (a, 2) \), or \( (2, 2, 1^a) \). In [4], we obtain a formula for the Schur expansion of LLT polynomials indexed by a 3-tuple of skew shapes, proving and generalizing a conjecture of Haglund [11].

This paper grew out of an attempt to push these results further. The approach we pursue here and in [4,5] combines ideas of Fomin–Greene [8], Lam [14], and Assaf [2,3]. D₀ graphs, which we now define, are central objects in this approach. These graphs were studied in [2] (with slightly different conventions), and the D graphs of [3] corresponding to LLT polynomials are D₀ graphs.

Definition 1.1 Let \( \mathcal{W}_n \) denote the set of words of length \( n \) with no repeated letter in the alphabet \( \{1, 2, \ldots, N\} \). A D₀ graph is a graph on a vertex set \( W \subseteq \mathcal{W}_n \) with edges colored from the set \{2, 3, \ldots, n − 1\} such that

1. each i-edge is one of the four pairs
   
   \{v bac w, v bca w\} or \{v acb w, v cab w\} (Knuth edges), or
   \{v bac w, v acb w\} or \{v bca w, v cab w\} (rotation edges)
for some letters $a < b < c$ and words $v, w$ such that $v$ has length $i - 2$,

(ii) each element of $W \cap \{v \text{bac} w, v \text{bca} w, v \text{acb} w, v \text{cab} w\}$ belongs to exactly one $i$-edge for all letters $a < b < c$ and words $v, w$ such that $v$ has length $i - 2$.

See Fig. 1 for an example. Also, Fig. 2 (Sect. 3.1) depicts the $D_0$ graph on the vertex set $S_4$ with only rotation edges. Knuth and rotation edges correspond to the operators $d_i$ and $\tilde{d}_i$ of [3] (see Sect. 3.1).

**Definition 1.2** The generating function of a $D_0$ graph $G$ is

$$\sum_{w \in \text{Vert}(G)} Q_{\text{Des}(w)}(x),$$

where $Q_{\text{Des}(w)}(x)$ denotes Gessel’s fundamental quasisymmetric function [9], $\text{Des}(w)$ is the descent set of $w$, and $\text{Vert}(G)$ denotes the vertex set of $G$.

In this paper and the companion paper [5], we study the generating functions of $D_0$ graphs using the theory of noncommutative Schur functions. Extensive computer investigations and results of [2–4] led us to speculate that $D_0$ graphs always have Schur positive generating functions. However, this is not true. In this paper, we solve a linear program to find a $D_0$ graph on a vertex set $\tilde{W}^* \subseteq S_8$ whose generating function is not Schur positive. We go on to show that $D$ graphs in the sense of [3] do not always have Schur positive generating functions by constructing a $D$ graph on the same set $\tilde{W}^*$.

Given the abundance of Schur positivity in this setting, these examples were quite surprising and demand further investigation of the question

What hypotheses must a $D_0$ graph satisfy to guarantee Schur positivity? \hfill (1)

See Sect. 8 for further discussion.

We now describe the theory that led us to these examples.

### 1.1 Noncommutative Schur functions

The reader may find it helpful here to take a look at the paper [8] of Fomin and Greene, though we do not formally depend on it in any way. Let
\[ U = \mathbb{Z}\langle u_1, u_2, \ldots, u_N \rangle \]

be the free associative algebra in the noncommuting variables \( u_1, u_2, \ldots, u_N \). We frequently write \( a \) for the variable \( u_a \) and think of the monomials of \( U \) as words in the alphabet \( \{1, 2, \ldots, N\} \).

The noncommutative elementary symmetric functions are given by

\[
ed(u) = \sum_{N \geq i_1 > i_2 > \cdots > i_d \geq 1} u_{i_1}u_{i_2} \cdots u_{i_d} \in U
\]

for any positive integer \( d \); set \( e_0(u) = 1 \) and \( e_d(u) = 0 \) for \( d < 0 \).

In this paper, we define the noncommutative Schur functions by the following noncommutative analog of the Jacobi–Trudi formula:

\[
\mathfrak{J}_{\lambda}(u) = \sum_{\pi \in S_t} \text{sgn}(\pi) e_{\lambda_1' + \pi(1) - 1}(u) e_{\lambda_2' + \pi(2) - 2}(u) \cdots e_{\lambda_t' + \pi(t) - t}(u),
\]

where \( \lambda \) is any partition and \( \lambda' = (\lambda'_1, \ldots, \lambda'_t) \) is the conjugate partition of \( \lambda \).

The Fomin–Greene theory of noncommutative Schur functions is related to D0 graphs by the following algebra. Define the algebra \( U/I_{KR}^{st} \) to be the quotient of \( U \) by the relations

\[
b(ac - ca) = (ac - ca)b \quad \text{for } a < b < c, \quad (2)
w = 0 \quad \text{for words } w \text{ with a repeated letter}.
\]

Here, \( I_{KR}^{st} \) denotes the corresponding two-sided ideal of \( U \); the K stands for Knuth and R for rotation, and “st” is short for “standard word” to remind the reader of relation (3).

We consider \( U \) to be endowed with the symmetric bilinear form \( \langle \cdot, \cdot \rangle \) for which monomials form an orthonormal basis. We show that a zero-one vector (in the monomial basis) belonging to \( I_{KR}^{st} \) is the same as the sum of the vertices of a D0 graph (Proposition–Definition 3.2). We also prove that the elementary symmetric functions \( e_d(u) \) commute in \( U/I_{KR}^{st} \) (Lemma 2.2), which is the first step required to apply the Fomin–Greene approach. Using these facts, we recast a result of Fomin–Greene to show that for any D0 graph \( G \),

\[
\left( \text{the coefficient of } s_\lambda(x) \text{ in the generating function of } G \right) = \mathfrak{J}_\lambda(u), \sum_{w \in \text{Vert}(G)} w.
\]

This identity shows that if there is a positive monomial expression for \( \mathfrak{J}_\lambda(u) \) in \( U/I_{KR}^{st} \), then the generating function of any D0 graph is Schur positive. The main theoretical result of this paper is an approximate converse of this statement, whose precise version we give shortly. Informally, it says that the Fomin–Greene approach to proving Schur positivity is a powerful one because it only fails if the symmetric functions to which it is applied are not actually all Schur positive.
Another notable theoretical result of this paper, which is similar to a result of [14], is

**Theorem 1.3** The noncommutative Schur function \( \mathcal{J}_\lambda(u) \) is a positive sum of monomials in \( \mathcal{U}/I_{\text{KR}}^{\text{st}} \) when \( \lambda \) is a hook shape or of the form \((a,2)\) or \((2,2,1^a)\).

### 1.2 Linear programming duality

We now give the precise statement of the “approximate converse” mentioned above. Fix a positive integer \( d \). Let \( w_1, \ldots, w_m \) be the words of \( \mathcal{U} \) of length \( d \) (all the words, not just those in \( \mathcal{W}_d \)). Let \( R_m \geq 0 \) denote the polyhedron \( \{ \sum_i x_i w_i \mid x_i \geq 0 \} \subseteq \mathbb{R}^m \) and let \( c_d = \sum_{w \in \mathcal{W}_d} w \in \mathbb{R}^m \).

**Theorem 1.4** Let \( \lambda \) be a partition of \( d \). Let \( J^{(1)}, \ldots, J^{(l)} \) be two-sided ideals of \( \mathcal{U} \) such that for each \( j \in [l] \),

- \( J^{(j)} \) is generated by monomials (i.e., words in \( \mathcal{U} \)) and binomials of the form \( v - w \), where \( v \) and \( w \) are words of the same length,
- \( J^{(j)} \supseteq I_{\text{KR}}^{\text{st}} \),
- \( w^j \in J^{(j)} \) if and only if \( w^j \notin \mathcal{W}_d \), for each word \( w^j \) of length \( d \).

Set \( J = \bigcap_j J^{(j)} \). The following are equivalent:

(i′) \( \mathcal{J}_\lambda(u) \) is not a real positive sum of monomials in \( \mathbb{R} \otimes \mathcal{U}/J \).

(v′) There exists an \( f \in R_m \geq 0 \) such that \( c_d - f \in \sum_j \left( (\mathbb{R} J^{(j)})^\perp \cap \mathbb{R}^m \right) \) and \( \langle \mathcal{J}_\lambda(u), f \rangle < 0 \).

These conditions are labeled (i′) and (v′) to match Theorem 6.2, the full version of Theorem 1.4. Note that if (v′) holds, then \( f \) lies in \( (\mathbb{R} J^{(j)})^\perp \cap \mathbb{R}^m \) and hence by (4) is (a \( \mathbb{R}_{>0} \)-weighted version of) the sum of vertices of a \( D_0 \) graph whose generating function is not Schur positive. The proof of this theorem uses linear programming duality.

### 1.3 \( D_0 \) graphs and \( D \) graphs are not always Schur positive

One of the main goals of this project [4,5] was to find a positive expression for \( \mathcal{J}_\lambda(u) \) in \( \mathcal{U}/I_{\text{KR}}^{\text{st}} \). By applying (4) to certain \( D_0 \) graphs constructed in [3], this would give an elegant and uniform formula for the Schur expansion of LLT polynomials. It is possible to carry this out for some \( \lambda \) and in certain quotients of \( \mathcal{U}/I_{\text{KR}}^{\text{st}} \) (e.g., Theorem 1.3 and [4, Theorem 4.1]). The main purpose of this paper, however, is a negative result which shows that for \( \lambda = (2,2,2,2) \), both conditions (i′) and (v′) in Theorem 1.4 hold. We exhibit a set \( \tilde{\mathcal{W}}^* \subseteq S_8 \) such that \( f := \sum_{w \in \tilde{\mathcal{W}}^*} w \in (I_{\text{KR}}^{\text{st}})^\perp \) and \( \langle \mathcal{J}_{(2,2,2,2)}(u), f \rangle = -1 \) (we do not know in general whether \( f \) can always be chosen to be a zero-one vector if (v′) holds, but it happens to be so for our choice of \( \lambda \) and \( J^{(j)} \) here). Hence there is a \( D_0 \) graph \( H^* \) on the vertex set \( \tilde{\mathcal{W}}^* \) whose generating function is not Schur positive.

As already mentioned, this example was quite surprising given our speculation based on computer experimentation and [2–4]. It naturally led us to the question (1)
above, particularly focusing on whether axioms from [3] are enough to guarantee Schur positivity. Though we will not go into the details of these axioms until Sect. 3.4, we briefly mention their relation to D₀ graphs. A D graph as defined in [3] is a colored graph (with some extra data) that satisfies the following properties from that paper: axioms 1, 2, 3, 4′a, 4′b, and 5 and LSP₄ and LSP₅. Most of these properties are clearly satisfied for D₀ graphs, but some require substantial proof and two of them do not always hold. For instance, D₀ graphs do not always satisfy axiom 5, which states that i-edges commute with j-edges for |i − j| ≥ 3. Using Theorem 1.3, we prove that a D₀ graph is a D graph if and only if it satisfies axioms 4′b and 5. A similar result is proved in [2] using different methods.

After finding the example above, we investigated whether imposing axiom 5 is enough to guarantee Schur positivity. In Sect. 7.4, we describe an algorithm that starts with the vertex set \( \tilde{W}^* \) and grows a D₀ graph on this set by adding edges that are forced by axiom 5. This produces a D₀ graph satisfying axiom 5 whose generating function is not Schur positive, so this axiom is not enough. The first graph we produced with this method was not a D graph because it did not satisfy axiom 4′b. With a considerably more intricate algorithm, we were able to produce a graph \( \mathcal{G}^* \) on a subset of \( \tilde{W}^* \) satisfying axioms 5 and 4′b. It has 4950 vertices and is described in the accompanying data files. Moreover, it satisfies a slightly stronger version of axiom 4′b, which we call axiom 4′′b (see Sect. 7.7).

**Theorem 1.5** There exists a D₀ graph \( \mathcal{G}^* \) satisfying axioms 4′′b and 5 whose generating function is not Schur positive. Hence D graphs do not always have Schur positive generating functions.

### 1.4 Organization

Section 2 gives a more thorough introduction to the theory of noncommutative Schur functions just discussed in Sect. 1.1. In Sect. 3 we define D₀ graphs and the D graphs of Assaf and relate D₀ graphs to the algebra \( \mathcal{U}/I_{kr}^{st} \). Section 4 contains some important theoretical results: the full statement and proof of Theorem 1.3 and the corollary that a D₀ graph is a D graph if and only if it satisfies axioms 4′b and 5. In Sect. 5 we show how LLT polynomials can be expressed as the generating functions of certain D₀ graphs and relate our setup to Lam’s [14] and the graphs \( \mathcal{G}^{(k)}_{c,D} \) defined by Assaf in [3]. In Sect. 6 we state and prove the full version of Theorem 1.4. We next solve a linear program related to Theorem 1.4 in Sects. 7.1–7.3, and in the remainder of Sect. 7, we use it to construct the D graph \( \mathcal{G}^* \). Some facts about this graph are given in Sect. 7.8 along with a guide to the accompanying data files giving its full description. Finally, in Sect. 8 we discuss the difficulties that must be overcome to answer question (1) and suggest more precise versions of this question.

## 2 The Fomin–Greene theory of noncommutative Schur functions

D₀ graphs are closely tied to the algebra \( \mathcal{U}/I_{kr}^{st} \). Here, we introduce the theory of noncommutative Schur functions in the algebra \( \mathcal{U}/I_{kr}^{st} \), expanding on the short account
given in Sect. 1.1. This will be useful later for proving several facts about $D_0$ graphs. The companion paper [5] contains a more thorough study of this theory.

2.1 Noncommutative elementary symmetric and Schur functions

The noncommutative elementary symmetric functions in subsets of the variables are given by

$$e_d(S) = \sum_{\substack{i_1 > i_2 > \cdots > i_d \\ i_1, \ldots, i_d \in S}} u_{i_1} u_{i_2} \cdots u_{i_d} \in \mathcal{U},$$

for any subset $S$ of $[N]$ and positive integer $d$; set $e_0(S) = 1$ and $e_d(S) = 0$ for $d < 0$. We also maintain the notation $e_d(u) = e_d([N])$ from Sect. 1.1 throughout the paper.

Let $\lambda$ be a partition, let $\lambda'$ be the conjugate partition of $\lambda$, and let $t$ be the number of parts of $\lambda'$ (which is equal to $\lambda_1$). Recall from Sect. 1.1 that the noncommutative Schur function $J_\lambda(u)$ is given by the following noncommutative version of the Jacobi–Trudi formula:

$$J_\lambda(u) = \sum_{\pi \in S_t} \operatorname{sgn}(\pi) e_{\lambda'_1+\pi(1)-1}(u) e_{\lambda'_2+\pi(2)-2}(u) \cdots e_{\lambda'_t+\pi(t)-t}(u),$$

considered as an element of $\mathcal{U}$.

2.2 From words to generating functions

Let $w = w_1 \cdots w_n$ be a word. We write $\operatorname{Des}(w) := \{i \in [n-1] \mid w_i > w_{i+1}\}$ for the descent set of $w$. Let

$$Q_{\operatorname{Des}(w)}(x) = \sum_{\substack{1 \leq i_1 \leq \cdots \leq i_n \\ j \in \operatorname{Des}(w) \implies i_j \leq i_{j+1}}} x_{i_1} \cdots x_{i_n}$$

be Gessel’s fundamental quasisymmetric function [9] in the commuting variables $x_1, x_2, \ldots$. Note that $Q_{\operatorname{Des}(w)}(x)$ depends on $n$ even though this does not appear in the notation.

Define the linear map

$$\Delta : \mathcal{U} \to \mathbb{Z}[x_1, x_2, \ldots] \text{ by } w \mapsto Q_{\operatorname{Des}(w)}(x).$$

The generating function of an element $f$ of $\mathcal{U}$ is defined to be $\Delta(f)$. This is compatible with the definition of the generating function of a $D_0$ graph from the introduction in that the generating function of a $D_0$ graph $G$ is equal to the generating function of $\sum_{w \in \operatorname{Vert}(G)} w$. 

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2.3 The Fomin–Greene setup

Let $\langle \cdot, \cdot \rangle$ be the symmetric bilinear form on $\mathcal{U}$ for which the monomials form an orthonormal basis. Note that any element of $\mathcal{U}/I$ has a well-defined pairing with any element of $I^\perp$ for any two-sided ideal $I$ of $\mathcal{U}$. Here,

$$I^\perp := \{ f \in \mathcal{U} | \langle z, f \rangle = 0 \text{ for all } z \in I \}$$

denotes the orthogonal complement of $I$.

We state our variant of Theorem 1.2 of [8] and results in Section 6 of [14].

**Theorem 2.1** Let $I$ be a two-sided ideal of $\mathcal{U}$. If $e_k(u)e_\ell(u) = e_\ell(u)e_k(u)$ in $\mathcal{U}/I$ for all $k, \ell$, then for any $f \in I^\perp$, the quasisymmetric function $\Delta(f)$ is symmetric and its Schur expansion is given by

$$\Delta(f) = \sum_\lambda s_\lambda(x) \langle J_\lambda(u), f \rangle,$$

where the sum is over all partitions $\lambda$.

The idea of the proof is that whenever the $e_d(u)$ commute in some quotient of $\mathcal{U}$, the subalgebra they generate is the surjective image of the ring of symmetric functions in commuting variables and hence all the usual identities hold, including the Jacobi–Trudi formula. See [5] for details.

The following lemma is similar to [8, Lemma 3.1]. In [5], we will prove a result that generalizes both the lemma below and that in [8]. Recall that $\mathcal{U}/I_{KR}^{st}$ is the quotient of $\mathcal{U}$ by the relations (2)–(3).

**Lemma 2.2** There holds $e_k(u)e_\ell(u) = e_\ell(u)e_k(u)$ in the algebra $\mathcal{U}/I_{KR}^{st}$, for all $k, \ell$.

**Proof** We closely follow the proof of [8, Lemma 3.1], with only a few key modifications. For $i \leq j$, let

$$E_{j,i}(x) = (1 + xu_j)(1 + xu_{j-1}) \cdots (1 + xu_i) = \sum_{d=0}^{j-i+1} x^d e_d([i, i+1, \ldots, j]),$$

where $x$ commutes with all of the $u_i$. Define $E_{j,i}(x) = 1$ if $i = j + 1$.

The statement of the lemma is equivalent to saying that $E_{N,1}(x)$ and $E_{N,1}(y)$ commute, where $x$ and $y$ are scalar variables. We will prove that $E_{j,i}(x)$ and $E_{j,i}(y)$ commute by induction on $j - i$.

