Kazhdan-Lusztig Polynomials for 321-Hexagon-Avoiding Permutations

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In memory of Rodica Simion

Abstract. In (Deodhar, *Geom. Dedicata*, 36(1) (1990), 95–119), Deodhar proposes a combinatorial framework for determining the Kazhdan-Lusztig polynomials $P_{x,w}$ in the case where W is any Coxeter group. We explicitly describe the combinatorics in the case where $W = \mathfrak{S}_n$ (the symmetric group on n letters) and the permutation w is 321-hexagon-avoiding. Our formula can be expressed in terms of a simple statistic on all subexpressions of any fixed reduced expression for w. As a consequence of our results on Kazhdan-Lusztig polynomials, we show that the Poincaré polynomial of the intersection cohomology of the Schubert variety corresponding to w is $(1+q)^{l(w)}$ if and only if w is 321-hexagon-avoiding. We also give a sufficient condition for the Schubert variety X_w to have a small resolution. We conclude with a simple method for completely determining the singular locus of X_w when w is 321-hexagon-avoiding. The results extend easily to those Weyl groups whose Coxeter graphs have no branch points (B_n, F_4, G_2).

Keywords: 321-hexagon-avoiding, Kazhdan-Lusztig polynomials, Schubert varieties, singular locus, defect graph

1. Introduction

In [21], Kazhdan and Lusztig constructed certain representations of the Hecke algebra associated to a Coxeter group W in order to elucidate representation-theoretic questions concerning W itself. To do this, they introduced a class of polynomials now known as the Kazhdan-Lusztig polynomials. These polynomials were quickly seen to play an important role in Lie theory. For instance, they give a natural setting for expressing multiplicities of Jordan-Hölder series of Verma modules (see [1, 11]). Introductions to these polynomials can be found in [9, 16, 20].

While there are many interpretations of, and uses for, these polynomials, their combinatorial structure is far from clear. Kazhdan and Lusztig originally defined the polynomials in terms of a complicated recursion relation. In [21], it was conjectured that the coefficients of these polynomials are non-negative. This has been proved for many important W (such as (affine) Weyl groups) [22], but not for arbitrary Coxeter groups. There has been limited

success in finding non-recursive formulas for the Kazhdan-Lusztig polynomials. Brenti [7, 8] has given a non-recursive formula in terms of an alternating sum over paths in the Bruhat graph. Lascoux and Schützenberger [27] have given an explicit formula for $P_{x,w}$ in the case where W is the symmetric group and x, w are Grassmannian permutations. Zelevinsky [36] has even constructed a small resolution of X_w in this case. Lascoux [26] extends the results of [27] to twisted vexillary permutations. Finally, Shapiro, Shapiro and Vainshtein [33] and Brenti and Simion [10] find explicit formulas for certain classes of permutations.

Deodhar [15] proposes a combinatorial framework for determining the Kazhdan-Lusztig polynomials for an arbitrary Coxeter group. The algorithm he describes is shown to work for all Weyl groups. However, the algorithm is impractical for routine computations. In this paper, we utilize Deodhar's framework to calculate $P_{x,w}$ for 321-hexagon-avoiding elements $w \in \mathfrak{S}_n$. For these elements, Deodhar's algorithm turns out to be trivial. As a result, in these cases we get a very explicit description of the polynomials. The algorithm consists of calculating Deodhar's defect statistic on each subexpression of a given reduced expression. We also show that the property of w being 321-hexagon-avoiding is equivalent to several nice properties on w in the Hecke algebra and in the cohomology of the corresponding Schubert variety X_w. In particular, we have the following (the necessary definitions can be found in Sections 2 and 3):

Theorem 1   *Let* $\mathbf{a} = s_{i_1} \cdots s_{i_r}$ *be a reduced expression for* $w \in \mathfrak{S}_n$. *The following are equivalent*:

1. *w is 321-hexagon-avoiding.*
2. *Let $P_{x,w}$ denote the Kazhdan-Lusztig polynomial for $x \leq w$. Then*

$$P_{x,w} = \sum q^{d(\sigma)} \tag{1}$$

   where $d(\sigma)$ is the defect statistic and the sum is over all masks σ on $\mathbf{a}$ whose product is x.

3. *The Poincaré polynomial for the full intersection cohomology group of X_w is*

$$\sum_i \dim(\mathrm{IH}^{2i}(X_w))q^i = (1+q)^{l(w)}. \tag{2}$$

4. *The Kazhdan-Lusztig basis element C_w' satisfies $C_w' = C_{s_{i_1}}' \cdots C_{s_{i_r}}'$.*
5. *The Bott-Samelson resolution of X_w is small.*
6. *$\mathrm{IH}_*(X_w) \cong H_*(Y)$, where Y is the Bott-Samelson resolution of X_w.*

Remark 1   Equivalence of 2, 4 and 5 is implicit in Deodhar [15].