The cases $j - i = -1$ and $j - i = 0$ are clear. Now assume $i < j$. Let $[u_i, u_j]$ denote the commutator $u_iu_j - u_ju_i$. Using the induction hypothesis, we compute

$$E_{j,i}(x)E_{j,i}(y)$$
$$= E_{j,i+1}(x)(1 + xu_i)(1 + yu_j)E_{j-1,i}(y)$$
$$= E_{j,i+1}(x)(1 + yu_j)(1 + xu_i)E_{j-1,i}(y) + xyE_{j,i+1}(x)[u_i, u_j]E_{j-1,i}(y)$$
The third-to-last equality is by (3), and the second-to-last equality is by (2). □

In Sect. 3.1, we will discuss consequences of Theorem 2.1 and Lemma 2.2 for $D_0$ graphs. The heart of the Fomin–Greene approach is to express $\mathfrak{Z}_\lambda(u)$ as a positive combinatorial formula for $\Delta(f)$ for any positive sum of monomials $f$ lying in $I^\perp$.

2.4 Bijectivizations

For the ideal $I = I^m_{KR}$, the condition $f \in I^\perp$ from Theorem 2.1 is unintuitive, and the problem of expressing $\mathfrak{Z}_\lambda(u)$ as a positive sum of monomials in $\mathcal{U}/I$ is computationally difficult. It is therefore fruitful to first consider the easier condition and problem for bijectivizations of $\mathcal{U}/I^m_{KR}$.

**Definition 2.3** A bijectivization of an algebra $\mathcal{U}/I$ is an algebra $\mathcal{U}/J$ such that $I \subseteq J$ and $J$ is generated by monomials (i.e., words in $\mathcal{U}$) and binomials of the form $v - w$, where $v$ and $w$ are words of the same length. To any bijectivization $\mathcal{U}/J$, we associate the following equivalence relation: Two words $v$ and $w$ of $\mathcal{U}$ are equivalent if $v - w \in J$.

We also say that a word is nonzero if it does not belong to $J$ and that an equivalence class of words is nonzero if all of its elements are nonzero.

If $J$ is as in the previous definition, then the space $J^\perp$ has $\mathbb{Z}$-basis $\{\sum_{w \in C} w\}$, where $C$ ranges over the nonzero equivalence classes of $\mathcal{U}/J$. Moreover, the problem of expressing $\mathfrak{Z}_\lambda(u)$ as a positive sum of monomials in $\mathcal{U}/J$ can be made explicit as follows: Let $w^1, \ldots, w^m$ denote the words of $\mathcal{U}$ of length $n$. For each partition $\lambda$ of $n$, we can write $\mathfrak{Z}_\lambda(u) = \sum_i c_i w^i$, $c_i \in \mathbb{Z}$ (an equality in $\mathcal{U}$). Then $\mathfrak{Z}_\lambda(u)$ is a positive sum of monomials in $\mathcal{U}/J$ if and only if $\sum_{w \in C} c_i \geq 0$ for each nonzero equivalence class $C$ of $\mathcal{U}/J$. 
Example 2.4 Let $\mathcal{U}/I_{\text{plac}}^\text{st}$ be the quotient of the plactic algebra by the additional relation (3), i.e., the quotient of $\mathcal{U}$ by (3) and the Knuth relations
\[
\text{acb} = \text{cab}, \\
\text{bac} = \text{bca},
\]
for letters $a < b < c$. Then $\mathcal{U}/I_{\text{plac}}^\text{st}$ is a bijectivization of $\mathcal{U}/I_{\text{KR}}^\text{st}$. The nonzero equivalence classes are the Knuth equivalence classes consisting of words with no repeated letter.

Another bijectivization of $\mathcal{U}/I_{\text{KR}}^\text{st}$ is the quotient of $\mathcal{U}$ by (3) and the relations
\[
\text{acb} = \text{bac}, \\
\text{cab} = \text{bca},
\]
corresponding to rotation edges. This algebra was studied by Novelli and Schilling in [18]. It follows easily from their results that two words $v, w \in \mathcal{W}_n$ are equivalent if and only if they have the same number of inversions, they are permutations of the same set of letters, and $\min(v)$ and $\max(v)$ occur in the same order in both words.

Example 2.5 Here is a rich source of examples of bijectivizations of $\mathcal{U}/I_{\text{KR}}^\text{st}$. For each subset $S \subseteq [N]$ of size 3, declare it to be either a Knuth triple or a rotation triple. The triples bijectivization of $\mathcal{U}/I_{\text{KR}}^\text{st}$ associated to these data is the quotient of $\mathcal{U}$ by the relations
\[
\text{acb} = \text{cab} \quad \text{if } a < b < c \text{ is a Knuth triple} \\
\text{bac} = \text{bca} \quad \text{if } a < b < c \text{ is a Knuth triple} \\
\text{acb} = \text{bac} \quad \text{if } a < b < c \text{ is a rotation triple} \\
\text{cab} = \text{bca} \quad \text{if } a < b < c \text{ is a rotation triple} \\
w = 0 \quad \text{for words } w \text{ with a repeated letter.}
\]

Remark 2.6 Extensive computer experimentation supports the following statement: The symmetric function $\Delta(\sum_{w \in C} w)$ is Schur positive for any nonzero equivalence class $C$ of any triples bijectivization. However, no proof of this is known. See Sect. 8 for further discussion.

In Sect. 5, we define certain bijectivizations of $\mathcal{U}/I_{\text{KR}}^\text{st}$ to apply the Fomin–Greene approach to LLT polynomials and certain graphs related to LLT polynomials from [3].

2.5 Automorphisms of $\mathcal{U}/I_{\text{KR}}^\text{st}$

Certain natural maps on $\mathcal{U}$ induce well-defined maps on the quotient $\mathcal{U}/I_{\text{KR}}^\text{st}$. Similar results are proven in [16] for the plactic monoid. For a word $w = w_1w_2\cdots w_n$, let $\text{rev}(w)$ denote the word $w_nw_{n-1}\cdots w_1$.

Proposition 2.7 (i) Let $\theta : [N] \to \mathbb{Z}$ be an order-preserving injection and let $\theta_{\mathcal{U}} : \mathcal{U} \to \mathcal{U}$, $u_i \mapsto u_{\theta(i)}$ be the corresponding algebra homomorphism, where we
set $u_i = 0$ if $i \notin \mathbb{N}$. Then $\theta_U(I_{KR}^{st}) \subseteq I_{KR}^{st}$ and hence $\theta_U$ induces an algebra homomorphism $U/I_{KR}^{st} \to U/I_{KR}^{st}$.

(ii) The analog of statement (i) holds for $\theta$ an order-reversing injection.

(iii) Let $\text{rev} : U \to U$ denote the algebra anti-automorphism given by $w \mapsto \text{rev}(w)$. Then $\text{rev}(I_{KR}^{st}) = I_{KR}^{st}$ and hence $\text{rev}$ induces an algebra anti-automorphism $U/I_{KR}^{st} \to U/I_{KR}^{st}$.

Proof Statement (i) is clear since for an order-preserving injection $\theta$ and any $1 \leq a < b < c \leq N$, there holds

$$\theta_U(b(ac - ca) - (ac - ca)b) = b'(a'c' - c'a') - (a'c' - c'a')b' \in I_{KR}^{st},$$

for some $a' < b' < c'$. Note that there is no problem if $a', b', c'$ do not all lie in $\mathbb{N}$ since if, say, $c' \notin \mathbb{N}$ then $c' := u_{c'} = 0$, so the right side of (5) is 0.

If $\theta$ is an order-reversing injection, then for any $1 \leq a < b < c \leq N$,

$$\theta_U(b(ac - ca) - (ac - ca)b) = b'(c'a' - a'c') - (c'a' - a'c')b'$$

$$= -(b'(a'c' - c'a') - (a'c' - c'a')b') \in I_{KR}^{st},$$

for some $a' < b' < c'$. To verify (iii), we compute

$$\text{rev}(b(ac - ca) - (ac - ca)b)$$

$$= (ca - ac)b - b(ca - ac) = b(ac - ca) - (ac - ca)b \in I_{KR}^{st}.$$

$\Box$

3 D$_0$ graphs and D graphs

Here, we define D$_0$ graphs differently than in the introduction and relate them to the algebra $U/I_{KR}^{st}$. We then recall the axioms defining a D graph from [3].

3.1 D$_0$ graphs

Let $W \subseteq U$ denote the set of words with no repeated letter, let $W_n \subseteq W$ denote the set of words of length $n$ with no repeated letter, and let $S_n$ denote the set of permutations of $n$. We write $|v|$ for the length of a word $v$.

A KR square is a 4-tuple of elements of $W$ of the form

$$v[abc]w = (v bac w, v bca w, v acb w, v cab w),$$

where $a < b < c$ are letters and $v$ and $w$ are words. We also say (6) is a KR$_i$ square, for $i = |v| + 2$. We abuse notation and identify the tuple $v[abc]w$ with its set of elements when convenient. We say that a KR square $X$ is a KR square of $W_n$ or a KR square of $S_n$ if $X \subseteq W_n$ or $X \subseteq S_n$, respectively.
Definition 3.1 A partial $D_0$ graph of degree $n$ is a graph $G$ on a vertex set $W \subseteq W_n$ with edges colored from the set $\{2, 3, \ldots, n-1\}$ such that for each KR, square $X = v[abc]w$, exactly one of the following possibilities occurs:

1. $X \cap W = \emptyset$.
2. $X \cap W$ is equal to $\{v bac w, v bca w\}$ or $\{v acb w, v cab w\}$ and is an $i$-edge,
3. $X \cap W$ is equal to $\{v ba c w, v ac b w\}$ or $\{v b c a w, v c a b w\}$ and is an $i$-edge,
4. $X \subseteq W$ and $\{v bac w, v bca w\}$ and $\{v acb w, v cab w\}$ are $i$-edges,
5. $X \subseteq W$ and $\{v bac w, v acb w\}$ and $\{v bca w, v cab w\}$ are $i$-edges,
6. $X \subseteq W$ and no edge has both ends in $X$.

If (vi) never occurs, then we say that $G$ is a $D_0$ graph of degree $n$.

Recall from Definition 1.1 that an edge $[x, y]$ of $G$ is a Knuth edge (resp. rotation edge) if $[x, y]$ is as in (ii) and (iv) (resp. (iii) and (v)); we call this the type of the edge so that each edge has two kinds of labels—color and type; we can then speak of the type of the $i$-edge at $x$, the color of a Knuth edge at $x$, the rotation $j$-edges of $G$, etc.; a Knuth $i$-edge (resp. rotation $i$-edge) is denoted $i$ (resp. $i$) in figures. Note that the type and color of an edge $[x, y]$ can be recovered from the vertex labels $x, y$, with one exception: If $x = vacw, y = vca bw$, then $[x, y]$ has type Knuth and color either $|v| + 1$ or $|v| + 2$.

In agreement with standard terminology (see, e.g., [20, A1]), a Knuth transformation is a transformation of the form $x \rightsquigarrow y$ whenever $[x, y]$ is as in (ii) and (iv) above. We define a rotation transformation to be a transformation of the form $x \rightsquigarrow y$ whenever $[x, y]$ is as in (iii) and (v) above. These transformations are related to the $d_j$ and $\tilde{d}_j$ of [3] as follows: For permutations $x$ and $y$, the transformation $x \rightsquigarrow y$ is a Knuth (resp. rotation) transformation at positions $i-1, i, i+1$ if and only if $d_i(x^{-1}) = y^{-1}$ (resp. $\tilde{d}_i(x^{-1}) = y^{-1}$).

Examples of $D_0$ graphs are given in Figs. 1, 2, and 4.

Given a partial $D_0$ graph $G$ with vertex set $W$, a KR square of $G$ is just a KR square, but has the following extra data associated to it. The type of a KR square $X = v[abc]w$ of $G$ is

\begin{align*}
\text{Irrelevant} & \quad (\emptyset) \text{ if } X \cap W = \emptyset, \\
\text{Undetermined} & \quad (0) \text{ if } X \cap W = X \text{ and no edge of } G \text{ has both ends in } X, \\
\text{Knuth} & \quad (K) \text{ if } \{v bac w, v bca w\} \text{ or } \{v acb w, v cab w\} \text{ (or both) are edges of } G, \\
\text{Rotation} & \quad (R) \text{ if } \{v bac w, v acb w\} \text{ or } \{v bca w, v cab w\} \text{ (or both) are edges of } G.
\end{align*}

3.2 KR sets

The vertex sets of $D_0$ graphs are the same as zero-one vectors of $(I_{KR}^*)^\perp$, as we now show. In light of Theorem 2.1, these sets are important objects in their own right and are in some ways more fundamental than $D_0$ graphs.

Proposition-Definition 3.2 For a subset $W$ of $W_n$, the following are equivalent:

1. $W$ is the vertex set of a $D_0$ graph.
For every KR square $X$ of $W_n$, the set $W \cap X$ is empty, is all of $X$, or consists of two words which differ by a Knuth transformation or rotation transformation.

If $W$ satisfies these conditions, then we say that $W$ is a KR set.

Proof By comparing the definition of a $D_0$ graph to (ii), it is clear that (i) implies (ii). To see that (ii) implies (i), note that the KR$_i$ squares of $W_n$ are pairwise disjoint. Hence if $W$ is as in (ii) and $t_i$ is the number of KR$_i$ squares $X$ such that $X \subseteq W$, then there are $2 \sum t_i$ $D_0$ graphs with vertex set $W$ corresponding to the $\sum t_i$ independent choices for the types of these KR squares.

We now prove the equivalence of (ii) and (iii). Let $X = v[abc]w$ be a KR square and let $\mathbb{Z}X$ be the $\mathbb{Z}$-module with $\mathbb{Z}$-basis $v[abc]w = (v\ bac\ w, v\ bca\ w, v\ acb\ w, v\ cab\ w)$.

Consider the vector

$$h_X := v\ bac\ w - v\ bca\ w - v\ acb\ w + v\ cab\ w = [1\ -1\ -1\ 1] \in \mathbb{Z}X.$$ 

The zero-one vectors orthogonal to $h_X$ are

$$[0\ 0\ 0\ 0], [1\ 1\ 1\ 1], [1\ 1\ 0\ 0], [0\ 0\ 1\ 1], [1\ 0\ 1\ 0], [0\ 1\ 0\ 1].$$

Fig. 2 $D_0$ graph on $S_4$ with only rotation edges. In the notation of Sect. 5.3, this is the Assaf LLT$_3^1$ D graph $\mathcal{G}^1_3$, restricted to $S_4$. 

(ii) For every KR square $X$ of $W_n$, the set $W \cap X$ is empty, is all of $X$, or consists of two words which differ by a Knuth transformation or rotation transformation.

(iii) $\sum_{w \in W} w \in (I_{\text{KR}}^1)^\perp$. 

If $W$ satisfies these conditions, then we say that $W$ is a KR set.
Therefore, since the $\mathbb{Z}$-module $I_{KR}^{st} \cap \mathbb{Z}W_n$ is spanned by the elements $h_X$ over all KR squares $X$ of $W_n$, an element $\sum_{w \in W} w \in \mathbb{Z}W_n$ belongs to $(I_{KR}^{st})^\perp$ if and only if $\sum_{w \in W \cap X} w$ is one of the six vectors in (7) for all KR squares $X$. The equivalence of (ii) and (iii) then follows because those pairs of words of $X$ which differ by a Knuth transformation or rotation transformation are exactly the supports of the last four vectors of (7).

We define (a slight generalization of Definition 1.2) the generating function of a partial $D_0$ graph $H$ to be

$$\Delta\left( \sum_{w \in \text{Vert}(H)} w \right) = \sum_{w \in \text{Vert}(H)} Q_{\text{Des}(w)}(x).$$

Note that this only depends on the KR set $\text{Vert}(H)$ and not on the edges of $H$. Theorem 2.1 and Lemma 2.2 then have the following corollary.

**Corollary 3.3** The generating function of any (partial) $D_0$ graph $H$ is a symmetric function. The coefficient of $s_\lambda(x)$ in this function is $\langle J_\lambda(u), \sum_{w \in \text{Vert}(H)} w \rangle$.

### 3.3 Preliminary definitions for D graphs

Before recalling the axioms of a D graph from [3], we must first recall several definitions from that paper.

**Definition 3.4** ([3, Definition 3.3]) A signed, colored graph\(^1\) of degree $n$ is an (undirected) graph $G$ with vertex set $V$ whose edges are colored from the set $\{2, 3, \ldots, n-1\}$, together with a signature function $\sigma : V \to \{+1, -1\}^{n-1}$.

A signed, colored graph satisfies axiom 0 if the $i$-degree of every vertex is at most 1. All signed, colored graphs considered in this paper satisfy axiom 0. Let $G$ be a signed, colored graph satisfying axiom 0. The notation $E_i(v) = w$ means that $\{v, w\}$ is an $i$-edge of $G$. A vertex $v$ of $G$ admits an $i$-neighbor if there is an $i$-edge $\{v, w\}$ for some $w$.

**Remark 3.5** It is sometimes convenient to think of $E_i$ in the definition above as an involution of $V$, with fixed points those vertices not admitting an $i$-neighbor. However, to avoid confusion, we consider the expression $E_i(v)$ to be undefined if $v$ does not admit an $i$-neighbor.

Any (partial) $D_0$ graph $G$ of degree $n$ may also be regarded as a signed, colored graph whose edge colors are the same as those of $G$ (but edge types are ignored) and whose signature function on each word $w \in \text{Vert}(G)$ is given by

$$\sigma(W)_i = \begin{cases} +1 & \text{if } w_i \leq w_{i+1}, \\
-1 & \text{if } w_i > w_{i+1}, \end{cases} \text{ for } i \in [n-1].$$

\(^1\) These are slightly less general than the signed, colored graphs considered in [3].
For example, \( \sigma(72158346) = - - + - + - + \). The signature \( \sigma(w) \) of \( w \) is just another encoding of the descent set \( \text{Des}(w) \), the two being related by \( \sigma(w)_i = - \) if and only if \( i \in \text{Des}(w) \).

**Definition 3.6** Given a \( D_0 \) graph \( G \) with vertex set \( W \subseteq \mathcal{W}_n \) and an interval \( K = \{i, i + 1, \ldots, j\} \), \( 1 \leq i \leq j \leq n \), the \( K \)-restriction of \( G \), denoted \( \text{Res}_K G \), is the graph with

(i) vertex set \( W \), with each vertex \( w \in W \) labeled by the word \( w_i w_{i+1} \cdots w_j \),

(ii) signature function \( \hat{\sigma} \) defined by \( \hat{\sigma}(w) = \sigma_{s+i-1}(w) \), for all \( s \in [j-i] \), \( w \in W \),

(iii) an \( (s-i+1) \)-edge for each \( s \)-edge of \( G \) (with the same ends as in \( G \)), for all \( s \in \{i+1, \ldots, j-1\} \).

For a signed, colored graph \( \mathcal{G} \), we define the \( K \)-restriction of \( \mathcal{G} \), \( \text{Res}_K \mathcal{G} \), in the same way, the only difference being that in place of (i) we simply define \( \text{Vert}(\text{Res}_K \mathcal{G}) \) to be \( \text{Vert}(\mathcal{G}) \).

If \( \mathcal{G} \) is a \( D_0 \) graph or a signed, colored graph and \( w \) is a vertex of \( \mathcal{G} \), we define \( \text{Res}_K(\mathcal{G}, w) \) to be the component of \( \text{Res}_K \mathcal{G} \) containing \( w \).

For example, here is a \( D_0 \) graph (top line) and its \([2, 3, 4]\)-restriction (bottom line):

\[
\begin{array}{c}
23451 \quad 23415 \\
345 \quad 341 \quad 24135 \quad 41235 \\
\end{array}
\]

**Remark 3.7** The reason for the somewhat awkward definition of the vertex set of \( \text{Res}_K \mathcal{G} \) in (i) is because two distinct vertices \( w, w' \in W \) can have the same label \( w_i w_{i+1} \cdots w_j = w'_i w'_{i+1} \cdots w'_j \). This also means that \( \text{Res}_K \mathcal{G} \) is not a \( D_0 \) graph in general. But this is harmless because every connected component of \( \text{Res}_K \mathcal{G} \) is a \( D_0 \) graph. (To view a component \( H \) of \( \text{Res}_K \mathcal{G} \) as a \( D_0 \) graph, we should forget the original set \( W \) and only retain the vertex labels \( \{w_i w_{i+1} \cdots w_j \mid w \in \text{Vert}(H)\} \) of \( H \).

**Definition 3.8** Let \( \mathcal{G} \) be a signed, colored graph satisfying axiom 0. Any component \( H \) of \( \text{Res}_{[i-2, i+1]} \mathcal{G} \) is a path or an even cycle. For \( 2 < i < n \), an \((i-1)\)-i-string for \( H \) is a sequence \( \langle x^1, x^2, \ldots, x^t \rangle \) consisting of all the vertices of \( H \) (without repetition) such that the pairs \( \{x^1, x^2\}, \{x^2, x^3\}, \ldots \) alternate between \( i \)-edges and \( i-1 \)-edges (starting with either an \( i \)-edge or an \( i-1 \)-edge). We also say that \( \langle x^1, x^2, \ldots, x^t \rangle \) is an \((i-1)\)-i-string if there exists an \( H \) such that it is an \((i-1)\)-i-string for \( H \).

**Definition 3.9** ([3, Definition 5.3]) A vertex \( v \) of a signed, colored graph \( \mathcal{G} \) satisfying axiom 0 has \( i \)-type \( W \) if \( v \) admits an \( i \)-neighbor and an \( i-1 \)-neighbor and \( \sigma(v)_i = -\sigma(E_{i-1}(v))_i \).

For example, the vertices in Fig. 2 that have 3-type \( W \) are 2143, 1423, 3412, 4132.

**Definition 3.10** ([3, Definition 5.7]) Let \( \mathcal{G} \) be a signed, colored graph of degree \( n \) satisfying axiom 0. For \( 4 \leq i < n \), a flat i-chain of \( \mathcal{G} \) is a sequence \( \langle x^1, x^2, \ldots, x^{2h-1}, x^{2h} \rangle \) of distinct vertices admitting \( i-2 \)-neighbors such that

\[
x^{2j-1} = E_i(x^{2j}) \quad \text{and} \quad x^{2j+1} = E_{i-2}(E_{i-1}E_{i-2})^{m_j}(x^{2j}),
\]
for nonnegative integers $m_j$ such that $(E_{i-1}E_{i-2})^{m_j}(x^{2j})$ does not have $(i - 1)$-type W.

In accordance with Remark 3.5, we assume that the applications of $E_j$ in this definition correspond to $j$-edges. A flat 4-chain of a $D_0$ graph of degree 8 is shown in Fig. 6.

Remark 3.11 To understand this definition, it is helpful to first consider the case in which the $m_j$ are all 0. For instance, if $G$ is a $D_0$ graph in which all $i - 2$-edges and $i - 1$-edges are Knuth, then the flat $i$-chains of $G$ have this property. A flat $i$-chain in this case all the $m_j$ are 0 is a sequence $(x^1, x^2, \ldots, x^{2h})$ of distinct vertices such that

- the pairs $\{x^1, x^2\}, \{x^2, x^3\}, \ldots, \{x^{2h-1}, x^{2h}\}$ alternate between $i$-edges and $i - 2$-edges, starting and ending with an $i$-edge, and
- $x^1$ and $x^{2h}$ admit $i - 2$-neighbors.

Remark 3.12 Let $(x^1, x^2, \ldots, x^{2h})$ be a flat $i$-chain of a $D_0$ graph $G$. The vertices $x^{2j}$ and $x^{2j+1}$ are related as follows: Let $H$ be the component of $Res_{[i-3,i]}G$ containing $x^{2j}$ and $x^{2j+1}$. By Proposition 4.4 (below), $H$ is either a 2-cycle, a path with two edges, or a path with four edges. The component $H$ cannot be a 2-cycle because in this case both $x^{2j}$ and $x^{2j+1}$ have $(i - 1)$-type W. If $H$ is a path with two edges, then we must have $x^{2j+1} = E_{i-2}(x^{2j})$.

Finally, suppose $H$ is a path with four edges and let $(y^1, \ldots, y^5)$ be the $(i - 2)$-$(i - 1)$-string for $H$ such that $(y^1, y^2)$ is an $i - 1$-edge. Then the vertices of $H$ having $(i - 1)$-type W are $y^2$ and $y^3$. Hence by the definition of a flat $i$-chain, $x^{2j+1} \in \{y^4, y^5\}$. We also must have $m_j \in \{0, 1\}$. Checking each possibility for $x^{2j+1}$ and $m_j$ shows that exactly one of the following must hold:

- $x^{2j} = y^2, m_j = 1, x^{2j+1} = y^5$,
- $x^{2j} = y^4, m_j = 0, x^{2j+1} = y^5$,
- $x^{2j} = y^5, m_j = 0, x^{2j+1} = y^4$.

In particular, the $m_j$ and $x^{2j+1}$ in the definition of a flat $i$-chain are determined uniquely by $x^{2j}$.

### 3.4 D graphs

Let $G$ be a signed, colored graph with vertex set $V$. The following axioms from [3] are needed to define D graphs:

(axiom 1) $G$ satisfies axiom 0 and $w \in V$ admits an $i$-neighbor if and only if $\sigma(w)_{i-1} = -\sigma(w)_i$;

(axiom 2) for each $i$-edge $[w, x]$, $\sigma(w)_j = -\sigma(x)_j$ for $j = i - 1, i$, and $\sigma(w)_h = \sigma(x)_h$ for $h < i - 2$ and $h > i + 1$;

(axiom 3) for each $i$-edge $[w, x]$, if $\sigma(w)_{i-2} = -\sigma(x)_{i-2}$, then $\sigma(w)_{i-2} = -\sigma(w)_{i-1}$, and if $\sigma(w)_{i+1} = -\sigma(x)_{i+1}$, then $\sigma(w)_{i+1} = -\sigma(w)_i$;

(axiom 4′a) for every $w \in V$ such that

---

2 In the statement of axiom 4′a in [3], the conditions on $w$ are $w \in W_i(G)$ has a nonflat $i - 1$-edge, which are equivalent to the conditions in (8) assuming axioms 1 and 2.
is defined to be
\[ \sum_{1} \]
the generating function of \( \text{Res}_{[i-3, i]}(G, w) \) is equal to that of \( \text{Res}_{[i-2, i+1]}(G, w) \);
(axiom 4') if \((x^1, x^2, \ldots, x^{2h-1}, x^{2h})\) is a flat \( i \)-chain and \( x^j \) has \((i + 1)\)-type \( W \) for some \( 2 < j < 2h - 1 \), then either \( x^1, \ldots, x^j \) have \((i + 1)\)-type \( W \) or \( x^j, \ldots, x^{2h} \) have \((i + 1)\)-type \( W \) (or both);
(axiom 5) if \( \{w, x\} \) is an \( i \)-edge and \( \{x, y\} \) is a \( j \)-edge for \( |i - j| \geq 3 \), then \( \{w, v\} \) is a \( j \)-edge and \( \{v, y\} \) is an \( i \)-edge for some \( v \in V \).

Remark 3.13  Note that we must assume \( G \) satisfies axiom 0 in the definition of axiom 4' since this is assumed in the definition of a flat \( i \)-chain. The version of axiom 4' stated here is from an earlier version of [3] posted on 04-2014. We use the 04-2014 version because it implies the version in [3] (posted 08-2014) and is more straightforward to check. For reference, the 08-2014 version is:

if \( x \in C_i(G) \) has \((i + 1)\)-type \( W \), then there exists a maximal length flat \( i \)-chain \((x^1, x^2, \ldots, x^{2h-1}, x^{2h})\) with \( x = x^j \) such that either \( x^1, \ldots, x^j \) have \((i + 1)\)-type \( W \) or \( x^j, \ldots, x^{2h} \) have \((i + 1)\)-type \( W \) (or both).

Here,
\[
C_i(G) := \{ x \in \text{Vert}(G) \mid x = x_j \text{ on a flat } i \text{-chain of length } 2h \text{ with } 2 < j < 2h - 1 \}.
\]

For comparison, here is the version of axiom 4' from [1] (posted 10-2013):

if \( x \in C_i^{\text{simple}}(G) \) has \((i + 1)\)-type \( W \) and \( E_{i-2}(x) \) does not, then \((E_{i-2}E_i)^m(x)\) has \((i + 1)\)-type \( W \) for all \( m \geq 1 \) for which \((E_{i-2}E_i)^{m-1}(x)\) admits an \( i \)-neighbor.

Here,
\[
C_i^{\text{simple}}(G) := \left\{ x \in \text{Vert}(G) \mid \left. E_{i-2}E_iE_{i-2}(x), E_iE_{i-2}(x), E_{i-2}(x), x, E_i(x), E_{i-2}E_i(x) \right\} \right. \text{ are well defined and distinct}
\]
where we have assumed \( G \) satisfies axioms 1 and 2 to translate from the notation of [1].

The generating function of a signed, colored graph \( G \) with signature function \( \sigma \) is defined to be \( \sum_{x \in \text{Vert}(G)} q_{\text{Des}(x)}(x) \), where \( \text{Des}(v) \) is defined to be the descent set encoded by \( \sigma(v) \), i.e., \( i \in \text{Des}(v) \) if and only if \( \sigma(v)_i = - \). When \( G \) is also a \( D_0 \) graph, this generating function is the same as the generating function of \( G \) previously defined (Definition 1.2).

Definition 3.14  ([3, Definition 4.5]) A signed, colored graph \( G \) is locally Schur positive for degree \( d \) (LSP\(_d\)) if the generating function of every component of every \( K \)-restriction of \( G \) is Schur positive, for all intervals \( K \) of size \( d \).

Note that \( G \) being LSP\(_d\) depends only on the signature function of \( G \) and not on the edges of \( G \).
Definition 3.15 A D$_5$ graph is a D$_0$ graph that satisfies axiom 5.

Recall Definition 5.37 from [3]: A signed, colored graph is a D graph if it satisfies axioms 1, 2, 3, 4$'$a, 4$'$b, 5, and LSP$_4$ and LSP$_5$.

In the next section we will prove that a D$_0$ graph satisfying axioms 4$'$b and 5 is a D graph (Theorem 4.10).

4 Basic properties of D$_0$ graphs

Here, we show that D$_0$ graphs satisfy LSP$_4$ and LSP$_5$ using noncommutative Schur functions. We also show that they satisfy axioms 1, 2, 3, and 4$'$a as well as some other basic properties.

4.1 Components, unions, and complements

D$_0$ graphs are well behaved under some basic set operations.

Proposition 4.1 (a) The connected components of a D$_0$ graph are D$_0$ graphs.
(b) The union of two D$_0$ graphs is a D$_0$ graph if their vertex sets are disjoint subsets of $W_n$.
(c) If $\mathcal{G}$ is a D$_0$ graph on a vertex set $W \subseteq W_n$, then there is a D$_0$ graph on the vertex set $W_n \setminus W$.

Proof It is easy to see that any connected component of a D$_0$ graph satisfies (i)–(v) in Definition 3.1, hence (a). Statement (b) also follows easily from the definition of D$_0$ graphs. For (c), note that $W_n$ and $W$ are KR sets; hence $\sum_{w \in W_n \setminus W} w \in (I_{KR})^\perp$ by Proposition–Definition 3.2. Therefore, there is a D$_0$ graph on the vertex set $W_n \setminus W$, again by Proposition–Definition 3.2.

4.2 Local structure of D$_0$ graphs

For a word $w \in W$, the standardization of $w$, denoted $w^{st}$, is the permutation obtained from $w$ by relabeling its smallest letter by 1, its next smallest letter by 2, etc.

Proposition 4.2 If $\mathcal{G}$ is a connected D$_0$ graph of degree n on a vertex set $W$, then there is a unique D$_0$ graph $\mathcal{G}^{st}$ on the set $W^{st} := \{w^{st} \mid w \in W\} \subseteq S_n$ such that the standardization map induces a graph isomorphism $\mathcal{G} \rightarrow \mathcal{G}^{st}$ which preserves edge color and type and vertex signatures.

Proof This is straightforward from the fact that Knuth and rotation transformations only depend on the relative order of three distinct letters, not on their exact values. The assumption that $\mathcal{G}$ is connected is necessary to ensure that the standardization map restricted to the vertices of $\mathcal{G}$ is injective.

Remark 4.3 For most of this paper we work with $W_n$ instead of $S_n$ because the former has the convenient property that any subword of some $w \in W$ also belongs to $W$. However, by the previous proposition, we could phrase all our results in terms of subsets of $S_n$ and lose no generality.
Proposition 4.4 If \( G \) is a \( D_0 \) graph and \( K \) is an interval of size 4, then the connected components of (the underlying colored graph of) \( \text{Res}_K \, G \) are of the form:

\[
\begin{align*}
\bullet & \quad 2 \quad \bullet \\
\bullet & \quad 3 \quad \bullet \\
\bullet & \quad 2 \quad \bullet \quad 3 \\
\end{align*}
\]

Proof Let \( H \) be a connected component of \( \text{Res}_K \, G \). By Remark 3.7 and Proposition 4.2, we can assume that \( H \) is a \( D_0 \) graph on a subset of \( S_4 \). Since every vertex of \( H \) has \( i \)-degree at most 1, \( H \) is a path or an even cycle. Moreover, \( H \) cannot be a path with an even number of vertices since this would imply that the generating function of \( H \) is either

\[
\begin{align*}
Q_{[1]}(x) + Q_{[2,3]}(x) + (h - 1)(Q_{[1,3]}(x) + Q_{[2]}(x)) \\
= Q_{[1]}(x) + Q_{[2,3]}(x) + (h - 1)s_{(2,2)}(x), \quad \text{or} \\
Q_{[1,2]}(x) + Q_{[3]}(x) + (h - 1)(Q_{[1,3]}(x) + Q_{[2]}(x)) \\
= Q_{[1,2]}(x) + Q_{[3]}(x) + (h - 1)s_{(2,2)}(x),
\end{align*}
\]

where \( 2h = |\text{Vert}(H)| \). But this is impossible since these functions are not symmetric while the generating function of \( H \) is Schur positive (by Corollary 4.9, below).

Now let \((x^1, \ldots, x^t)\) be a 2–3-string for \( H \). Suppose for a contradiction that \( H \) is not one of the three graphs above. Then either \( t \geq 7 \) or \( H \) is a cycle of length >2. Set \( w = x^{(t+1)/2} \). The desired contradiction follows from the claim

at least one of \( w, E_2(w), E_3(w), E_3 E_2(w), E_2 E_3(w) \)

does not admit both a 2-neighbor and a 3-neighbor. (9)

Before proving (9), we show the following for any vertex \( v \) of \( H \):

Suppose \( v_4 \in \{1, 4\} \). If \( v \) admits both a 2-neighbor and a 3-neighbor, then \( E_2(v) \) does not. (10)

Suppose \( v_1 \in \{1, 4\} \). If \( v \) admits both a 2-neighbor and a 3-neighbor, then \( E_3(v) \) does not. (11)

To prove (10), suppose \( v_4 = 4 \), the case \( v_4 = 1 \) being similar. If \( v \) admits a 2-neighbor, then exactly one of \( \sigma_2(v) \), \( \sigma_2(E_2(v)) \) is +. Since \( v_4 = 4 \), there holds \( \sigma_3(v) = \sigma_3(E_2(v)) = + \), so exactly one of \( v \), \( E_2(v) \) admits a 3-neighbor. Statement (10) follows. The proof of (11) is similar.

We now prove (9) by showing that at least one of \( w, E_2(w), E_3(w) \) satisfies the first hypothesis of (10) or (11). If \( \{w_2, w_3\} \neq \{1, 4\} \), then \( w \) satisfies the first hypothesis of (10) or (11). If \( \{w_2, w_3\} = \{1, 4\} \), then \( E_2(w) \) (resp. \( E_3(w) \)) satisfies the first hypothesis of (10) or (11) if the 2-edge (resp. 3-edge) at \( w \) is a rotation edge. The only
remaining possibility is that the 2-edge and 3-edge at \( w \) are Knuth, but this implies that \( H \) is a cycle of length 2, contrary to our supposition. This completes the proof of (9). \( \square \)

We can now show that axiom 4’ a in the definition of a D graph always holds for \( D_0 \) graphs. This was also proved as part of [2, Theorem 6.1] by a computer check. A similar result is proved in [3, Theorem 5.38] using similar methods.

**Proposition 4.5** \( D_0 \) graphs satisfy axiom 4’ a.

**Proof** Let \( G \) be a \( D_0 \) graph. Since axiom 4’ a for \( G \) depends only on \( \text{Res}_K G \) for \( |K| = 5 \), by Proposition 4.2 we may assume that the vertices of \( G \) lie in \( S_5 \) and the \( i \) in the definition of axiom 4’ a is 4. Let \( \{ w, v \} \) be an \( i-1 \)-edge of \( G \) as in (8). Since \( G \) satisfies axioms 1 and 2 (see Theorem 4.10, below), the conditions (8) on \( w \) imply that \( \text{Res}_{[1, 4]}(G, w) \) and \( \text{Res}_{[2, 5]}(G, w) \) each contain at least 3 edges. Then by Proposition 4.4, \( \text{Res}_{[1, 4]}(G, w) \) is a path with 4 edges and \( \text{Res}_{[2, 5]}(G, w) \) is a path with 4 edges.

Since a Knuth transformation only changes two adjacent letters, the conditions \( \sigma_{i-3}(w) \neq \sigma_{i-3}(v) \) and \( \sigma_i(w) \neq \sigma_i(v) \) imply that the 3-edge \( \{ w, v \} \) must be a rotation edge. In fact, one can check that these conditions imply that \( \{ w, v \} \) is equal to \( \{ 21534, 23154 \} \) or \( \{ 23154, 21534 \} \). Both cases are similar, so assume the former. It is easy to see that no matter the type of the 4-edge at \( 21534 \), the vertex \( E_4(21534) \) does not admit a 3-neighbor. Hence the 3-4-string containing \( w \) is \( \{ E_4(21534), 21534, 23154, E_4(21534), E_3E_4(21534) \} \); see Fig. 3 (the vertices of \( G \) and types of the edges need not be as in the figure, but the numbers on the edges and the signatures of the words must be as in the figure). It follows that the signatures of the vertices of \( \text{Res}_{[2, 5]}(G, w) \) are \( (++, +-, +-, -, ++, +, +, -) \) and therefore its generating function is \( s_{(2, 2)}(x) + s_{(3, 1)}(x) \). A similar argument shows that this is also the generating function of \( \text{Res}_{[1, 4]}(G, w) \).