Remark 2   Lusztig [28] and Fan and Green [19] have already studied those elements w for which part 4 of the main theorem hold. In the terminology of these papers, such a w is "tight." Also, Fan and Green show the implication 4 $\Longrightarrow$ 1 of Theorem 1.

Remark 3 For concreteness, this paper refers only to $\mathfrak{S}_n$. However, 2 through 6 hold for all Weyl groups. In addition, our combinatorial characterization of $1 \Longleftrightarrow 2$ can be extended to the other "non-branching" Weyl groups B_n, F_4, G_2 (see [35]). One need simply replace "321-avoiding" by "short-braid-avoiding" in any statements made (e.g., "321-hexagon-avoiding" $\mapsto$ "short-braid-hexagon-avoiding"). The characterization in 1 fails to hold for D_n, E_6, E_7, E_8 primarily due to failure of Lemma 1. An appropriate analogue of hexagon-avoiding for these other Weyl groups would fix this deficiency.

The organization of the paper is as follows. In Section 2 we introduce necessary background definitions. In Section 3 we introduce the notion of pattern avoidance and in Section 4 we present Deodhar's combinatorial framework. A critical tool used to prove Theorem 1 is the defect graph explored in Section 5. In Section 6 this graph is used to prove Theorem 1. Section 7 contains an application of Theorem 1 to a conjecture of Haiman. Section 8 determines the singular locus of Schubert varieties corresponding to 321-hexagon-avoiding permutations. Finally, Section 9 contains a table enumerating the elements of $\mathfrak{S}_n$ for which Theorem 1 applies. We do not know a closed form for this sequence.

2. Preliminaries

Let $\mathfrak{S}_n$ denote the symmetric group on n letters. Choose the standard presentation $\mathfrak{S}_n = \langle s_1, \ldots, s_{n-1} : s_i^2 = 1, s_i s_j = s_j s_i$ for $|i - j| > 1$, and $s_i s_{i+1} s_i = s_{i+1} s_i s_{i+1} \rangle$. Let $S = \{s_i\}_{i \in [1 \ldots n-1]}$ denote the generating set for $\mathfrak{S}_n$. An *expression* is any product of generators s_i. The *length* $l(w)$ of an element $w \in \mathfrak{S}_n$ is the minimum r for which we have an expression $w = s_{i_1} \cdots s_{i_r}$. A *reduced expression* $w = s_{i_1} \cdots s_{i_r}$ is an expression for which $l(w) = r$. If $v, w \in \mathfrak{S}_n$, then $v \leq w$ will signify that v is below w in the Bruhat-Chevalley order (see, e.g., [20]). This order is characterized by $v \leq w$ if and only if every reduced expression for w contains a subexpression for v.

For the remainder of this section, all of our definitions apply to any finite Weyl group W. However, following this section, we will restrict our attention to the case where $W = \mathfrak{S}_n$.

In order to define the Kazhdan-Lusztig polynomials, we now recall the notion of the Hecke algebra $\mathcal{H}$ associated to a finite Weyl group W. $\mathcal{H}$ has basis T_w indexed by the elements of W. For all generators s of W, we have

$$T_s T_w = T_{sw} \text{ if } l(sw) > l(w), \tag{3}$$

$$T_s^2 = (q-1)T_s + qT_e \tag{4}$$

(where e is the identity element of W). This is an algebra over $A = \mathbb{Q}(q^{1/2})$. Following [21], we define an involution on A by $\overline{q^{1/2}} = q^{-1/2}$. Extend this to an involution on $\mathcal{H}$ by setting

$$\iota \left(\sum_w \alpha_w T_w \right) = \sum_w \bar{\alpha}_w (T_{w^{-1}})^{-1}. \tag{5}$$

From [21], we have that the Kazhdan-Lusztig polynomials are determined uniquely by the following:

Theorem 2 (*Theorem* 1.1, [21])   *For any $w \in W$, there is a unique element $C'_w \in \mathcal{H}$ such that*

1. $C'_w = q^{-l(w)/2} \sum_{x \leq w} P_{x,w} T_x$, *and*
2. $\iota(C'_w) = C'_w$,

where $P_{x,w} \in A$ is a polynomial in q of degree at most $\frac{1}{2}(l(w) - l(x) - 1)$ for $x < w$, $P_{w,w} = 1$, and $P_{x,w} = 0$ if $x \not\leq w$.

As mentioned above, it is conjectured in [21] that the coefficients of $P_{x,w}$ are non-negative.