\( \square \)

### 4.3 Noncommutative flagged Schur functions

For the inductive computation of the noncommutative Schur functions \( \mathfrak{J}_\lambda(u) \) in the next subsection, we need their flagged generalization.
For any positive integer \(d\) and \(m \in \{0, 1, \ldots, N\}\), recall that
\[
e_d([m]) = \sum_{m \geq i_1 > i_2 > \cdots > i_d \geq 1} u_{i_1} u_{i_2} \cdots u_{i_d} \in \mathcal{U},
\]
where \([0] := \{\}\). Also recall \(e_0([m]) = 1\) and \(e_d([m]) = 0\) for \(d < 0\). Note that
\[
e_d([0]) = \begin{cases} 1 & \text{if } d = 0, \\ 0 & \text{otherwise}. \end{cases}
\]
We will use the following fact several times in the proof of Theorem 4.6 below:
\[
e_d([m]) = m e_{d-1}([m-1]) + e_{d}([m-1]) \quad \text{if } m > 0 \text{ and } d \text{ is any integer}. \tag{12}
\]
Given a weak composition \(\alpha = (\alpha_1, \ldots, \alpha_l)\) and \(n = (n_1, n_2, \ldots, n_l) \in \{0, 1, \ldots, N\}^l\), define the noncommutative column flagged Schur function \(J_\alpha(n) = J_\alpha(n)(u)\) by
\[
J_\alpha(n) = \sum_{\pi \in S_l} \text{sgn}(\pi) e_{\alpha_1 + \pi(1)-1}([n_1])e_{\alpha_2 + \pi(2)-2}([n_2]) \cdots e_{\alpha_l + \pi(l)-l}([n_l]).
\]
Note that if \(\lambda\) is a partition then \(J_\lambda(u) = J_{\lambda'}(N, N, \ldots, N)\), so the noncommutative column flagged Schur functions generalize the noncommutative Schur functions defined earlier.
It follows from Lemma 2.2 that
\[
J_\alpha(n) \equiv -J_{\alpha_1, \ldots, \alpha_{j-1}, \alpha_{j+1}-1, \alpha_j+1, \ldots, \alpha_l}(n) \pmod{I_{\text{KR}}^{\text{st}}} \quad \text{whenever } n_j = n_{j+1}. \tag{13}
\]
In particular,
\[
J_\alpha(n) \equiv 0 \pmod{I_{\text{KR}}^{\text{st}}} \quad \text{whenever } \alpha_j = \alpha_{j+1} - 1 \text{ and } n_j = n_{j+1}. \tag{14}
\]

### 4.4 Local Schur positivity of \(D_0\) graphs

We now prove that \(D_0\) graphs satisfy LSP4 and LSP5 by showing that certain noncommutative Schur functions are positive sums of monomials in \(\mathcal{U}/I_{\text{KR}}^{\text{st}}\).

We first review some terminology and fix conventions related to diagrams and tableaux. Partition diagrams are drawn with the English (matrix-style) convention so that row (resp. column) labels start with 1 and increase from north to south (resp. west to east). Let \(\lambda\) be a partition. A semistandard Young tableau \(T\) of shape \(\lambda\) is the diagram of \(\lambda\) together with a letter occupying each of its cells such that entries strictly increase from north to south in each column and weakly increase from west to east in each row. Write \(T_{r,c}\) for the entry of \(T\) in the \(r\)th row and \(c\)th column. The row reading word of \(T\), denoted \(\text{rowword}(T)\), is the word obtained by concatenating the rows of \(T\) (reading each row left to right), starting with the bottom row. The column reading
word of T, denoted colword(T), is the word obtained by concatenating the columns of T (reading each column bottom to top), starting with the leftmost column.

For example, rowword(\begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & \end{bmatrix}) = 53412 and colword(\begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{bmatrix}) = 52143.

For a partition \( \lambda \) and a tuple \( n = (n_1, \ldots, n_l) \) of nonnegative integers, let \( \text{SYT}(\lambda)^n \) denote the set of semistandard Young tableaux of shape \( \lambda \) having no repeated letter such that the entries in column \( c \) lie in \([n_c]\).

We now state and prove the full version of Theorem 1.3 from the introduction. It is similar to Theorems 17 and 19 of [14].

**Theorem 4.6** Let \( n = (n_1, n_2, \ldots, n_l) \) with \( 0 \leq n_1 \leq n_2 \leq \cdots \leq n_l \).

(i) Let \( \lambda \) be the hook shape \( (a, 1^b) \) \((a \geq 1, b = l - 1 \geq 0)\). Then in \( \mathcal{U}/I_{\text{st KR}}^\text{st} \),

\[
J_{\lambda}(n) = \sum_{T \in \text{SYT}(\lambda')^n} \text{colword}(T). \tag{15}
\]

(ii) If \( a \geq 2, \lambda = (a, 2) \), and \( l = 2 \), then in \( \mathcal{U}/I_{\text{st KR}}^\text{st} \),

\[
J_{\lambda}(n) = \sum_{T \in \text{SYT}(\lambda')^n, T_{1,2} > T_{2,1}} \text{colword}(T) + \sum_{T \in \text{SYT}(\lambda')^n, T_{1,2} < T_{2,1}} \text{rowword}(T). \tag{16}
\]

In particular, \( J_{\lambda}(u) \) is a positive sum of monomials in \( \mathcal{U}/I_{\text{st KR}}^\text{st} \) if \( \lambda \) is a hook shape or of the form \((a, 2)'\).

**Proof** Throughout the proof, we write \( x \equiv y \) to mean that \( x \) and \( y \) are congruent mod \( I_{\text{st KR}}^\text{st} \). We first prove (i). The proof is by induction on \( a, b, \) and the \( n_i \). If \( n_1 = 0 \), then the first row of the matrix \( \left[ e_{\lambda_{1,c}} + c - r([n_r]) \right]_{r,c \in [l]} \) is zero, and hence its determinant \( J_{\lambda}(n) \) is 0. The right side of (15) is certainly also 0 in this case because \( \text{SYT}(\lambda')^n \) is empty.

We now may assume \( n_1 > 0 \). Set \( n^- = (n_1 - 1, n_2, \ldots, n_l) \). First suppose \( a \geq 2 \). Then (12) yields

\[
J_{(a, 1^b)}(n) = n_1 J_{(a-1, 1^b)}(n^-) + J_{(a, 1^b)}(n^-) \equiv \sum_{T \in \text{SYT}(\lambda')^n, T_{a,1} = n_1} \text{colword}(T) + \sum_{T \in \text{SYT}(\lambda')^{n^-}} \text{colword}(T) = \sum_{T \in \text{SYT}(\lambda')^n} \text{colword}(T).
\]

The congruence is by induction on \( n_1 \). The last equality is by the fact that \( \{ T \in \text{SYT}(\lambda')^n | T_{a,1} = n_1 \} \sqcup \text{SYT}(\lambda')^{n^-} \) is a set partition of \( \text{SYT}(\lambda')^n \).
Now suppose \( a = 1 \). Applying (12), we obtain
\[
J_{(1,1^b)}(n) = n_1J_{(0,1^b)}(n^-) + J_{(1,1^b)}(n^-)
\]
\[
= n_1\left(J_{(1^b)}(n_2, n_3, \ldots) - J_{(1^b)}(n_1 - 1, n_3, \ldots)\right) + J_{(1,1^b)}(n^-)
\]
\[
\equiv \sum_{T \in SYT(\lambda')} \text{colword}(T) + \sum_{T \in SYT(\lambda')^n^-} \text{colword}(T)
\]
\[
= \sum_{T \in SYT(\lambda')^n} \text{colword}(T).
\]

Note that for \( \alpha = (0, 1^b) \), \( J_\alpha(n^-) \) is a (noncommutative version of) the determinant of the matrix \( \left[ e_{\alpha c + \epsilon - r}([n^- c]) \right]_{r, c \in [l]} \), which has first column \( [1 1 0 \cdots 0]^T \). The second equality then follows from computing this determinant by expanding along this column. The congruence is by induction on \( b \), and the last equality is by the fact that \( \{ T \in SYT(\lambda')^n \mid T_{1,1} = n_1 \} \sqcup SYT(\lambda')^n^- \) is a set partition of \( SYT(\lambda')^n \).

We now prove (ii). The statement for \( a > 2 \) reduces to the \( a = 2 \) case by a similar argument to the \( a \geq 2 \) case in the proof of (i). So we may assume \( \lambda = (2, 2) \).

For each subset \( S \) of \( \{ u_1, \ldots, u_N \} \), let \( (U/I_{K^R}^{st})_S \) denote the subspace of \( U/I_{K^R}^{st} \) spanned by the permutations of \( S \). By Proposition 2.7 (i) and the fact that \( U/I_{K^R}^{st} \) is the direct sum of the subspaces \( (U/I_{K^R}^{st})_S \), the result for general \( n \) reduces to the case \( n_1 \leq |\lambda| = 4 \). It therefore suffices to show
\[
J_\lambda(1, 4) \equiv 0, \quad (17)
\]
\[
J_\lambda(2, 4) \equiv 2143, \quad (18)
\]
\[
J_\lambda(3, 4) \equiv 2143 + 3412, \quad (19)
\]
\[
J_\lambda(4, 4) \equiv 2143 + 3412, \quad (20)
\]

since these right-hand sides are equal to
\[
\sum_{T \in SYT(\lambda')^{n_1 + 4}, T_{1,2} > T_{2,1}} \text{colword}(T) + \sum_{T \in SYT(\lambda')^{n_1 + 4}, T_{1,2} < T_{2,1}} \text{rowword}(T),
\]
for \( n_1 = 1, 2, 3, 4 \), respectively.

The verification of (17) and (18) is immediate from the definition of \( J_\lambda(n) \). For (19), we compute directly
\[
J_{22}(3, 4) = 2143 + 3412 + 3241 - 3214
\]
\[
= 2143 + 3412 + 3(14 - 41)2 + 32(41 - 14)
\]
\[
\equiv 2143 + 3412 + 32(14 - 41) + 32(41 - 14)
\]
\[
= 2143 + 3412.
\]

Finally, (20) follows from (19) and
\[
J_{22}(4, 4) = 4J_{12}(3, 4) + J_{22}(3, 4) \equiv 4J_{12}(3, 3) + J_{22}(3, 4) \equiv J_{22}(3, 4).
\]
Here, the first equality is by (12), the first congruence is because words with repeated letters are 0 in $U/I_{KR}$, and the second congruence is by (14).

The final ingredient to prove that $D_0$ graphs satisfy LSP$_4$ and LSP$_5$ is a result about how the noncommutative Schur functions behave under the anti-automorphism $\text{rev} : U/I_{KR} \rightarrow U/I_{KR}$ of Proposition 2.7 (iii).

The noncommutative homogeneous symmetric functions are given by

$$h_d(u) = \sum_{1 \leq i_1 \leq i_2 \leq \cdots \leq i_d \leq N} u_{i_1} u_{i_2} \cdots u_{i_d} \in U.$$ 

Let $\Lambda(u)$ be the subalgebra of $U/I_{KR}$ generated by $e_1(u), e_2(u), \ldots$, and let $\Lambda(x)$ denote the ring of symmetric functions in the commuting variables $x_1, x_2, \ldots$. By Lemma 2.2, there is an algebra homomorphism

$$\Psi : \Lambda(x) \rightarrow \Lambda(u), \quad e_d(x) \mapsto e_d(u).$$

Lemma 4.7 There holds $\Psi(h_d(x)) = h_d(u)$. Hence the $h_d(u)$ belong to $\Lambda(u)$ and pairwise commute in $U/I_{KR}$.

Proof By Theorem 4.6 (i), $\mathfrak{J}_d(u) = h_d(u)$ in $U/I_{KR}$. The first statement then follows from

$$\mathfrak{J}_d(u) = \det(e_{1 + j - i}(u)) = \Psi(\det(e_{1 + j - i}(x))) = \Psi(h_d(x)),$$

where the last equality is by the Jacobi–Trudi formula in the commuting variables $x_1, x_2, \ldots$. The concluding statement follows from the fact that the algebra $\Lambda(u)$ is commutative.

Proposition 4.8 In $U/I_{KR}$, there holds $\text{rev}(\mathfrak{J}_d(u)) = \mathfrak{J}_{d'}(u)$.

Proof By the version of the Jacobi–Trudi formula expressing $s_\lambda(x)$ in terms of the $h_d(x)$ and the version expressing $s_\lambda(x)$ in terms of the $e_d(x)$,

$$\det(h_{\lambda_i + j - i}(x)) = s_\lambda(x) = \det(e_{\lambda_i' + j - i}(x)). \quad (21)$$

The identity $\text{rev}(e_d(u)) = h_d(u)$ holds in $U/I_{KR}$ because of relation (3). Hence in $U/I_{KR}$,

$$\mathfrak{J}_{d'}(u) = \det(e_{\lambda_i + j - i}(u)) = \text{rev}(\det(h_{\lambda_i + j - i}(u))) = \text{rev}(\mathfrak{J}_d(u)).$$

The last equality is obtained by applying $\Psi$ to (21) and using Lemma 4.7.

Corollary 4.9 $D_0$ graphs satisfy LSP$_4$ and LSP$_5$.

Proof Let $H$ be the $K$-restriction of a $D_0$ graph for $K$ of size 4 or 5. Theorem 4.6 and Proposition 4.8 imply that $\mathfrak{J}_d(u)$ is a positive sum of monomials in $U/I_{KR}$ for all $\lambda$ of size $\leq 5$. Then by Corollary 3.3 and Remark 3.7, the generating function of each connected component of $H$ is Schur positive.
The following theorem summarizes the results of this section. The similar result [2, Theorem 6.1] is proved by a computer check.

**Theorem 4.10** $D_0$ graphs satisfy axioms 1, 2, 3, 4, 4’ and LSP$_4$ and LSP$_5$. Hence a $D_0$ graph is a $D$ graph if and only if it satisfies axioms 4’b and 5.

**Proof** Axiom 1 is built into the definition of a $D_0$ graph because if $w$ is a vertex of a $D_0$ graph, then

\[ w \text{ admits an } i\text{-neighbor} \iff w \text{ belongs to a KR}_i \text{ square} \iff \sigma_{i-1}(w) \neq \sigma_i(w). \]

Axiom 2 is also clear because Knuth and rotation transformations only involve three consecutive letters.

Axiom 4’a was proved in Proposition 4.5 and LSP$_4$ and LSP$_5$ were just proved in Corollary 4.9. Assuming axiom 1, axiom 3 is equivalent to the condition that any component of any $K$-restriction with $|K| = 4$ has more than 1 edge. This is implied by LSP$_4$ (for more about this, see [3, Remark 5.2]).

\[ \square \]

**5 LLT polynomials**

LLT polynomials are certain $q$-analogs of products of skew Schur functions, first defined by Lascoux, Leclerc, and Thibon in [15]. There are two versions of LLT polynomials (which we distinguish following the notation of [10]): the combinatorial LLT polynomials of [15] defined using spin and the new variant combinatorial LLT polynomials of [13] defined using inversion numbers. Although the theory of noncommutative Schur functions is well suited to studying the former (see [14]), we prefer to work with the latter to follow [3,4] and because inversion numbers are easier to calculate than spin.

In this section, we first recall an expression for LLT polynomials in terms of quasisymmetric functions from [3]. We then introduce a simplified version $\mathcal{U}_q/J^{1\text{Lam, st}}_k$ of Lam’s algebra of ribbon Schur operators from [14] and show how LLT polynomials and their Schur expansions can be interpreted in terms of this algebra. We then connect $\mathcal{U}_q/J^{1\text{Lam, st}}_k$ to the algebra $\mathcal{U}/I^{\text{st}}_{\text{KR}}$ and the graphs $\mathcal{G}^{(k)}_{c,D}$ defined by Assaf [3].

**5.1 LLT polynomials in terms of quasisymmetric functions**

Recall our conventions for partition diagrams from Sect. 4.4. A skew shape $\lambda/\mu$, where $\mu \subseteq \lambda$ are partitions, is the diagram obtained by removing the cells of $\mu$ from the diagram of $\lambda$. The content of a cell $(i,j)$ of a skew shape is $j - i$. A skew shape with contents is an equivalence class of skew shapes, where two skew shapes are equivalent if there is a content and order-preserving bijection between their diagrams. A $k$-tuple of skew shapes with contents is a $k$-tuple $\beta = (\beta^{(0)}, \ldots, \beta^{(k-1)})$ such that each $\beta^{(i)}$ is a skew shape with contents. The shifted content of a cell $z$ of $\beta$ is

\[ \tilde{c}(z) = k \cdot c(z) + i, \]

\[ \tilde{c}(z) = k \cdot c(z) + i, \]

\[ \tilde{c}(z) = k \cdot c(z) + i, \]

\[ \tilde{c}(z) = k \cdot c(z) + i, \]

\[ \tilde{c}(z) = k \cdot c(z) + i, \]

\[ \tilde{c}(z) = k \cdot c(z) + i, \]
when \( z \in \beta^{(i)} \) and where \( c(z) \) is the usual content of \( z \) regarded as a cell of \( \beta^{(i)} \).

For a \( k \)-tuple \( \beta = (\beta^{(0)}, \ldots, \beta^{(k-1)}) \) of skew shapes with contents such that each \( \beta^{(i)} \) contains no \( 2 \times 2 \) square and its shifted contents lie in \([N]\),

\[
\forall z \in \beta^{(i)} \text{ and where } c(z) \text{ is the usual content of } z \text{ regarded as a cell of } \beta^{(i)}.
\]

\[
\text{define } W'_k(\beta) \subseteq \mathcal{W} \text{ to be the set of words } v \text{ such that}
\]

- \( v \) is a rearrangement of the shifted contents of \( \beta \),
- for each \( i \) and each pair \( z, z' \) of cells of \( \beta^{(i)} \) such that \( z' \) lies immediately east or south of \( z \), the letter \( \tilde{c}(z) \) occurs before \( \tilde{c}(z') \) in \( v \).