Several of the conditions in Theorem 1 require some notation regarding cohomology. So let W be the Weyl group of some semi-simple algebraic group G with Borel subgroup B. C_w will denote the Schubert cell in the flag variety G/B corresponding to $w \in W$ (see, e.g., [6]). X_w will denote the corresponding Schubert variety, $X_w = \cup_{v \leq w} C_v$. For any variety X (such as some X_w), we let $\mathrm{IH}^i(X)$ denote the i-th (middle) intersection cohomology group of X. Suppose that $f : Y \longrightarrow X$ is a resolution of singularities of X. The map f is said to be a *small resolution* if for every $r > 0$,

$$\operatorname{codim}\{x \in X : \dim f^{-1}(x) \geq r\} > 2r. \tag{6}$$

A commonly used resolution of the singularities of X_w is the Bott-Samelson resolution (see [5, 13]). Theorem 1 yields an easy criterion for determining when such a resolution is small.

3.   Pattern avoidance and heaps

It will be useful to view elements of $\mathfrak{S}_n$ as permutations on $[1, 2, \ldots, n]$. To this end, we identify s_i with the transposition $(i, i+1)$. Let $w(i)$ be the image of i under the permutation w. Hence, we have a one-line notation for a permutation w given by writing the image of $[1, 2, \ldots, n]$ under the action of w: $[w(1), w(2), \ldots, w(n)]$.

The results of this paper pertain to a particular set of elements of $\mathfrak{S}_n$. This subset will be defined using the notion of pattern avoidance. Let $v \in S_k$ and $w \in S_l$. Say that w *avoids* v (or is v-avoiding) if there do not exist $1 \leq i_1 < \cdots < i_k \leq l$ with $w(i_1), w(i_2), \ldots, w(i_k)$ in the same relative order as $v(1), v(2), \ldots, v(k)$. We are interested in two particular instances of pattern avoidance. The first is where $v = [321]$. It is shown by Billey-Jockusch-Stanley [2] that the 321-avoiding permutations in $\mathfrak{S}_n$ are precisely those for which no reduced expression contains a substring of the form $s_i s_{i \pm 1} s_i$. In the context of reduced expressions, 321-avoiding permutations are called *short-braid-avoiding* (terminology due to Zelevinsky, according to [18]). Short-braid-avoiding permutations have been studied by Fan and Stembridge [17, 18, 30, 31].

The second instance of pattern-avoidance with which we will be concerned is most easily visualized via a poset associated to w. So let $w \in \mathfrak{S}_n$ be 321-avoiding and fix some reduced expression $\mathbf{a} = s_{i_1} \cdots s_{i_r}$ for w. By [32], all reduced expressions for such a 321-avoiding w are equivalent up to moves of the form $s_i s_j \to s_j s_i$ for $|i - j| > 1$. This allows us to associate a well-defined poset to w (rather than just to $\mathbf{a}$, see [30]). Let the generators $\{s_{i_j}\}_{j=1}^r$ in our reduced expression label the elements of our poset. For an ordering, we take

Figure 1. Let $w = s_9 s_6 s_7 s_8 s_2 s_1 s_3 s_2 s_4 s_5 s_6$. The left image shows the result of the embedding $s_{i_j} \mapsto (i_j, \mathrm{lvl}_L(s_{i_j}))$. On the right is the result of pushing the "connected components" together.

the transitive closure of

$$s_{i_j} \preceq s_{i_k} \text{ if } s_{i_{j+1}} \cdots s_{i_{k-1}} s_{i_k} = s_{i_k} s_{i_{j+1}} \cdots s_{i_{k-1}} \quad \text{and} \quad s_{i_j} s_{i_k} \neq s_{i_k} s_{i_j}.$$

We now wish to embed this poset in the plane in a very particular way. Effectively, what we do is send a generator s_{i_j} to the point in the plane $(i_j, \mathrm{lvl}(s_{i_j}))$ where $\mathrm{lvl}(s_{i_j})$ measures the maximal length of a chain $s_{i_b} \preceq \cdots \preceq s_{i_j}$ over all $b \leq j$. However, in order for our embedding to have the properties we need, this procedure needs to be adjusted slightly.

So, as above, embed this poset in the plane via $s_{i_j} \mapsto \mathrm{pt}(j) \overset{\mathrm{def}}{=} (i_j, \mathrm{lvl}(s_{i_j}))$, where we define $\mathrm{lvl}(s_{i_j})$ as follows: Let k be as small as possible in the interval $[1, \ldots, j]$ such that s_{i_j} commutes with s_{i_l} for all l with $k \leq l \leq j$. Now, initially, define a level function by: $\mathrm{lvl}_L(s_{i_j}) = 0$ if $k = 1$ and $\mathrm{lvl}_L(s_{i_j}) = \mathrm{lvl}_L(s_{i_{k-1}}) + 1$ if $k \geq 2$.

For most purposes, $\mathrm{lvl}_L(\cdot)$ gives us what we'd like. However, with $\mathrm{lvl}_L(\cdot)$ as the level function, "connected components" do not necessarily abut. Figure 1 gives an example of the embedding $(i_j, \mathrm{lvl}_L(s_{i_j}))$ and how it can be improved by coalescing "connected components."

So, we first define connected components by imposing an equivalence $\sim$ on the generators in our expression for w: Let $s_{i_j} \sim s_{i_k}$ if $i_j = i_k \pm 1$ and $\mathrm{lvl}_L(s_{i_j}) = \mathrm{lvl}_L(s_{i_k}) \pm 1$. Extend this equivalence transitively. Now, since we are assuming that w is 321-avoiding, the components have a canonical partial order. It is then a simple matter to uniformly adjust the levels of all members of a particular connected component to allow distinct components to abut as much as possible and hence "coalesce." Define $\mathrm{lvl}(s_{i_j})$ to be this adjustment of the level $\mathrm{lvl}_L(s_{i_j})$.

We will refer to the realization $s_{i_j} \mapsto (i_j, \mathrm{lvl}(s_{i_j}))$ of our poset as $\mathrm{Heap}(w)$. The notion of $\mathrm{Heap}(w)$ is due to Viennot [34], see also the work of Stembridge [30] in the context of fully-commutative elements. Note that s_{i_j} can cover s_{i_k} if and only if $|i_j - i_k| = 1$.

We are now ready to introduce the second class of patterns that we wish to avoid. Say that w is *hexagon-avoiding* if it avoids each of the patterns in

$$\{[4, 6, 7, 1, 8, 2, 3, 5], [4, 6, 7, 8, 1, 2, 3, 5],$$
$$[5, 6, 7, 1, 8, 2, 3, 4], [5, 6, 7, 8, 1, 2, 3, 4]\}. \tag{7}$$

If we set

$$u = s_3 s_2 s_1 s_5 s_4 s_3 s_2 s_6 s_5 s_4 s_3 s_7 s_6 s_5, \tag{8}$$

then the permutations in (7) correspond to u, us_4, $s_4 u$, $s_4 u s_4$.

The heap of any hexagon-avoiding permutation must not contain the hexagon in figure 2. Permutations that are 321-avoiding and hexagon-avoiding (321-hexagon-avoiding) can, in
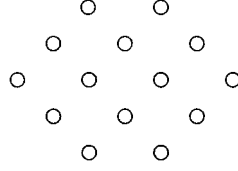
Figure 2. Heap(u) for u as in (8).

fact, be characterized as those for which no reduced expression contains a substring of either of the forms

$$u^j = s_{j+3}s_{j+2}s_{j+1}s_{j+5}s_{j+4}s_{j+3}s_{j+2} \cdot$$
$$\qquad s_{j+6}s_{j+5}s_{j+4}s_{j+3}s_{j+7}s_{j+6}s_{j+5} \quad \text{for any } j \geq 0, \tag{9}$$
$$s_j s_{j\pm1} s_j \quad \text{for any } j \geq 1. \tag{10}$$

It is this characterization of 321-hexagon-avoiding elements that we will use in the rest of the paper.

Remark 4 Computationally, it is much more efficient (polynomial time) to recognize 321-hexagon-avoiding patterns via pattern avoidance rather than by scanning through all reduced expressions for a particular subexpression (exponential time).

The heaps of 321-avoiding elements have a very important property that will be exploited in the proof of Theorem 1. To develop this property, it will be useful to define the following two subsets of the unit integer lattice for each j, $1 \leq j \leq r$:

The *lower cone*: $\text{Cone}_\wedge(j) = \{(i_j + \alpha, \text{lvl}(s_{i_j}) - \beta) \in \mathbb{Z}^2 : |\alpha| \leq \beta\}$.

The *upper cone*: $\text{Cone}^\vee(j) = \{(i_j + \alpha, \text{lvl}(s_{i_j}) + \beta) \in \mathbb{Z}^2 : |\alpha| \leq \beta\}$.

The *boundary* of $\text{Cone}_\wedge(j)$ (or $\text{Cone}^\vee(j)$) corresponds to the points in this cone where $|\alpha| = |\beta|$ (see figure 3).

The following lemma yields a very nice property of 321-avoiding permutations. In Remark 5, we interpret this result visually in terms of Heap(w).