Example 5.1 Let \( \beta \) be the 3-tuple \( \begin{array}{c} \begin{array}{c} 1 \end{array} \\ \begin{array}{c} 2 \end{array} \end{array}, \begin{array}{c} \begin{array}{c} 4 \end{array} \\ \begin{array}{c} 5 \end{array} \end{array}, \begin{array}{c} \begin{array}{c} 6 \end{array} \\ \begin{array}{c} 7 \end{array} \end{array} \end{array} = (2, 32, 33)/(1, 11, 21) \) of skew shapes with contents. Its shifted contents are

\[
\begin{array}{c} \begin{array}{c} 1 \end{array} \\ \begin{array}{c} 2 \end{array} \end{array}, \begin{array}{c} \begin{array}{c} 3 \end{array} \\ \begin{array}{c} 4 \end{array} \end{array}, \begin{array}{c} \begin{array}{c} 5 \end{array} \\ \begin{array}{c} 6 \end{array} \end{array} \end{array}.
\]

Some elements of \( W'_3(\beta) \), together with their 3-inversion numbers, are

\[
\begin{array}{|c|c|c|c|c|c|}
\hline
v & 2413857 & 3417285 & 4871235 & 8341275 & 2853417 \\
\hline
\text{inv}'_3(v) & 3 & 4 & 4 & 5 & 5 \\
\hline
\end{array}
\]

The next proposition is an adaptation of [3, Corollary 4.3], which expresses the new variant combinatorial LLT polynomials in terms of quasisymmetric functions. We take this as the definition of these polynomials; they were originally defined in [13] as a sum over \( k \)-tuples of semistandard tableaux with an inversion statistic. Be aware that the words used here are inverses of those used in [3]; see [4, §2.5–2.6] for details.

Proposition 5.2 ([4, Proposition 2.8]) Let \( \beta \) be a \( k \)-tuple of skew shapes with contents satisfying (22). The new variant combinatorial LLT polynomial indexed by \( \beta \) is

\[
G_{\beta}(x; q) = \sum_{v \in W'_k(\beta)} q^{\text{inv}'_k(v)} Q_{\text{Des}(v)}(x).
\]

Remark 5.3 There is a statement similar to Proposition 5.2 without the restriction (22) on \( \beta \); however in order to be compatible with the convention in this paper of only focusing on words with no repeated letter, we chose to simplify the discussion in this section to this special case. For the same reason, we work with a quotient of Lam’s algebra by the relation (3) instead of the original algebra defined by Lam. See [5] for the full treatment without this simplification.
5.2 Lam’s algebra of ribbon Schur operators

Lam [14] defines an algebra of ribbon Schur operators, which gives an elegant algebraic framework for LLT polynomials. It sets the stage for applying the theory of noncommutative Schur functions from [8] to the problem of computing Schur expansions of LLT polynomials. We now introduce a simplified version of this algebra and review how the Schur expansions of certain LLT polynomials can be interpreted using this algebra and Theorem 2.1.

Let \( \mathbb{Q}(q) \) be the field of rational functions in the indeterminate \( q \) with coefficients in \( \mathbb{Q} \) and let \( \mathcal{U}_q = \mathbb{Q}(q) \otimes_{\mathbb{Z}} \mathcal{U} \). Let \( \mathcal{U}_q / J_{\text{Lam}, \text{st}}^{1} \) be the quotient of \( \mathcal{U}_q \) by the following relations (let \( J_{\text{Lam}, \text{st}}^{1} \) denote the corresponding two-sided ideal of \( \mathcal{U}_q \)):

\[
\begin{align*}
ac &= ca & \text{for } c - a > k, \quad (23) \\
ab &= q^{-1}ba & \text{for } 0 < b - a < k, \quad (24) \\
w &= 0 & \text{for words } w \text{ with a repeated letter.} \quad (25)
\end{align*}
\]

The new variant \( q \)-Littlewood–Richardson coefficients, denoted \( c_{\lambda}^\beta(q) \), are the coefficients of the Schur expansion of the new variant combinatorial LLT polynomials, i.e.,

\[
G_{\beta}(x; q) = \sum_{\lambda} c_{\lambda}^\beta(q) s_{\lambda}(x).
\]

The new variant \( q \)-Littlewood–Richardson coefficients are known to be polynomials in \( q \) with nonnegative integer coefficients [10, 17]. We now express these coefficients (or rather, the subset of them that fit with our simplified setup) using the theory of noncommutative Schur functions as was done in [14].

**Proposition 5.4** Let \( \beta \) be a \( k \)-tuple of skew shapes with contents satisfying (22). Then

\[
f := \sum_{v \in W_k'(\beta)} q^{\text{inv}'(v)} v \in (J_{k}^{\text{Lam}, \text{st}})^{\perp},
\]

and the new variant combinatorial LLT polynomial can be written as

\[
G_{\beta}(x; q) = \Delta(f).
\]

Hence the new variant \( q \)-Littlewood–Richardson coefficient is given by

\[
c_{\lambda}^\beta(q) = \langle \mathfrak{J}_\lambda(u), f \rangle.
\]

**Proof** For the first statement, we must show that \( \langle v(ca - ac)w, f \rangle = 0 \), for any \( c - a > k \) (as in (23)) and words \( v, w \). This is clear since \( \text{inv}'(vcaw) = \text{inv}'(vacw) \), and \( vcaw \in W_k'(\beta) \) if and only if \( vacw \in W_k'(\beta) \). We must also show that \( \langle v(qab - ba)w, f \rangle = 0 \), for any \( 0 < b - a < k \) (as in (24)) and words \( v, w \). This holds because
vabw ∈ W′_k(β) if and only if vbaw ∈ W′_k(β), and

\[ q^{-\text{inv}'_k(vabw)}(v(ab - ba)w, f) = q^{-\text{inv}'_k(vabw)}vabw - q^{-\text{inv}'_k(vabw)}vbaw, f = 0, \]

where the first equality is by \( \text{inv}'_k(vabw) = \text{inv}'_k(vbaw) - 1 \).

The second statement is immediate from the definition of \( G_\beta(x; q) \) (Proposition 5.2) and \( \Delta \).

For the last statement, it is not hard to show that the relations (23)–(25) imply the relations (2)–(3), and hence \( U_q/J_{k,\text{st}}^\text{Lam} \) is a quotient of \( \mathbb{Q}(q) \otimes_{\mathbb{Z}} (U/I_{k,\text{KR}}) \) (see the proof of Proposition 5.7). Hence the last statement follows from Lemma 2.2 and an easy modification of Theorem 2.1 to the coefficient field \( \mathbb{Q}(q) \). \( \square \)

Though working with the algebra \( U_q/J_{k,\text{st}}^\text{Lam} \) over \( \mathbb{Q}(q) \) is particularly convenient for expressing \( q \)-Littlewood Richardson coefficients as in Proposition 5.4, to relate to Assaf’s work it is convenient to have a version of this algebra without the \( q \). Accordingly, define \( I_{k,\text{st}}^\text{Lam} := U \cap J_{k,\text{st}}^\text{Lam} \subseteq U_q \), where \( U \subseteq U_q \) is the \( \mathbb{Z} \)-subalgebra of \( U_q \) generated by 1 and the \( u_i \).

**Proposition 5.5** The nonzero equivalence classes of \( U/I_{k,\text{st}}^\text{Lam} \) are

\[ \{ v \in W'_k(\beta) \mid \text{inv}'_k(v) = t \} \]

for \( \beta \) as in (22) and \( t \in \mathbb{N} \) such that this set is nonempty.

**Proof** Since applying a relation (23) or (24) to a word does not change the relative position of two letters that differ by \( k \), it follows that if \( v \equiv w \mod I_{k,\text{st}}^\text{Lam} \), then \( \text{inv}'_k(v) = \text{inv}'_k(w) \), and \( v \) and \( w \) belong to the same \( W'_k(\beta) \) for some \( \beta \). Hence each set \( \{ v \in W'_k(\beta) \mid \text{inv}'_k(v) = t \} \) is a union of nonzero equivalence classes. To see that this is actually a nonzero equivalence class, observe that any word in \( W'_k(\beta) \) can be transformed into a power of \( q \) times the word \( w(\beta) \) by a sequence of applications of (23) and (24). Here,

\[ w(\beta) := w^0w^1 \cdots w^{k-1}, \]

where \( w^j \) is the word obtained by reading the shifted contents of \( \beta^{(j)} \) along antidiagonals, starting from the northwesternmost and reading each antidiagonal from southwest to northeast. For the \( \beta \) in Example 5.1, \( w^0 = 3, w^1 = 417, w^2 = 285, \) and \( w(\beta) = 3417285 \). Therefore, if \( x, y \in \{ v \in W'_k(\beta) \mid \text{inv}'_k(v) = t \} \), then

\[ x \equiv q^{\text{inv}'_k(x) - \text{inv}'_k(w(\beta))}w(\beta) = q^{\text{inv}'_k(y) - \text{inv}'_k(w(\beta))}w(\beta) \equiv y \mod J_{k,\text{st}}^\text{Lam}. \]

Hence \( x \equiv y \mod J_{k,\text{st}}^\text{Lam} \). \( \square \)

### 5.3 Assaf’s LLT bijectivizations

We now relate Lam’s [14] algebraic approach to studying LLT polynomials to Assaf’s [3] approach using D graphs. To do this, we first define the following bijectivizations
of $U/I_{st}^{\text{KR}}$ and related D₀ graphs. Let $U/I_k^{\text{Assaf}, \text{st}}$ denote the quotient of $U$ by the following relations (let $I_k^{\text{Assaf}, \text{st}}$ denote the corresponding two-sided ideal of $U$):

$$\begin{align*}
\text{bac} &= \text{bca} \quad \text{for } c - a > k \text{ and } a < b < c, \\
\text{acb} &= \text{cab} \quad \text{for } c - a > k \text{ and } a < b < c, \\
\text{bac} &= \text{acb} \quad \text{for } c - a \leq k \text{ and } a < b < c, \\
\text{bca} &= \text{cab} \quad \text{for } c - a \leq k \text{ and } a < b < c, \\
w &= 0 \quad \text{for words } w \text{ with a repeated letter.}
\end{align*}$$

(26) (27) (28) (29) (30)

It is easy to see that these relations imply the relations (2)–(3), and hence $U/I_{st}^{\text{Assaf}, \text{st}}$ is a bijectivization of $U/I_{st}^{\text{KR}}$. These algebras generalize the plactic algebra since $U/I_{st}^{\text{Assaf}, 1} = U/I_{\text{plac}}^{\text{st}}$ (see Example 2.4).

**Definition 5.6** Define $G_{st}^{\text{st}}$ to be the D₀ graph on the vertex set $W$ such that

the type of the KR square $v[abc]w$ of $G_{st}^{\text{st}}$ is

$$\begin{cases}
\text{Knuth} & \text{if } c - a > k, \\
\text{rotation} & \text{if } c - a \leq k.
\end{cases}$$

We define an Assaf LLT $k$ D graph to be a union of connected components of $G_{st}^{\text{st}}$.

By construction, the nonzero equivalence classes of $U/I_{st}^{\text{Assaf}, \text{st}}$ (see Sect. 2.4) are the components of $G_{st}^{\text{st}}$.

**Proposition 5.7** The algebra $U/I_{k}^{\text{Lam}, \text{st}}$ is a quotient of $U/I_k^{\text{Assaf}, \text{st}}$.

**Proof** Clearly, the relations (26) and (27) are implied by (23). Next, we compute using (24) twice,

$$\text{bac} \equiv \text{qabc} \equiv \text{acb} \mod J_{k}^{\text{Lam}, \text{st}} \quad \text{for } c - a \leq k \text{ and } a < b < c.$$  

It follows that (28) holds in $U/I_{k}^{\text{Lam}, \text{st}}$. The relation (29) is similar. □

By the previous proposition, each nonzero equivalence class $\{v \in W'_k(\beta) \mid \text{inv}'_k(v) = t\}$ of $U/I_{k}^{\text{Lam}, \text{st}}$ is a union of nonzero equivalence classes of $U/I_k^{\text{Assaf}, \text{st}}$. This means that each set $\{v \in W'_k(\beta) \mid \text{inv}'_k(v) = t\}$ with $\beta$ and $t$ as in Proposition 5.5 is the vertex set of a union of connected components of $G_{k}^{\text{st}}$, define $G_{k}^{\text{st}}(\beta, t)$ to be this union of components.

We can now rephrase the connection between the graphs $G_{k}^{\text{st}}$ and LLT polynomials from [3, §4.2] in our language:

**Corollary 5.8** Let $\beta$ be as in (22). There holds $\sum_{v \in W'_k(\beta), \text{inv}'_k(v) = t} v \in (I_k^{\text{Assaf}, \text{st}}) \perp$. The expression for LLT polynomials from Proposition 5.4 can be rewritten as

$$G_{\beta}(x; q) = \sum_{t} q^t \Delta\left( \sum_{v \in W'_k(\beta), \text{inv}'_k(v) = t} v \right) = \sum_{t} q^t (\text{gen. function of } G_{k}^{\text{st}}(\beta, t)).$$
For each \( k \)-tuple \( \beta \) of skew shapes with contents satisfying (22), the graph \( \bigsqcup \mathcal{G}^\text{st}_k(\beta, t) \) is isomorphic to the graph \( \mathcal{G}^{(k)}_{c,D} \) defined in [3, §4.2] as a signed, colored graph, where \( c, D \) are the content vector and \( k \)-descent set corresponding to \( \beta \) as in [3, Equation 4.2] (see also [4, Proposition 2.6]).

It is clear that the \( \mathcal{G}^\text{st}_k \) satisfy axiom 5, and it is shown in [3] that the graphs \( \mathcal{G}^{(k)}_{c,D} \) and hence the \( \mathcal{G}^\text{st}_k \) satisfy axiom \( 4'b \).

**Theorem 5.9** ([3, Theorem 5.38]) The \( D_0 \) graphs \( \mathcal{G}^\text{st}_k \) are \( D \) graphs. Hence, as their name suggests, the Assaf LLT \( k \) \( D \) graphs are \( D \) graphs.

**Example 5.10** Figure 4 depicts the graph \( \bigsqcup \mathcal{G}^\text{st}_3(\beta, t) \) for \( \beta = (2/1, 22/11, 2) \). Hence by Corollary 5.8,

\[
\mathcal{G}_{\beta}(x; q) = q^2 s_{41} + q^3(s_{32} + s_{311}) + q^4(s_{311} + s_{221}) + q^5 s_{2111}.
\]

### 6 Linear programming and Schur positivity

Here, we state and prove the full version of Theorem 1.4 from the introduction, which relates the monomial positivity of \( \mathcal{J}_\lambda(u) \) in a quotient of \( \mathcal{U}/I^\text{st}_{\mathcal{KR}} \) to the Schur positivity of generating functions of certain \( D_0 \) graphs. Its proof uses linear programming duality.

#### 6.1 Background on linear programming

We review some terminology related to linear programs. A good reference for this background is [19, Chapter 7].

Let \( A \) be a \( t \times m \) real matrix and \( \mathbf{b} \in \mathbb{R}^t \), \( \mathbf{c} \in \mathbb{R}^m \) be column vectors. The linear program LP associated to these data is the optimization problem minimize \( \mathbf{c}^T \mathbf{x} \) over all \( \mathbf{x} \in \mathbb{R}^m \) satisfying the linear constraints
The linear program dual to LP, denoted \( LP^\vee \), is to maximize \( b^T y \) over all \( y \in \mathbb{R}^t \) satisfying the linear constraints
\[
A^T y \leq c, \\
y \geq 0.
\]

A solution of a linear program is a vector satisfying the stated constraints (e.g., \( x \in \mathbb{R}^m \) is a solution of LP if and only if \( Ax \geq b, \ x \geq 0 \)). The feasible region is the set of all solutions. A linear program is feasible if the feasible region is nonempty and infeasible otherwise. A linear program whose objective is to minimize \( c^T x \) is bounded if this quantity is bounded below as \( x \) ranges over the feasible region. Similarly, a linear program whose objective is to maximize \( b^T y \) is bounded if this quantity is bounded above as \( y \) ranges over the feasible region.

**Theorem 6.1** (Duality Theorem) Exactly one of the following is true for the linear program LP and its dual \( LP^\vee \):
- LP and \( LP^\vee \) are feasible and bounded and
  \[
  \min\{c^T x \mid Ax \geq b, \ x \geq 0\} = \max\{b^T y \mid A^T y \leq c, \ y \geq 0\}.
  \]
- LP is unbounded and \( LP^\vee \) is infeasible.
- \( LP^\vee \) is unbounded and LP is infeasible.
- LP and \( LP^\vee \) are infeasible.

If the first bullet point holds above, then \( \min\{c^T x \mid Ax \geq b, \ x \geq 0\} \) is the optimal value of LP; any solution \( x^* \) of LP such that \( c^T x^* \) equals the optimal value is an optimal solution. Similarly, an optimal integer solution of LP is an integer vector \( x^* \) such that \( c^T x^* \) is the minimum of \( c^T x \) over all integer vectors \( x \) in the feasible region; this minimum value is the optimal integer value of LP. We use similar terminology for the dual.

### 6.2 Linear programs for monomial positivity of \( \mathcal{J}_\lambda(u) \)

Below we define three linear programs \( LP_\cap, LP_\cap=, \) and \( LP_\cap^\vee \), and then in Theorem 6.2 we relate them to the problem of expressing \( \mathcal{J}_\lambda(u) \) as a positive sum of monomials in a quotient of \( \mathcal{U}/T_{KR}^d \). We must first fix some notation.

Throughout this subsection, fix a positive integer \( d \) and a partition \( \lambda \) of \( d \). Let \( U_d \) denote the degree \( d \) homogeneous component of \( \mathcal{U} \), and for any homogeneous ideal \( J \) of \( \mathcal{U} \), let \( J_d \) denote the degree \( d \) homogeneous component of \( J \). Let \( w^1, \ldots, w^m \) be the words of \( \mathcal{U} \) of length \( d \). We work in the vector space \( \mathbb{R}\mathcal{U}_d := \mathbb{R} \otimes_{\mathbb{Z}} \mathcal{U}_d \cong \mathbb{R}^m \) and identify any vector \( x \in \mathbb{R}^m \) with the element \( \sum x_i w^i \in \mathbb{R}\mathcal{U}_d \). In particular, the element \( \mathcal{J}_\lambda(u) \in \mathcal{U}_d \) is identified with a vector in \( \mathbb{R}^m \).

Let \( J^{(1)}, \ldots, J^{(l)} \) be ideals of \( \mathcal{U} \) such that for each \( j \in [l] \)
• the quotient $U/J^{(j)}$ is a bijectivization of $U/I_{KR}^{st}$,
• the union of the nonzero equivalence classes of $U/J^{(j)}$ of degree $d$ is $\mathcal{W}_d$.

For each $j \in [l]$, let $h_1^{(j)}, \ldots, h_{t_j}^{(j)}$ be the $\mathbb{Z}$-basis of $(J_d^{(j)})^\perp$ described in Sect. 2.4; each $h_i^{(j)}$ is a zero-one vector (in the basis $w^1, \ldots, w^m$) whose support is a nonzero equivalence class of $U/J^{(j)}$.