Lemma 1 (*Lateral Convexity*) *Label the generators of $\mathfrak{S}_n$ such that $s_i s_j = s_j s_i$ if and only if $|i - j| > 2$ (the standard labeling). Then $w \in \mathfrak{S}_n$ is 321-avoiding if and only if any two occurrences of some s_i in a reduced expression for w are separated by both an s_{i-1} and an s_{i+1}.*

Remark 5 Lemma 1 can be rephrased as follows. Suppose that $w = s_{i_1} \cdots s_{i_r}$ is 321-avoiding and pt(j), pt(k) $\in$ Heap(w) with $\text{lvl}(s_{i_j}) < \text{lvl}(s_{i_k})$. Suppose further that for each $m \in [i_j, i_k]$ (if $i_j \leq i_k$) or $m \in [i_k, i_j]$ (if $i_j > i_k$), there is a point $(m, \text{lvl}(s_{i_l})) \in \text{Cone}_\wedge(s_{i_k})$ $\cap \text{Cone}^\vee(s_{i_j}) \cap$ Heap(w) for some l, $j \leq l \leq k$. Then the entire diamond $\text{Cone}_\wedge(s_{i_k}) \cap$
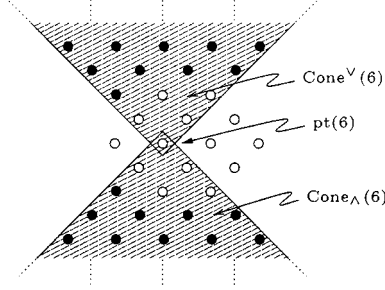
Figure 3.   Heap(u) overlaid with Cone$_\wedge$(6) and Cone$^\vee$(6). The white nodes are in Heap(u). The black nodes are in one of the cones, but not in Heap(u).

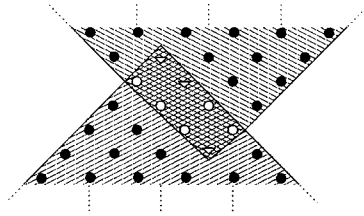*Figure 4.*   If it is known that the triangular nodes are in Heap(w), then Lemma 1 tells us that all the white circles are also in Heap(w).

Cone$^\vee(s_{i_j})$ is contained in Heap(w). This is illustrated in figure 4. This interpretation relies on Lateral Convexity, that w is 321-avoiding, and the "coalescing" performed in the embedding that defines Heap(w).

Proof of Lateral Convexity: Suppose $w \in \mathfrak{S}_n$ is 321-avoiding. Choose a reduced expression for w for which a pair of s_i's is as close together as possible for some i. These two copies of s_i must be separated by at least one of $s_{i\pm1}$, otherwise our expression would not be reduced. But then our reduced expression looks like $u_1 s_i u_2 s_{i\pm1} u_3 s_i u_4$ where $l(w) = 3 + \sum_{j=1}^{4} l(u_j)$. If $s_i u_2 = u_2 s_i$ and $u_3 s_i = s_i u_3$, then w has a reduced expression $u_1 u_2 s_i s_{i\pm1} s_i u_3 u_4$. Such a w is not 321-avoiding, which is a contradiction. So either u_2 or u_3 must contain $s_{i\mp1}$.

For the reverse implication, suppose that every two copies of the same generator s_i in some reduced expression for w are separated by both an s_{i-1} and an s_{i+1}. It is a theorem of Tits [32], that any two reduced expressions for $w \in \mathfrak{S}_n$ can be obtained from each other by a sequence of moves of the following two types:

$$C_1 : s_i s_j = s_j s_i, \quad \text{if } |i - j| > 1, \tag{11}$$
$$C_2 : s_i s_j s_i = s_j s_i s_j, \quad \text{if } i = j \pm 1. \tag{12}$$

But, under our hypothesis, we are never able to apply a C_2 move for such a w. So all reduced expressions for w must be obtainable by a sequence of C_1 moves. Hence, w is 321-avoiding.   □

4. Deodhar's framework

For 321-hexagon-avoiding permutations, we will give an explicit combinatorial formula for the Kazhdan-Lusztig polynomials. This will be done in a framework developed by Deodhar [15] (using slightly different notation). The necessary concepts are reviewed in this section.

Our construction of the Kazhdan-Lusztig polynomials will be in terms of subexpressions of a fixed reduced expression $\mathbf{a} = s_{i_1} \cdots s_{i_r}$. To this end, we define a *mask* σ (associated to $\mathbf{a}$) to be any binary word $(\sigma_1, \ldots, \sigma_r)$ in the alphabet $\{0, 1\}$. Set $\sigma[j] \stackrel{\text{def}}{=} (\sigma_1, \ldots, \sigma_j)$ for $1 \leq j \leq r$. (So $\sigma = \sigma[r]$.) We'll use the notation

$$s_{i_j}^{\sigma_j} = \begin{cases} s_{i_j}, & \text{if } \sigma_j = 1, \\ 1, & \text{if } \sigma_j = 0. \end{cases} \tag{13}$$

Hence, $w^{\sigma[j]} \stackrel{\text{def}}{=} s_{i_1}^{\sigma_1} \cdots s_{i_j}^{\sigma_j}$ is a (not necessarily reduced) subexpression of w. Let $\pi(w^{\sigma[j]})$ denote the corresponding element of $\mathfrak{S}_n$. $\mathcal{P}(\mathbf{a})$ will denote the set of (2^r possible) masks of $\mathbf{a}$. Note that $\mathcal{P}(\mathbf{a})$ can be viewed as the power set of $\{1, \ldots, r\}$. Finally, for $x \in \mathfrak{S}_n$, set $\mathcal{P}_x(\mathbf{a}) \subset \mathcal{P}(\mathbf{a})$ to be the subset consisting of those masks σ such that $\pi(w^{\sigma}) = x$.

Define the *defect set* $\mathcal{D}(\sigma)$ of the fixed reduced expression $\mathbf{a}$ and associated mask σ to be

$$\mathcal{D}(\sigma) = \left\{ j : 2 \leq j \leq n,\ l\big(\pi\big(w^{\sigma[j-1]}\big) \cdot s_{i_j}\big) < l\big(\pi(w^{\sigma[j-1]})\big) \right\}. \tag{14}$$

Note that j's membership in $\mathcal{D}(\sigma)$ is independent of σ_k for $k \geq j$. The elements of $\mathcal{D}(\sigma)$ are simply called *defects* (of the mask σ).

Example 1 Let $w = s_3 s_2 s_1 s_4 s_3 s_2 s_5 s_4 s_3$, $\sigma = (1, 1, 0, 1, 0, 1, 0, 1, 0)$. Then $w^{\sigma} = w^{\sigma[9]} = s_3 s_2 s_4 s_2 s_4$, $\pi(w^{\sigma}) = s_3$, and $\mathcal{D}(\sigma) = \{6, 8, 9\}$. If $x = s_1 s_3 s_5$, then

$$\begin{aligned} \mathcal{P}_x(\mathbf{a}) = \{ \sigma' &= (0, 0, 1, 0, 0, 0, 1, 0, 1), \\ \sigma'' &= (0, 0, 1, 0, 1, 0, 1, 0, 0), \\ \sigma''' &= (1, 0, 1, 0, 0, 0, 1, 0, 0), \\ \sigma'''' &= (1, 0, 1, 0, 1, 0, 1, 0, 1) \}. \end{aligned} \tag{15}$$

So, $\mathcal{D}(\sigma') = \emptyset$, $\mathcal{D}(\sigma'') = \{9\}$, $\mathcal{D}(\sigma''') = \{5, 9\}$, and $\mathcal{D}(\sigma'''') = \{5\}$.

Deodhar, in [15, Lemma 4.1, Definition 4.2, Proposition 4.5], gives a more combinatorial characterization of the Kazhdan-Lusztig polynomials. Specifically, he proves that one can always find a subset $\mathcal{S} \subseteq \mathcal{P}(\mathbf{a})$ that yields the Kazhdan-Lusztig polynomials. This is an amazing result. However, in general, the procedure to find this subset $\mathcal{S}$ is somewhat complicated. But we can restrict our attention to the case where $\mathcal{S} = \mathcal{P}(\mathbf{a})$. In this case, Deodhar's result can be translated as follows:

Theorem 3 *Let W be any finite Weyl group and* **a** *be a reduced expression for some* $w \in W$. *Set*

$$P_x(\mathbf{a}) = \sum_{\sigma \in \mathcal{P}_x(\mathbf{a})} q^{|\mathcal{D}(\sigma)|}. \tag{16}$$

If $\deg P_x(\mathbf{a}) \leq \frac{1}{2}(l(w) - l(x) - 1)$ *for all* $x \in W$, *then* $P_x(\mathbf{a})$ *is the Kazhdan-Lusztig polynomial* $P_{x,w}$ *for all* $x \in W$.

Most of the content of Theorem 3 is that the $P_x(\mathbf{a})$ satisfy a recursive formula equivalent to Theorem 2.

5. The defect graph

The purpose of the defect graph is to furnish us with a simple criterion for ensuring that $|\mathcal{D}(\sigma)| \leq \frac{1}{2}(l(w) - l(\pi(w^\sigma)) - 1)$ as required by Theorem 3. However, it is advantageous to first rephrase this inequality in another language. So again we introduce some notation. Partition the defect set $\mathcal{D}(\sigma) = \mathcal{D}^0(\sigma) \cup \mathcal{D}^1(\sigma)$ where $\mathcal{D}^\epsilon(\sigma)$ consists of those $j \in \mathcal{D}(\sigma)$ for which $\sigma_j = \epsilon \in \{0, 1\}$. Let $\mathbf{a}[j] \stackrel{\text{def}}{=} s_{i_1} \cdots s_{i_j}$ for $1 \leq j \leq r$. Also, set $d_j(\sigma) \stackrel{\text{def}}{=} |\mathcal{D}(\sigma[j])|$, $d(\sigma) \stackrel{\text{def}}{=} |\mathcal{D}(\sigma)|$, $x[j] \stackrel{\text{def}}{=} \pi(w^{\sigma[j]})$ and $w[j] \stackrel{\text{def}}{=} \pi(\mathbf{a}[j])$. Finally, set

$$\Delta_{\sigma[j]} \stackrel{\text{def}}{=} \frac{l(w[j]) - l(x[j]) - 1}{2} - |\mathcal{D}(\sigma[j])|. \tag{17}$$