We next define matrices and vectors for the linear programs. Let $A$ be the $((\sum t_j) \times m)$ matrix given by

\[
A = \begin{bmatrix}
A_1 \\
A_2 \\
\vdots \\
A_l
\end{bmatrix}, \quad \text{where } A_j = \begin{bmatrix}
-h_1^{(j)} \\
\vdots \\
-h_{t_j}^{(j)}
\end{bmatrix}.
\]

Define the column vector $b \in \mathbb{R}^{\sum t_j}$ by

\[
b = \begin{bmatrix}
b^1 \\
b^2 \\
\vdots \\
b^l
\end{bmatrix}, \quad \text{where } b^j = A_j \tilde{J}_\lambda(u) = \begin{bmatrix}
\langle \tilde{J}_\lambda(u), h_1^{(j)} \rangle \\
\vdots \\
\langle \tilde{J}_\lambda(u), h_{t_j}^{(j)} \rangle
\end{bmatrix} \in \mathbb{R}^{t_j}.
\]

Let $c \in \mathbb{R}^m$ be the zero-one vector whose support is $\mathcal{W}_d$, i.e.,

\[
c_i = \begin{cases}
1 & \text{if } w^i \in \mathcal{W}_d, \\
0 & \text{if } w^i \notin \mathcal{W}_d.
\end{cases}
\]

The linear program $LP_\cap$ is to minimize $c^T x$ over all $x \in \mathbb{R}^m$ satisfying

\[
Ax \geq b, \\
x \geq 0.
\]

Define the linear program $LP_{\cap,=}$ to be the same as $LP_\cap$ except with the constraint $Ax \geq b$ replaced by $Ax = b$.

The linear program dual to $LP_\cap$, denoted $LP_{\cap}^\vee$, is to maximize $b^T y$ over all $y \in \mathbb{R}^{\sum t_j}$ satisfying

\[
A^T y \leq c, \\
y \geq 0.
\]

**Theorem 6.2** Maintain the notation above. In particular, we are assuming that $d$ and $\lambda$ have been fixed and for each $j \in [l]$, $U/J^{(j)}$ is a bijectivization of $U/I_{KR}^{st}$.

Let $J = \bigcap J^{(j)}$. Recall that $w^1, \ldots, w^m$ are the words of $U_d$. Let $\mathbb{R}_{\geq 0}^m$ denote the polyhedron $\{ \sum_i x_i w^i \mid x_i \geq 0 \} \subseteq \mathbb{R}U_d$. Set $M = c^T \tilde{J}_\lambda(u)$. The following are equivalent:
\((i)\) \(J_\lambda(u)\) lies in the image of \(\mathbb{R}^m_{\geq 0}\) in \(\mathbb{R}U_d/\mathbb{R}J_d\).

\((ii)\) The linear program \(\text{LP}_{\cap}\) is feasible.

\((iii)\) The linear program \(\text{LP}_\cap\) has optimal value \(M\).

\((iv)\) The linear program \(\text{LP}_\vee\cap\) has optimal value \(M\).

\((v)\) For every \(g \in \sum_j ((\mathbb{R}J_d)^j)^- \cap \mathbb{R}^m_{\geq 0}\) such that \(g \leq c\), \(\langle J_\lambda(u), c - g \rangle \geq 0\).

Statement \((i)\) is another way of saying that \(J_\lambda(u)\) is a positive real sum of monomials in \(\mathbb{R} \otimes \mathbb{Z} U_d/\mathbb{R}d\). Note that \((\mathbb{R}J_d)^- = \sum_j ((\mathbb{R}J_d)^j)^-\) and \(c \in J_d^+\), and hence \((v)\) says that \(\langle J_\lambda(u), f \rangle \geq 0\) for certain \(f\) that are a positive real sum of monomials and lie in \((\mathbb{R}J_d)^+\). Thus \((i)\) certainly implies \((v)\), but the converse is not obvious. This theorem therefore provides us with a deeper understanding of the key ingredient required for the Fomin–Greene approach (see the discussion at the end of Sect. 2.3).

**Proof** First note that \(J_d(j) = \ker(A_j)\), i.e., \(J_d(j) = \{x \in U_d \mid A_j x = 0\}\). Hence \(J_d = \ker(A)\). There also holds \(A J_\lambda(u) = b\) by (31).

We therefore have, for \(x \in \mathbb{R}^m\),

\[
\begin{align*}
x \text{ is a solution of } \text{LP}_{\cap,} & \iff A (J_\lambda(u) - x) = 0 \text{ and } x \geq 0 \\
& \iff J_\lambda(u) - x \in \mathbb{R}J_d \text{ and } x \geq 0.
\end{align*}
\]

This proves the equivalence of \((i)\) and \((ii)\).

To prove that \((ii)\) and \((iii)\) are equivalent, we first establish some basic facts. The rows of \(A_j\) are the nonzero equivalence classes of \(U_d/\mathbb{R}J_d(j)\) of degree \(d\) and a \(\mathbb{Z}\)-basis of \((\mathbb{R}J_d(j))^-\). Hence

\[
\begin{align*}
1^T A_j &= c^T, \\
1^T b^j &= 1^T A_j J_\lambda(u) = c^T J_\lambda(u) = M, \\
c &\in (J_d(j))^+ \subseteq J_d^+,
\end{align*}
\]

where \(1 \in \mathbb{R}^{t_j}\) denotes the all-ones vector.

We now prove \((iii)\) implies \((ii)\). Suppose \(\text{LP}_{\cap}\) has an optimal solution \(x^*\) with optimal value \(M = c^T x^*\). We must show that \(A_j x^* = b^j\). By (33), the inequality \(b^j \leq A_j x^*\), and (32) we obtain

\[
M = 1^T b^j \leq 1^T A_j x^* = c^T x^* = M,
\]

so the inequality is an equality. It follows that \(A_j x^* = b^j\), as desired.

To prove \((ii)\) implies \((iii)\), suppose \(x\) is a solution of \(\text{LP}_{\cap,}\). By the proof of the equivalence of \((i)\) and \((ii)\), \(J_\lambda(u) - x \in \mathbb{R}J_d\). Hence by (34), \(c^T (J_\lambda(u) - x) = 0\), which gives \(c^T x = c^T J_\lambda(u) = M\). Hence \(\text{LP}_{\cap}\) has optimal value \(M\). To see that \(\text{LP}_{\cap}\) has optimal value \(\geq M\), we compute using (33) and (32) that for any solution \(x\) of \(\text{LP}_{\cap}\),

\[
M = 1^T b^j \leq 1^T A_j x = c^T x.
\]
Statements (iii) and (iv) are equivalent by the Duality Theorem since LP∩ and LP∨ are always feasible: LP∩ is always feasible because Ax ≥ b whenever the xi are sufficiently large, and LP∨ is always feasible because y = 0 is always a solution.

To prove the equivalence of (iv) and (v), we first claim that as y ranges over the feasible region of LP∨, the vector g = ATy ∈ Rm ranges over

\[ \left( \sum _{j} \left( (\mathbb{R} J_d^{(j)})^\perp \cap \mathbb{R}_m^m \right) \right) \cap \{ z \in \mathbb{R}_m^m \mid z \leq c \}. \]

This follows from the fact that the rows of A_j are the nonzero equivalence classes of U/I^{(j)} of degree d and hence are a monoid basis of \( (\mathbb{R} J_d^{(j)})^\perp \cap \mathbb{R}_m^m \).

Let g = ATy. We compute using A\( J_\lambda(u) = b \),

\[ \langle J_\lambda(u), g \rangle = g^T J_\lambda(u) = y^T A J_\lambda(u) = y^T b. \]

We conclude that

\[ \langle J_\lambda(u), c - g \rangle = M - b^T y \geq 0 \iff b^T y \leq M. \quad (35) \]

Hence by (35) and the claim above, every solution y of LP∨ has b^T y ≤ M if and only if (v) holds. Moreover, if we let y be the vector with a 1 in its first t1 coordinates and 0’s elsewhere, then g = ATy = c and b^T y = M, so LP∨ has optimal value ≥ M. Hence (iv) is equivalent to the statement that LP has optimal value ≤ M, and we just showed this to be equivalent to (v).

7 A D graph whose generating function is not Schur positive

For this section, we set N = 8 so that U = \( \mathbb{Z}\langle u_1, \ldots, u_8 \rangle \). Let LLTLP8 be the linear program LP∨ from Theorem 6.2 with d = 8, \( \lambda = (2, 2, 2, 2) \), and the following bijectivizations of U/I_{\text{KR}}^st:

\[ U/J^{(k)} = U/I_{k}^{\text{Lam},st} \text{ for } k = 1, 2, \ldots, 8, \text{ and } U/J^{(9)} = U/I_{\text{plac}}^\text{st}. \]

The bijectivizations U/I_k^{\text{Lam},st} and U/I_{\text{plac}}^\text{st} are defined in Sect. 5.2 and Example 2.4, respectively.

We will see that an optimal integer solution of LLTLP8 yields a D0 graph whose generating function is not Schur positive. We go on to construct a D graph on the same vertex set as this D0 graph.

7.1 The linear program LLTLP8

Here is some specific data about the linear program LLTLP8. Since we are optimizing b^T y, we may delete all entries of b that are 0 and delete the corresponding rows of A.

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Also, since all of the columns of $A$ and entries of $c$ corresponding to $w \notin \mathcal{W}_{d}$ are zero, we may as well delete these columns and entries. Let $A', A'_i, b', c'$, etc., denote the matrices and vectors associated to this smaller linear program obtained by removing zeros, and let this linear program be $\text{LLTLP}'_{8}$. Note that $c'$ is the all-ones vector. Also note that $A'$ has columns indexed by $\mathcal{W}_{d} = S_{8}$; assume we have fixed some ordering $v_{1}, \ldots, v_{8}$ of $S_{8}$ which labels these columns.

To give an idea of the size of this linear program, here are the $b'_{i}$:

\[
\begin{align*}
(b'_{1})^{T} & = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix} \\
(b'_{2})^{T} & = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix} \\
(b'_{3})^{T} & = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix} \\
(b'_{4})^{T} & = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix} \\
(b'_{5})^{T} & = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix} \\
(b'_{6})^{T} & = \begin{bmatrix} 1 & 2 & 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix} \\
(b'_{7})^{T} & = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 2 & 1 \end{bmatrix} \\
(b'_{8})^{T} & = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix} \\
(b'_{9})^{T} & = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}
\end{align*}
\]

The rows of $A'_{9}$ correspond to the Knuth equivalence classes of shape $(2, 2, 2, 2)$ contained in $S_{8}$. More precisely, the rows of $A'_{k}$ are in bijection with $\text{SYT}(2, 2, 2, 2)$ so that the row labeled by $T \in \text{SYT}(2, 2, 2, 2)$ is the zero-one vector of length $8!$ whose support is \{ $i \in \{1, 2, \ldots, 8!\}$ \mid $P(v^{i}) = T$ \}. Here, $\text{SYT}(2, 2, 2, 2)$ denotes the set of standard Young tableaux of shape $(2, 2, 2, 2)$. For $k \leq 8$, the rows of $A'_{k}$ correspond to certain equivalence classes from Proposition 5.5.

### 7.2 Solving $\text{LLTLP}_{8}$

A weighted packing linear program is a linear program of the form: maximize $b^{T}y$ over the vectors $y \in \mathbb{R}^{t}$ satisfying

\[
A^{T}y \leq 1,
\]

\[
y \geq 0,
\]

where $A$ has entries in $\{0, 1\}$ and has nonzero rows, and $b$ has entries in $\mathbb{N}$. Let $S_{i}$ denote the support of the $i$th row of $A$. The integer solutions of this linear program correspond to packings of the $S_{i}$, i.e., collections of $S_{i}$ such that no two intersect. The optimization problem is to find a packing of maximum weight, where the weight of a packing \{ $S_{i}$ \mid $I \subseteq \{1, \ldots, t\}$ \} is $\sum_{i \in I} b_{i}$.

Any weighted packing linear program $\text{LP}_{\text{pack}}$ can be converted into a maximum independent set problem as follows: Let $A, b, S_{i}$ be the data associated to $\text{LP}_{\text{pack}}$ as above. Define $G(A, b)$ to be the graph with

- vertex set $V := \bigsqcup_{i=1}^{t} V_{i}$, where $V_{i}$ is a set of size $b_{i}$,
- edges between all vertices in $V_{i}$ and all vertices in $V_{j}$ if $S_{i} \cap S_{j} \neq \emptyset$ and $i \neq j$,
- no edge between any vertex in $V_{i}$ and any vertex in $V_{j}$ if $S_{i} \cap S_{j} = \emptyset$,
- no edge between any two vertices of $V_{i}$.
Define a map $\Theta$ by

$$\Theta : \{0, 1\}^t \rightarrow \text{subsets of } V, \quad y \mapsto \bigcup_{\{i \in [t] \mid y_i = 1\}} V_i.$$ 

**Proposition 7.1** Maintain the notation above. The map $\Theta$ yields a bijection between integer solutions of $\text{LP}_{\text{pack}}$ and independent sets of $G(A, b)$ that intersect each $V_i$ in all of $V_i$ or not at all. Moreover, $y^*$ is an optimal integer solution of $\text{LP}_{\text{pack}}$ if and only if $\Theta(y^*)$ is a maximum independent set of $G(A, b)$.

**Proof** First note that any integer solution of $\text{LP}_{\text{pack}}$ is a zero-one vector. The first statement then follows from the following chain of equivalences. For any $y \in \{0, 1\}^t$,

$$A^T y \leq 1$$

$$\iff S_i \cap S_j = \emptyset\text{ for each pair } i, j \text{ of distinct indices in the support of } y$$

$$\iff \text{there is no edge between } \Theta(y) \cap V_i \text{ and } \Theta(y) \cap V_j \text{ for all } i, j.$$ 

The second statement then follows from $b^T y = |\Theta(y)|$. \qed

For the linear program $\text{LLTL}_8'$, $b' \in \mathbb{N}^{121}$ and $G(A', b')$ has 126 vertices. The maximum size of an independent set is 15. This computation takes 1–2 s on a machine with a 32-core, 2.7 GHz processor and 25 GB of RAM using the branch and bound algorithm [7] built into Magma [6]. Hence by Proposition 7.1, $\text{LLTL}_8'$ has optimal integer value 15 and its optimal integer solutions are in bijection with independent sets of $G(A', b')$ of size 15.

### 7.3 An optimal integral solution of LLTL8

There are many optimal integer solutions of $\text{LLTL}_8'$. We now describe one such solution $y^*$ in detail and its consequences for Schur positivity of $D_0$ graphs.

Recall that the rows of $A'$ and rows of $y^*$ are naturally labeled by certain nonzero equivalence classes of the $U/J^{(i)}$. The solution $y^*$ is a zero-one vector whose support corresponds to the following equivalence classes: 13 of the 14 Knuth equivalence classes of shape $(2, 2, 2, 2)$, an equivalence class of $U/I_3^\text{Lam, st}$, and an equivalence class of $U/I_7^\text{Lam, st}$, with precise descriptions given by (36), (37), and (38), respectively.

\[
\begin{align*}
\{ w \in S_8 \mid P(w) \text{ has shape } (2, 2, 2, 2), \ P(w) \neq \begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \\ 7 & 8 \end{bmatrix} \} & \quad \text{(size } 13 \cdot 14), \quad (36) \\
\{ w \in S_8 \mid w \in W'_3(\beta_3), \ \text{inv}'_3(w) = 9 \} & \quad \text{(size } 126), \quad (37) \\
\{ w \in S_8 \mid w \in W'_7(\beta_7), \ \text{inv}'_7(w) = 18 \} & \quad \text{(size } 316), \quad (38)
\end{align*}
\]
where $\beta_3$ (resp. $\beta_7$) is the 3-tuple (resp. 7-tuple) of skew shapes with contents given by

$$\beta_3 = (33, 333, 333)/(22, 222, 222).$$

Its shifted contents are $\left(\begin{array}{ccc}
6 & 7 & 8 \\
3 & 4 & 5 \\
1 & 2 & 1
\end{array}\right)$. 

$$\beta_7 = (2, 2, 1, 1, 1, 1, 1)/(1, \emptyset, \emptyset, \emptyset, \emptyset, \emptyset).$$

Its shifted contents are $\left(\begin{array}{cccccccc}
7 & 1 & 8 & 2 & 3 & 4 & 5 & 6
\end{array}\right)$. 

For example, the equivalence class $(37)$ contains $78634521$ and the equivalence class $(38)$ contains $75183642$. 

Let $W^* \subseteq S_8$ be the union of the equivalence classes $(36)$, $(37)$, and $(38)$. Set $\bar{W}^* = S_8 \setminus W^*$. Let $g^* = A^Ty^*$, the zero-one vector (in the basis $\mathbf{v}^1, \ldots, \mathbf{v}^8$) whose support is $W^*$, which may be identified with the element $\sum_{w \in W^*} w \in U_8$. Let $f^* = c^* - g^* = \sum_{w \in W^*} w \in U_8$. Note that $f^*, g^* \in J^\perp$ and since the $U/J^{(j)}$ are bijectivizations of $U/I_{KR}^{st}. J^\perp \subseteq (I_{KR}^{st})^\perp$. Hence $W^*$ and $\bar{W}^*$ are KR sets. 

For the linear program LLTLP$_8$, the $M$ from Theorem 6.2 is given by $M = c^T_J(\mu) = |SYT(2, 2, 2, 2)| = 14$. Since LLTLP$_8$ has optimal value $\geq 15$, (iv) from Theorem 6.2 is false, and hence (i)–(v) are all false. This has two important consequences, which we summarize in the corollaries below. A further consequence will be discussed in Sect. 8. 

**Corollary 7.2** The generating function $\Delta(f^*)$ of $f^*$ is not Schur positive. Moreover, by Proposition–Definition 3.2, there is a $D_0$ graph on the vertex set $\bar{W}^*$ whose generating function is not Schur positive. 

To see in more detail why $\Delta(f^*)$ is not Schur positive, we compute as in the proof of Theorem 6.2:

$$\langle \mathfrak{J}(2,2,2,2)(\mathbf{u}), f^* \rangle = M - \langle \mathfrak{J}(2,2,2,2)(\mathbf{u}), g^* \rangle = M - y^Tb' = M - 15 = -1. $$

Hence the coefficient of $s_{(2,2,2,2)}(\mathbf{x})$ in $\Delta(f^*)$ is $-1$. It may also be instructive to see the Schur expansions of $\Delta(g^*)$ and $\Delta(f^*)$ in full:

$$\Delta(g^*) = s_{41111} + s_{32211} + 3s_{32111} + s_{311111} + 15s_{2222} + 2s_{2222} + 2s_{221111}. $$

$$\Delta(f^*) = \Delta\left(\sum_{w \in W^*} w - g^*\right) = \sum_{|\mu| = 8} |\text{SYT}(\mu)|s_{\mu}(\mathbf{x}) - \Delta(g^*)

= s_8 + 7s_{71} + 20s_{62} + 21s_{61} + 28s_{53} + 64s_{521} + 35s_{5111} + 14s_{44} + 70s_{431} + 56s_{422} + 90s_{4211} + 34s_{41111} + 42s_{332} + 56s_{3311} + 68s_{33221} + 61s_{32111} + 20s_{311111} - s_{2222} + 26s_{22211} + 18s_{221111} + 7s_{2111111} + 2111111. $$

**Corollary 7.3** There is no way to write $\mathfrak{J}(2,2,2,2)(\mathbf{u})$ as a positive sum of monomials (even over $\mathbb{R}$) that holds simultaneously in $U/J_{Lam, st}^k$, $k \in [8]$, and $U/I_{plac}^{st}$. Hence (by Proposition 5.7) there is also no way write $\mathfrak{J}(2,2,2,2)(\mathbf{u})$ as a positive sum of monomials over $\mathbb{R}$ that holds simultaneously in all the $U/I_{Assaf, st}^k$ for $k \in [8]$. 

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7.4 Forcing axiom 5

In this subsection we construct a $D_5$ graph (a $D_0$ graph satisfying axiom 5) whose generating function is not Schur positive. The basic idea is to start with a partial $D_0$ graph on the vertex set $\bar{W}$ from Sect. 7.3 and repeatedly add edges that are forced by axiom 5. To fully understand this construction, we first need the following functions which add edges to force axiom 5.

Recall from Sect. 3.1 that the type of a KR square of a partial $D_0$ graph is $\emptyset$, $0$, $K$, or $R$. Note that a partial $D_0$ graph $H$ is a $D_0$ graph if and only if the type of any KR square of $H$ is not 0.

Algorithm 7.4 The functions $\text{ForceAxiom5}$ and $\text{ForceAxiom5Step}$ below take as input a partial $D_0$ graph $H$ and output a partial $D_0$ graph containing $H$ or FAILURE.

function $\text{ForceAxiom5Step}(H)$
For every $|j - i| \geq 3$ and $i$-edge $\{v, w\}$ of $H$ such that $v$ admits a $j$-neighbor, ensure that the type $t_v^j$ of the KR$_j$ square containing $v$ is the same as the type $t_w^j$ of the KR$_j$ square containing $w$. This means

- if $t_v^j = t_w^j$, do nothing
- if $t_v^j \neq t_w^j$ and both types $t_v^j$, $t_w^j$ are not 0, then return FAILURE
- if $t_v^j \neq 0$ and $t_w^j = 0$, set $t_w^j := t_v^j$ and add the two corresponding edges to $H$
- if $t_w^j \neq 0$ and $t_v^j = 0$, set $t_v^j := t_w^j$ and add the two corresponding edges to $H$.

Return the resulting graph.

end function

function $\text{ForceAxiom5}(H)$
repeat
$H' := H$
$H := \text{ForceAxiom5Step}(H)$
until $H' = H$ or $H = \text{FAILURE}$
return $H$

end function

Note that $\text{ForceAxiom5Step}$ uses description (iii) of axiom 5 from Proposition 7.10 below. Since $\text{ForceAxiom5Step}$ checks that there are no violations to axiom 5 and only adds edges that are forced by axiom 5, the following proposition is immediate.

Proposition 7.5 If $\text{ForceAxiom5}$ outputs a $D_0$ graph, then this graph satisfies axiom 5. If $\text{ForceAxiom5}(H)$ outputs FAILURE, then there is no $D_5$ graph containing $H$.

Algorithm 7.6 The following recursive function takes as input a partial $D_0$ graph $H$ and outputs either a $D_5$ graph containing $H$ or FAILURE.
function GrowD5Graph(H)
  if there are no undetermined KR squares of H then
    return H
  end if
  Choose an undetermined KR square X of H. Declare the type of X to be Knuth, add the two corresponding edges to H, and let H’ denote the resulting graph.
  \[ H'' := \text{ForceAxiom5}(H') \]
  if \( H'' = \text{FAILURE} \) then
    return FAILURE
  end if
  return GrowD5Graph(H’’)
end function

Definition 7.7 Given a KR set \( W \), the minimal partial \( D_0 \) graph on \( W \) is the partial \( D_0 \) graph \( H \) on the vertex set \( W \) having as many undetermined KR squares as possible. Equivalently, \( H \) is the graph on the vertex set \( W \) such that \( \{ v, w \} \) is an \( i \)-edge if and only if \( \{ v, w \} = X \cap W \) for some KR, square \( X \).

Although Algorithm 7.6 comes nowhere close to searching the entire space of \( D_0 \) graphs on a vertex set for one that satisfies axiom 5, it is good enough to find a \( D_5 \) graph on the vertex set \( \bar{W}^* \) from Sect. 7.3. Specifically, let \( H^* \) denote the minimal partial \( D_0 \) graph on \( \bar{W}^* \). Order the KR squares of \( S_8 \) as follows:

associate to each KR, square \( v[abc]w \) the string \( i vbacw \) and then order these strings lexicographically.

If the smallest undetermined KR square of \( H \) is always chosen in GrowD5Graph, then GrowD5Graph(\( H^* \)) returns a \( D_5 \) graph on \( \bar{W}^* \). By Corollary 7.2, its generating function is not Schur positive. The largest component of this graph, which has 5322 vertices, is also a \( D_5 \) graph whose generating function is not Schur positive.

7.5 Reformulations of axiom 5

Here, we reformulate axiom 5 in terms of KR squares and give a slightly smarter version of the function ForceAxiom5.

Definition 7.8 For a partial \( D_0 \) graph \( H \) of degree \( n \), and indices \( |j - i| \geq 3 \), a KR\(_{i,j}\) hypercube \( Z \) of \( H \) consists of a matrix of KR squares of \( H \) of the form

\[
\begin{align*}
x[abc]yefdz & \quad x[abc]yefdz \quad xbacy[def]z \quad xbcay[def]z \\
x[abc]ydefz & \quad x[abc]ydefz \quad xacby[def]z \quad xcaby[def]z
\end{align*}
\]

\[
(39)
\]

together with their types, called the pattern of \( Z \), notated as
Fig. 5  Vertices and some of the edges potentially involved in a KR_{2,6} hypercube

\[ t = \begin{bmatrix} t_1^i & t_2^i & t_1^j & t_2^j \\ t_3^i & t_4^i & t_3^j & t_4^j \end{bmatrix}, \]  \hspace{1cm} (40)

where \( a < b < c \) and \( d < e < f \) are letters and \( x, y, z \) are words. Also, \( i = |x| + 2, j = |x| + |y| + 5 \) so that the four KR squares on the left (resp. right) of (39) are KR_{i} (resp. KR_{j}) squares.

Note that the pattern of any KR_{i,j} hypercube of a D_0 graph only contains the types \( \emptyset, K, \) and \( R \).

Example 7.9  If \( H \) is a partial D_0 graph containing all the vertices in Fig. 5 and only the bold edges, then

the pattern of \( \begin{bmatrix} [167]84253 & [167]84523 & 6178[245]3 & 6718[245]3 \\ [167]82543 & [167]85243 & 1768[245]3 & 7168[245]3 \end{bmatrix} \) is \( \begin{bmatrix} R & R & K & 0 \\ K & 0 & 0 & 0 \end{bmatrix} \).

For a partial D_0 graph containing only the eight vertices on the left of the figure, and the four bold edges between these vertices together with the four rotation 6-edges between these vertices, the pattern is \( \begin{bmatrix} R & \emptyset & R & K \\ K & \emptyset & R & R \end{bmatrix} \).

A partial pattern is a \( 2 \times 4 \)-matrix as in (40) whose entries are either unoccupied or one of the types \( \emptyset, 0, K, \) or \( R \). A pattern \( t \) contains a partial pattern \( \hat{t} \) if \( t \) and \( \hat{t} \) agree on the occupied entries of \( \hat{t} \).

If \( T \) and \( T' \) are sets of \( 2 \times 2 \) matrices, then let \( T \times T' \) denote the set of \( 2 \times 4 \) matrices

\( \{ [t | t'] | t \in T, t' \in T' \} \).

For example, if

\[ \begin{bmatrix} \emptyset & R \\ K & \emptyset \end{bmatrix} \]
\[ T = \left\{ \begin{bmatrix} K \\ R \end{bmatrix}, \begin{bmatrix} K \\ R \end{bmatrix} \right\}, \quad T' = \left\{ \begin{bmatrix} R \\ R \end{bmatrix}, \begin{bmatrix} R \\ R \end{bmatrix} \right\} , \] then

\[ T \times T' = \left\{ \begin{bmatrix} K \\ R \\ R \\ R \end{bmatrix}, \begin{bmatrix} K \\ R \\ R \\ R \end{bmatrix}, \begin{bmatrix} K \\ R \\ R \\ R \end{bmatrix}, \begin{bmatrix} K \\ R \\ R \\ R \end{bmatrix} \right\}. \]

It is convenient to reformulate axiom 5 in terms of KR square types, with no direct mention of edges.

**Proposition 7.10** The following properties of a $D_0$ graph $G$ are equivalent:

(i) $G$ satisfies axiom 5.

(ii) For every $|j - i| \geq 3$ and $i$-edge $\{v, w\}$ such that $v$ admits a $j$-neighbor, the type of the $j$-edge at $v$ is the same as the type of the $j$-edge at $w$.

(iii) For every $|j - i| \geq 3$ and $i$-edge $\{v, w\}$ such that $v$ admits a $j$-neighbor, the type of the KR$_j$ square containing $v$ is the same as the type of the KR$_j$ square containing $w$.

(iv) For every $j - i \geq 3$, the pattern of any KR$_{i,j}$ hypercube of $G$ does not contain any of the partial patterns in the following set of size 64:

\[
\begin{align*}
\text{(41)} & \quad \left\{ \begin{bmatrix} K \\ K \\ K \\ K \end{bmatrix}, \begin{bmatrix} K \\ K \\ K \\ K \end{bmatrix}, \begin{bmatrix} K \\ K \\ K \\ K \end{bmatrix}, \begin{bmatrix} K \\ K \\ K \\ K \end{bmatrix} \right\} \times \left\{ \begin{bmatrix} K \\ R \\ R \\ K \end{bmatrix}, \begin{bmatrix} K \\ R \\ R \\ K \end{bmatrix}, \begin{bmatrix} R \\ K \\ K \\ K \end{bmatrix}, \begin{bmatrix} R \\ K \\ K \\ K \end{bmatrix} \right\} \\
\text{(42)} & \quad \bigcup \left\{ \begin{bmatrix} R \\ R \\ R \\ R \end{bmatrix}, \begin{bmatrix} R \\ R \\ R \\ R \end{bmatrix}, \begin{bmatrix} R \\ R \\ R \\ R \end{bmatrix}, \begin{bmatrix} R \\ R \\ R \\ R \end{bmatrix} \right\} \times \left\{ \begin{bmatrix} K \\ R \\ R \\ K \end{bmatrix}, \begin{bmatrix} K \\ R \\ R \\ K \end{bmatrix}, \begin{bmatrix} R \\ K \\ K \\ K \end{bmatrix}, \begin{bmatrix} R \\ K \\ K \\ K \end{bmatrix} \right\} \\
\text{(43)} & \quad \bigcup \left\{ \begin{bmatrix} K \\ R \\ R \\ K \end{bmatrix}, \begin{bmatrix} K \\ R \\ R \\ K \end{bmatrix}, \begin{bmatrix} R \\ K \\ R \\ K \end{bmatrix}, \begin{bmatrix} R \\ K \\ R \\ K \end{bmatrix} \right\} \times \left\{ \begin{bmatrix} K \\ K \\ K \\ K \end{bmatrix}, \begin{bmatrix} K \\ K \\ K \\ K \end{bmatrix}, \begin{bmatrix} K \\ K \\ K \\ K \end{bmatrix}, \begin{bmatrix} K \\ K \\ K \\ K \end{bmatrix} \right\} \\
\text{(44)} & \quad \bigcup \left\{ \begin{bmatrix} K \\ K \\ R \\ R \end{bmatrix}, \begin{bmatrix} K \\ K \\ R \\ R \end{bmatrix}, \begin{bmatrix} K \\ K \\ R \\ R \end{bmatrix}, \begin{bmatrix} K \\ K \\ R \\ R \end{bmatrix} \right\} \times \left\{ \begin{bmatrix} R \\ R \\ R \\ R \end{bmatrix}, \begin{bmatrix} R \\ R \\ R \\ R \end{bmatrix}, \begin{bmatrix} R \\ R \\ R \\ R \end{bmatrix}, \begin{bmatrix} R \\ R \\ R \\ R \end{bmatrix} \right\}. 
\end{align*}
\]

(v) For every $j - i \geq 3$, the pattern of any KR$_{i,j}$ hypercube of $G$ appears below or is obtained from one of these by replacing some of the types $K$ or $R$ by $\emptyset$.
Proof The equivalence of (i), (ii), and (iii) follows from the fact that in a D₀ graph, the type of an i-edge is equal to the type of the KRᵢ square containing it.

To prove (iv) implies (iii), suppose \( \{v, w\} \) is an i-edge such that \( v \) admits a j-neighbor. Assume \( j > i \), the case \( j < i \) being similar. Let

\[
\begin{array}{cc}
  t_{11} & t_{12} \\
  t_{21} & t_{22}
\end{array}
\quad \begin{array}{cc}
  t_{31} & t_{32} \\
  t_{41} & t_{42}
\end{array}
\]

be the pattern of the KRᵢ, j hypercube of \( G \) that contains the KRᵢ square containing \( v \) and \( w \). Note that the KR j squares containing \( v \) and \( w \) cannot have type \( \emptyset \) or 0. Hence if \( \{v, w\} \) has type K (resp. R), then \( t \) not containing any of the partial patterns in (41) (resp. (42)) implies \( t_{11} = t_{22} \) and \( t_{31} = t_{42} \) (resp. \( t_{11} = t_{32} \) and \( t_{22} = t_{41} \)). It follows that the type of the KR j square containing \( v \) is the same as the type of the KR j square containing \( w \).

To help prove (iii) implies (iv), we first claim that (iii) implies the left 2 × 2 submatrix and the right 2 × 2 submatrix in the pattern of any KRᵢ, j hypercube of \( G \) does not contain \[
\begin{bmatrix}
  R & K \\
  K & R
\end{bmatrix}
\quad \text{and} \quad
\begin{bmatrix}
  K & R \\
  R & K
\end{bmatrix}
\]
and their rotations. (45)

To prove this claim, consider a KRᵢ, j hypercube of \( G \) as in (39) with pattern \( t \) as in (40). Since \( G \) is a D₀ graph, if \( t_{11} \in \{K, R\} \), then at least two of the vertices in \( \{abc|yedfz \}
\] are vertices of \( G \) and admit j-neighbors. So (iii) implies that at least one of \( t_{21} \), \( t_{31} \) is the same as \( t_{11} \). This proves that the left 2 × 2 submatrix of \( t \) does not contain \[
\begin{bmatrix}
  R & K \\
  K & R
\end{bmatrix}
\]
and \[
\begin{bmatrix}
  K & R \\
  R & K
\end{bmatrix}
\]. The other conclusions of the claim are proved in a similar way.

Now assume (iii) holds. Suppose for a contradiction that (iv) does not hold, i.e., there is a pattern

\[
\begin{array}{cc}
  t_{11} & t_{12} \\
  t_{21} & t_{22}
\end{array}
\quad \begin{array}{cc}
  t_{31} & t_{32} \\
  t_{41} & t_{42}
\end{array}
\]

of a KRᵢ, j hypercube of \( G \) as in (39) such that \( t \) contains one the partial patterns in (iv). All 64 possibilities are handled in a similar way, so assume \( t_{11} = R, t_{22} = R, t_{41} = K \). By (45), we must have \( t_{11} \in \{R, \emptyset\} \) and \( t_{31} \in \{K, \emptyset\} \). Since \( t_{11} = R \), at least one of the sets \( \{xbcayedfz, xacbyedfz\}, \{xbcayedfz, xcabyedfz\} \) is an i-edge of \( G \). But by (iii), the former being an i-edge implies \( t_{11} = t_{31} \in \{K, R\} \) and the latter being an i-edge implies \( t_{21} = t_{41} \in \{K, R\} \), contradiction.

To prove that (v) implies (iv), it suffices to check each of the 12 patterns appearing in (v) does not contain any of the partial patterns in (iv), which is straightforward.

We now prove (iv) implies (v). Let \( t \) be the pattern of any KRᵢ, j hypercube of \( G \). Let \( t_{1} \) (resp. \( t_{2} \)) be the left (resp. right) 2 × 2 submatrix of \( t \). Note that (iv) implies (45) since (iv) implies (iii). It follows that
\(t^i\) (resp. \(t^j\)) belongs to
\[
\begin{bmatrix}
K & K \\
K & K \\
R & R \\
R & R \\
K & K \\
K & K \\
R & K \\
R & K \\
R & R \\
R & R \\
\end{bmatrix},
\]
(46)
or is obtained from one of these by replacing some of the types \(K\) or \(R\) by \(\emptyset\).

If \(t^i\) contains \(\begin{bmatrix} K & R \end{bmatrix}\), then by (iv), line (43), \(t^j\) equals \(\begin{bmatrix} R & R \\
R & R \end{bmatrix}\) or is obtained from this by replacing some of the types by \(\emptyset\). It follows from (46) that \(t = \begin{bmatrix} K & R & R & R \\
K & R & R & R \end{bmatrix}\) or is obtained from this by replacing some of the types by \(\emptyset\). This pattern belongs to the list in (v), as desired. If \(t^i\) contains a rotation of \(\begin{bmatrix} K & R \end{bmatrix}\) or \(\begin{bmatrix} R & K \end{bmatrix}\), then a similar argument applies. If \(t^i\) contains only \(K\) or \(\emptyset\), then by (46) and (iv) (line (41)), \(t\) is equal to one of the patterns in the top row of the list in (v) or is obtained from one of these by replacing some of the types by \(\emptyset\). The case that \(t^i\) contains only \(R\) or \(\emptyset\) is similar. This exhausts all possibilities for \(t^i\) because by the definition of a \(D_0\) graph, if \(t\) does not consist entirely of \(\emptyset\)’s, then \(t^i\) contains two entries that are not \(\emptyset\) in the same row or column. \(\square\)

Say that a pattern \(t'\) of a \(KR_{i,j}\) hypercube \(Z\) covers another pattern \(t\) of \(Z\) if \(t'\) is obtained from \(t\) by replacing some of its 0’s and \(\emptyset\)’s by \(K\) or \(R\).

**Algorithm 7.11** The functions below take as input a partial \(D_0\) graph \(H\) and output a partial \(D_0\) graph containing \(H\) or FAILURE.

**function** AdvancedForceAxiom5Step\((H)\)

For each \(j - i \geq 3\) and \(KR_{i,j}\) hypercube of \(H\) with pattern
\[
t = \begin{bmatrix} t_{11} & t_{12} & t_{13} & t_{14} \\
t_{21} & t_{22} & t_{23} & t_{24} \end{bmatrix},
\]
and for each \(t_{rc}\) equal to 0, set \(t_{rc} = K\) (resp. \(t_{rc} = R\)) and add the two corresponding edges to \(H\) if each of the 12 patterns of Proposition 7.10 (v) that covers \(t\) has \(r, c\)-entry equal to \(K\) (resp. \(R\)). Let \(H'\) denote the resulting graph. If none of the 12 patterns covers \(t\), return FAILURE, otherwise return \(H'\).