We write Δ_σ for $\Delta_{\sigma[r]}$. Having $\Delta_\sigma \geq 0$ implies that the inequality in Theorem 3 holds. The defect graph will allow us to show that a condition equivalent to $\Delta_\sigma \geq 0$, stated in the following lemma, holds whenever w is 321-hexagon-avoiding.

Lemma 2 *Let* $\mathbf{a} = s_{i_1} \cdots s_{i_r}$ *be a reduced expression for some* $w \in \mathfrak{S}_n$. *Suppose* $\sigma = (\sigma_1, \ldots, \sigma_r) \in \mathcal{P}(\mathbf{a})$ *with* $\pi(w^\sigma) \neq w$. *Then* $\Delta_\sigma \geq 0$ *if and only if*

$$(\# \ of \ 0's \ in \ \{\sigma_1, \ldots, \sigma_r\}) \geq 2 \cdot |\mathcal{D}^0(\sigma)| + 1. \tag{18}$$

Proof: Let k be the smallest index for which $\sigma_k = 0$. Such a k must exist by our stipulation that $\pi(w^\sigma) \neq w$. Consider the sequence $w[k], w[k + 1], \ldots$. Since $s_{i_1} \cdots s_{i_k}$ is reduced, $\mathcal{D}(\sigma[k]) = \emptyset$. Hence, $\Delta_{\sigma[k]} = 0$. We now investigate the differences $\Delta_{\sigma[j]} - \Delta_{\sigma[j-1]}$ for $j > k$. There are four possibilities (note that in each case, $l(w[j]) = l(w[j - 1]) + 1$):

1. $j \notin \mathcal{D}(\sigma)$, $\sigma_j = 1$. Then $d_j(\sigma) = d_{j-1}(\sigma)$, $l(x[j]) = l(x[j - 1]) + 1$. So $\Delta_{\sigma[j]} - \Delta_{\sigma[j-1]} = 0$.
2. $j \notin \mathcal{D}(\sigma)$, $\sigma_j = 0$. Then $d_j(\sigma) = d_{j-1}(\sigma)$, $l(x[j]) = l(x[j-1])$. So $\Delta_{\sigma[j]} - \Delta_{\sigma[j-1]} = 1/2$.
3. $j \in \mathcal{D}(\sigma)$, $\sigma_j = 1$. Then $d_j(\sigma) = d_{j-1}(\sigma) + 1$, $l(x[j]) = l(x[j - 1]) - 1$. So $\Delta_{\sigma[j]} - \Delta_{\sigma[j-1]} = 0$.
4. $j \in \mathcal{D}(\sigma)$, $\sigma_j = 0$. Then $d_j(\sigma) = d_{j-1}(\sigma) + 1$, $l(x[j]) = l(x[j - 1])$. So $\Delta_{\sigma[j]} - \Delta_{\sigma[j-1]} = -1/2$.

So, the only cases we need to consider are the second and the fourth. From this it follows that for each $j > k$,

$$\Delta_{\sigma[j]} \geq 0 \quad \Longleftrightarrow \quad \text{\# of } 0's \text{ in}\{\sigma_{k+1}, \ldots, \sigma_j\} \geq 2 \cdot |\mathcal{D}^0(\sigma[j])|. \tag{19}$$

The conclusion of the lemma follows by induction upon setting $j = r$.

Recall that we need to show that (18) is satisfied for 321-hexagon-avoiding permutations for any choice of reduced expression. To do this, we define a graph G_σ whose vertices are in one-to-one correspondence with the defects of $\mathcal{D}^0(\sigma)$. In Lemmas 3, 4, and 5 we develop some technical results relating the shape of Heap(w) to the shape of G_σ. Then in Proposition 1 we show that G_σ is a forest if w is 321-hexagon-avoiding. The proof of this Proposition is rather intricate and is given as a "proof by picture." Finally, in Section 6 we conclude by a simple combinatorial argument that if G_σ is a forest, then (18) is satisfied.