**end function**

**function** AdvancedForceAxiom5\((H)\)

repeat
\(H' := H\)
\(H :=\) AdvancedForceAxiom5Step\((H)\)
until \(H' = H\) or \(H =\) FAILURE
return \(H\)

**end function**
To illustrate AdvancedForceAxiom5Step, the pattern \( t = \begin{array}{cc} R & 0 \\ K & 0 \end{array} \begin{array}{cc} 0 & 0 \\ 0 & 0 \end{array} \) can be completed to \( \begin{array}{cc} R & R \\ K & K \end{array} \begin{array}{cc} K & K \\ K & K \end{array} \) since this is the only one of the 12 patterns covering \( t \).

The following proposition is immediate from Proposition 7.10.

**Proposition 7.12** If AdvancedForceAxiom5 outputs a \( D_0 \) graph, then this graph satisfies axiom 5. If AdvancedForceAxiom5(\( H \)) outputs FAILURE, then there is no \( D_5 \) graph containing \( H \).

Recall that in Example 2.5 we defined triples bijectivizations of \( \mathcal{U}/I_{KR}^{st} \). Also of interest are graphs associated to these bijectivizations. These will be discussed in the next example and Sect. 8.

**Definition 7.13** For each assignment of Knuth or rotation to the subsets of size 3 of \([N]\) (as in Example 2.5), define a \( D_0 \) graph on the vertex set \( W \) by requiring:

the type of the KR square \( v[abc]w \) is \[
\begin{cases}
\text{Knuth} & \text{if } \{a, b, c\} \text{ is a Knuth triple}, \\
\text{rotation} & \text{if } \{a, b, c\} \text{ is a rotation triple}.
\end{cases}
\]

We say that a *triples \( D_0 \) graph* is a union of connected components of such a graph.

**Example 7.14** To better understand the subset of \( D_5 \) graphs inside the set of all \( D_0 \) graphs, the following enumerative results are instructive.

| Number of KR squares of \( \mathcal{S}_n \) | \( \frac{(n-2)n}{3} \) |
| Number of \( D_0 \) graphs on \( \mathcal{S}_n \) | \( \frac{(n-2)n}{3} \) |
| Number of triples \( D_0 \) graphs on \( \mathcal{S}_n \) | \( 2^\binom{n}{3} \) |
| Number of \( D_0 \) graphs on \( \mathcal{S}_6 \) | \( 2^{24 \cdot 20} \) |
| Number of \( D_5 \) graphs on \( \mathcal{S}_6 \) | \( 2^{16 \cdot 20} \cdot 12^{20} \) |

The first line comes from the fact that KR.i squares of \( \mathcal{S}_n \) are in bijection with words of length \( n-3 \) having no repeated letter, in the alphabet 1, 2, \ldots, \( n \). A \( D_0 \) graph on \( \mathcal{S}_n \) is determined by choosing the type of each KR square of \( \mathcal{S}_n \) independently, hence the second line. The number of triples \( D_0 \) graphs on \( \mathcal{S}_n \) is clear.

The number of \( D_5 \) graphs on \( \mathcal{S}_n \) seems difficult to compute for \( n > 6 \); however, the \( n = 6 \) case is particularly simple because each KR square is contained in at most one KR.i,j hypercube. There are \( 24 \cdot 20 \) KR squares of \( \mathcal{S}_6 \). Axiom 5 imposes no conditions on the KR3 and KR4 squares. The same goes for the KR2 squares of the form \( [abc]w \), where \( w \) is an increasing or decreasing word and for the KR5 squares of the form \( v[abc] \), where \( v \) is an increasing or decreasing word. This is a total of \( 16 \cdot 20 \) KR squares. There are \( \binom{6}{3} = 20 \) KR2,5 hypercubes of \( \mathcal{S}_6 \) corresponding to the subsets of \( \{1, 2, 3, 4, 5, 6\} \) of size 3, and these partition the remaining \( 8 \cdot 20 \) KR squares into 20 sets of size 8. By Proposition 7.10(v), there are 12 possibilities for the patterns of each of these hypercubes.
7.6 Forcing axioms 4’b and 5

We sketch the algorithm used to find a D graph whose generating function is not Schur positive.

Let $H$ be a partial D$_0$ graph. For each $4 \leq i \leq n - 2$, define $B_i(H) \subseteq \text{Vert}(H)$ to be the set of $w \in \text{Vert}(H)$ such that

- $E_{i-2}E_iE_{i-2}(w), E_iE_{i-2}(w), E_{i-2}(w), E_i(w), E_{i-2}E_i(w)$ are well defined and distinct,
- $w$ has $(i + 1)$-type W and $E_{i-2}(w)$ does not have $(i + 1)$-type W.

Define the following statistic on partial D$_0$ graphs $H$ taking values in $\mathbb{N} \sqcup \{\infty\}$:

$$\text{stat}4’b(H) := \begin{cases} \sum_{i=4}^{n-2} |B_i(H)| & \text{if } H \text{ satisfies axiom 4’b}, \\ \infty & \text{otherwise.} \end{cases}$$

Given a partial D$_0$ graph $H$, let $Q(H)$ be the graph with

- vertex set the undetermined KR squares of $H$, 
- an edge for every pair of undetermined KR squares that appear together in a KR$_{i,j}$ hypercube.

The space of all D$_5$ graphs containing a given partial D$_0$ graph $H$ is much too big to explore completely for one that satisfies axiom 4’b. To explore this space intelligently, we test the possibilities K or R for the undetermined KR squares of $H$ while not violating axioms 4’b and 5. We work on one component of $Q(H)$ at a time, and for small components, we explore both possibilities K or R for the undetermined KR squares, using the statistic stat4’b to decide which ones to keep. For concreteness, let us say that a subgraph of $Q(H)$ is small if it has $\leq 10$ vertices (see Remark 7.16).

**Algorithm 7.15** In the functions below, the input $H$ is a partial D$_0$ graph, $C$ and $Q$ are induced subgraphs of the graph $Q(H)$, and $C$ is assumed to be connected. Both functions return a partial D$_0$ graph containing $H$ together with a statistic in $\mathbb{N} \sqcup \{\infty\}$. Moreover, if GrowDGraphOneQComponent (resp. GrowDgraph) returns $G, z$ with $z < \infty$, then $G$ is a partial D$_0$ graph that satisfies axioms 4’b and 5 and has no undetermined KR squares belonging to the vertex set of $C$ (resp. $Q$). In particular, if GrowDgraph($H, Q(H)$) returns $G, z$ with $z < \infty$, then $G$ is a D$_0$ graph and a D graph. The function GrowDGraphOneQComponent calls AdvancedForceAxiom5 from Algorithm 7.11.

**Remark 7.16** In practice, we used complicated heuristics to determine the condition that $C$ is small and to choose a vertex of $C$ in the algorithm above. Also, we used a slightly simpler and faster version of AdvancedForceAxiom5.

**Remark 7.17** Instead of calling GrowDGraph with the minimal partial D$_0$ graph $H^*$ on $\bar{W}^*$, it is better to call it with a smaller partial D$_0$ graph constructed as follows: Let $H'$ be the D$_0$ graph obtained by setting each undetermined KR square of $H^*$ to type Knuth. Let $V$ be the vertex set of the largest component of $H'$ (there is a unique largest component); the size of $V$ is 6026, whereas the size of $\bar{W}^*$ is 39696. Let $H^*_{6026}$ be
function GrowDGraphOneQComponent(H, C)
    Choose a vertex \( X \) of \( C \), which is an undetermined KR square of \( H \).
    Let \( H^K \) (resp. \( H^R \)) be the graph obtained from \( H \) by setting the type of \( X \) to be Knuth (resp. rotation) and adding the two corresponding edges to \( H \).
    \( G^K := \) AdvancedForceAxiom5(\( H^K \))
    if \( G^K = \) FAILURE then
        return \( H, \infty \)
    end if
    Let \( Q^K \) be the graph obtained from \( C \) by removing all the vertices which are no longer undetermined KR squares in \( G^K \) (\( Q^K \) is an induced subgraph of \( Q(G^K) \)).
    \( G^K, \) stat\(_K := \) GrowDGraph(\( G^K, Q^K \))
    if \( C \) is small then
        \( G^R := \) AdvancedForceAxiom5(\( H^R \))
        if \( G^R = \) FAILURE then
            return \( H, \infty \)
        end if
        Let \( Q^R \) be the graph obtained from \( C \) by removing all the vertices which are no longer undetermined KR squares in \( G^R \).
        \( G^R, \) stat\(_R := \) GrowDGraph(\( G^R, Q^R \))
        if \( \text{stat}_K \leq \text{stat}_R \) then
            return \( G^K, \) stat\(_K \)
        else
            return \( G^R, \) stat\(_R \)
        end if
    else
        if \( \text{stat}_K < \infty \) then
            return \( G^K, \) stat\(_K \)
        else
            return GrowDGraph(\( G^R, Q^R \))
        end if
    end if
end function

function GrowDGraph(H, \( \mathcal{Q} \))
    Let \( C_1, \ldots, C_t \) be the components of \( \mathcal{Q} \), in increasing order of size (\( \mathcal{Q} \) may be empty in which case \( t := 0 \)).
    for \( i = 1 \) to \( t \) do
        \( H, \) stat := GrowDGraphOneQComponent(\( H, C_i \))
        if \( \text{stat} = \infty \) then
            return \( H, \infty \)
        end if
    end for
    return \( H, \) stat4\(_b(H) \)
end function

the minimal partial D\(_0\)-graph on \( V \) (by Proposition 4.1 (i) and Proposition–Definition 3.2, \( V \) is a KR set). The generating function of this graph is not Schur positive.

With \( H_{6026}^* \) as in Remark 7.17, the function call GrowDGraph(\( H_{6026}^*, \mathcal{Q}(H_{6026}^*) \)), or rather its modification with the heuristics and caveats of Remark 7.16, outputs a D graph. The largest component \( G^* \) of this graph is a D graph whose generating
function is not Schur positive. The graph $G^*$ is described in the data files accompanying this paper. See Sect. 7.8 for a guide to these files and some basic properties of $G^*$.

7.7 A strengthening of axiom $4'b$

We also considered a stronger version of axiom $4'b$, which we call axiom $4''b$.

**Definition 7.18** Let $G$ be a signed, colored graph of degree $n$ satisfying axiom 0. For $4 \leq i < n$, a weak flat $i$-chain of $G$ is a sequence $(x^1, x^2, \ldots, x^{2h-1}, x^{2h})$ of distinct vertices admitting $i - 2$-neighbors such that

- $x^{2j-1} = E_i(x^{2j})$,
- $x^{2j+1}$ is any vertex on the $(i - 2)-(i - 1)$-string containing $x^{2j}$ such that $E_{i-2}(x^{2j+1})$ does not have $(i - 1)$-type W.

**Remark 7.19** The vertices $x^{2j}$ and $x^{2j+1}$ in a weak flat $i$-chain are related just as in Remark 3.12, except that if $H$ is a path $(y^1, \ldots, y^5)$ with 4 edges as in that remark, then exactly one of the following possibilities must hold:

- $x^{2j} = y^2$, $x^{2j+1} = y^5$,
- $x^{2j} = y^4$, $x^{2j+1} = y^5$,
- $x^{2j} = y^4$, $x^{2j+1} = y^4$,
- $x^{2j} = y^3$, $x^{2j+1} = y^5$.

Axiom $4''b$ is the same as axiom $4'b$ except with weak flat $i$-chain in place of flat $i$-chain:

(axiom $4''b$) if $(x^1, x^2, \ldots, x^{2h-1}, x^{2h})$ is a weak flat $i$-chain and $x^j$ has $(i + 1)$-type W for some $2 < j < 2h - 1$, then either $x^1, \ldots, x^j$ have $(i + 1)$-type W or $x^j, \ldots, x^{2h}$ have $(i + 1)$-type W (or both).

Any flat $i$-chain is a weak flat $i$-chain, and hence any signed, colored graph satisfying axiom $4''b$ also satisfies axiom $4'b$. The $D_0$ graph $G^*$ constructed in Sect. 7.6 satisfies axiom $4''b$ in addition to axioms 5 and $4'b$.

7.8 Accompanying data files

The graph $G^*$ constructed in Sect. 7.6 has 4950 vertices, and its generating function is

$$6s_{4211} + 12s_{41111} + s_{332} + 3s_{3331} + 13s_{3221} + 37s_{32111} + 12s_{311111} - s_{2222} + 8s_{22211} + 2s_{221111}.$$ 

Figure 6 depicts a flat 4-chain of $G^*$ of length 10 and some of its neighboring vertices.

Let $V^*$ be the vertex set of $G^*$. The accompanying files present $G^*$ in several different formats and contain Maple code to check that $G^*$ satisfies axioms $4'b$ and 5.
Fig. 6 A flat 4-chain of $\mathcal{G}^*$ of length 10. The words that belong to the chain are outlined. All of the 3-neighbors and 5-neighbors of the vertices in the chain are also shown as well as the vertices along the 2–3-strings connecting consecutive vertices in the chain. Only the last two vertices of the chain, 78516243 and 78561243, have 5-type W, and hence this does not violate axiom $4'b$

(a) vertexset.txt gives the vertex set $V^* \subseteq S_8$ as a list of lists.
(b) involutions.txt gives the edges of $\mathcal{G}^*$ as involutions $E_2, \ldots, E_7$ of \{1, \ldots, 4950\} $\cong V^*$, where the isomorphism is given by the ordering of vertices in (a).
(c) involutionswithzeros.txt is the same as (b) except $E_i(v)$ is set to 0 if $v$ does not admit an $i$-neighbor.
(d) maplegraph.txt presents $\mathcal{G}^*$ as a Maple graph (no edge colors or types included).
(e) checkaxioms.txt contains Maple code to check that $\mathcal{G}^*$ is a $D_0$ graph and satisfies axioms $4'b$ and 5. Hence it is a D graph by Theorem 4.10. We also provide code to verify that the coefficient of $s(2,2,2,2)(x)$ in the generating function of $\mathcal{G}^*$ is $-1$. This file contains the data in vertexset.txt and involutionswithzeros.txt.

Remark 7.20 Checking that $\mathcal{G}^*$ is a D graph only depends on the code in checkaxioms.txt and the material in Sects. 2–4 (more specifically, Theorem 4.10 and the definition of a D graph in Sects. 3.3–3.4). (The material in Sects. 6–7 is important for understanding how $\mathcal{G}^*$ was found, but is not needed for checking it is a D graph.)

8 Concluding remarks

The following table summarizes our current knowledge of Schur positivity for the generating functions of various classes of $D_0$ graphs.
Class of $D_0$ graphs & Schur positive \\
All $D_0$ graphs & No \\
$D_0$ graphs satisfying axiom 5 & No \\
$D_0$ graphs satisfying axioms 4' and 5 & No \\
$D_0$ graphs satisfying axioms 4'' and 5 & No \\
All triples $D_0$ graphs (Definition 7.13) & Unknown \\
The Assaf LLT $k$ $D$ graphs (Definition 5.6) & Unknown \\
$D_0$ graphs $\mathcal{G}$ such that $\sum_{w \in \text{Vert}(\mathcal{G})} w \in (I_{\text{Assaf},st}^{\text{Lam}})^{\perp}$ & Yes \\
The graphs $\mathcal{G}^{st}_{\beta, t}$ (see §5.3) & Yes \\

Here, $I_{\text{Lam},st}^{\text{Lam}}$ is the two-sided ideal of $\mathcal{U}$ corresponding to the relations (3) together with

$$ac = ca$$

for $c - a > k$,

$$b(ac - ca) = (ac - ca)b$$

for $a < b < c$ and $c - a \leq k$.

Then $I_{\text{Lam},st}^{\text{Lam}} \supseteq I_{\text{KR}}^{st}$. In [4], we show that $\mathcal{Z}_\lambda(u)$ is a positive sum of monomials in $\mathcal{U}/I_{\text{Lam},st}^{\text{Lam}}$, which explains the second-to-last entry of the table. Also, the last entry of the table follows from the Schur positivity of LLT polynomials.

Despite the negative results of this paper, there is substantial evidence that many $D_0$ graphs have Schur positive generating functions. This includes computer experimentation of many researchers, the “Yes” entries in the table above, and to some extent the “Unknown” entries because substantial computer searches support Schur positivity in these cases. In addition, Theorem 4.6 can be generalized to show that the coefficient of $s_\lambda(x)$ in the generating function of any $D_0$ graph is nonnegative whenever $\lambda$ is a hook shape or of the form $(a, 2, 1^b)$. It remains a major open question to give some uniform explanation of these observations. Before formulating some specific questions along these lines, let us see exactly how the negative results of this paper make such an explanation difficult.

For the sake of concreteness, let us define a local property of a $D_0$ graph $\mathcal{G}$ to be one that only depends on $\text{Res}_K \mathcal{G}$ for $|K| \leq 6$. Then axioms 3, 4' $a$, 4' $b$, 4'' $b$ and LSP$_3$ are local in this sense. Understanding the Schur expansions of $D_0$ graphs using the theory of noncommutative Schur functions is well adapted to studying such properties. For example, if $I$ is a two-sided ideal of $\mathcal{U}$ generated in degree $\leq 6$ and $I \supseteq I_{\text{KR}}^{st}$, then the property that a $D_0$ graph $\mathcal{G}$ satisfies $\sum_{w \in \text{Vert}(\mathcal{G})} w \in I^{\perp}$ is a local property. These are the natural local properties from this perspective.

However, Sect. 7.3 shows the limitations of such properties for proving Schur positivity. If we want to prove that all Assaf LLT$_k$ $D$ graphs have Schur positive generating functions using a local property corresponding to an ideal $I$ as above, then we must prove that

(A) for all $k$ and all Assaf LLT$_k$ $D$ graphs $\mathcal{G}$, there holds $\sum_{w \in \text{Vert}(\mathcal{G})} w \in I^{\perp}$, 

(B) $\Delta(\sum_{w \in W} w)$ is Schur positive for every KR set $W$ such that $\sum_{w \in W} w \in I^{\perp}$.

Then we must have $I^{\perp} \supseteq (I_{\text{Assaf},st}^{\text{Lam}})^{\perp}$ for all $k$, hence $I^{\perp} \supseteq J^{\perp}$ for $J = \bigcap J^{(j)}$ with $J^{(j)}$ as in Sect. 7.3. But then (B) is false. Hence we must turn to nonlocal
properties, properties that depend on edges and not just vertices, or some “nonuniform” explanation of Schur positivity that handles each $k$ separately.

Here are some precise questions to guide us toward a better understanding of what makes a $D_0$ graph Schur positive:

- In which quotients $U/I$ of $U/I_{KR}^{G}$ can $\zeta_{\lambda}(u)$ be written as a positive sum of monomials? We believe the case $I$ is generated in degree 3 to be particularly important.
- For which quotients $U/I$ of $U/I_{KR}^{G}$ do all $D_5$ graphs $G$ satisfying $\sum_{w \in \text{Vert}(G)} w \in I^\perp$ have Schur positive generating functions?

The negative results of this paper suggest that answers to these questions will not be simple and that there may be no unique, most general condition that guarantees Schur positivity.

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