The edges of G_σ will depend on how the various defects and zeros in σ are intertwined. To measure this intertwining, we overlay strings on Heap(w). In particular, we will overlay the lines $y = \pm x + C$ for $C \in \mathbb{Z}$. At each point pt(j) of our heap we will move these strings according to the following rule: If $\sigma_j = 0$, then "bounce" the strings as in figure 5(a). If $\sigma_j = 1$, then "cross" the strings as in figure 5(b).

In either case, γ_1 and γ_2 are said to *meet* at pt(j) and each of γ_1, γ_2 is said to *encounter* pt(j). If we number the strings from left to right along the bottom of our heap, reading the order of the strings at the top gives the permutation $\pi(w^\sigma)$. Figure 6 gives an example.

Remark 6 In the heap model, defects occur when two strings meet that have previously crossed an odd number of times.

Remark 7 In our diagrams, we make the following conventions. First, every diamond point is known to be a defect. Second, white nodes are known to be in our heap. Third, the inclusion of black nodes within the heap is undetermined at the time the picture is first referenced.

Suppose $j \in \mathcal{D}(\sigma)$. For the strings meeting at pt(j) to have previously crossed, they both need to have changed direction at some point (see figure 7). Formally, there must be
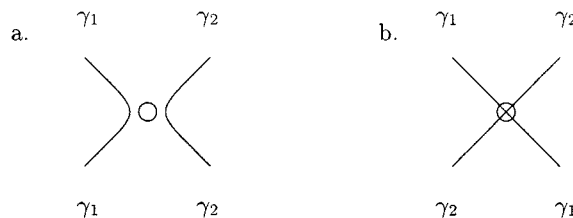

Figure 5.   Overlay of string diagram corresponding to some σ on Heap(w).
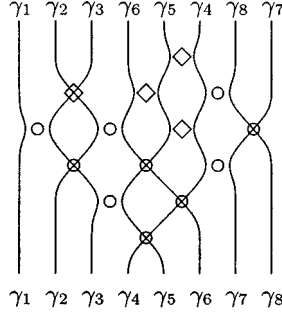
Figure 6. Heap(w) overlaid with a string diagram for the reduced expression $\mathbf{a} = s_4 s_3 s_2 s_1 s_5 s_4 s_3 s_2 s_6 s_5 s_4 s_7 s_6 s_5$ and $\boldsymbol{\sigma} = (1, 0, 1, 0, 1, 1, 0, 1, 0, 0, 1, 0, 0)$. Note that $\pi(w^\sigma) s_4 s_5 s_4 s_7$, giving the permutation $[1, 2, 3, 6, 5, 4, 8, 7]$. The defects are represented by diamonds. As an illustration of our terminology regarding strings, note that $\gamma_4 \gamma_7$ meet at pt(9) (for our reduced expression $\mathbf{a}$). And γ_6 encounters pt(j) for $j \in \{5, 6, 7, 11\}$ (also for $\mathbf{a}$).

a, b with $1 \le a \ne b < j$ and $\alpha, \beta > 0$ such that $(i_j, \mathrm{lvl}(s_{i_j})) = (i_a + \alpha, \mathrm{lvl}(s_{i_a}) + \alpha) = (i_b - \beta, \mathrm{lvl}(s_{i_b}) + \beta)$ where $\sigma_{i_a} = \sigma_{i_b} = 0$. Otherwise, the strings meeting at $(i_j, \mathrm{lvl}(s_{i_j}))$ could not have previously crossed.

Choose a, b as above and as large as possible. Call $\mathrm{lcz}(j) = \mathrm{pt}(a)$ the *left critical zero* and $\mathrm{rcz}(j) = \mathrm{pt}(b)$ the *right critical zero* of j (or of pt(j)). In terms of the heap, the left and right critical zeros ($\mathrm{lcz}(j)$ and $\mathrm{rcz}(j)$) are the closest zeros to pt(j) on the boundary of $\mathrm{Cone}_\wedge(j)$.

Now, for $j \in \mathcal{D}^0(\boldsymbol{\sigma})$, $\{\mathrm{lcz}(j), \mathrm{rcz}(j), \mathrm{pt}(j)\}$ are the *critical zeros* of j. For this reason, we will sometimes refer to pt(j) as the *middle critical zero* of j (denoted $\mathrm{mcz}(j)$). A point pt(j) is *shared* if pt(j) is a critical zero for two separate defects.

There is one final construct we will need to prove Theorem 1. Define a graph G_σ associated to σ as follows. Let the vertex set of G_σ be $\{\mathrm{ver}(j)\}_{j \in \mathcal{D}^0(\boldsymbol{\sigma})}$. The edge set consists of those $(\mathrm{ver}(j), \mathrm{ver}(k))$ for which

$$\{\mathrm{lcz}(j), \mathrm{rcz}(j), \mathrm{mcz}(j)\} \cap \{\mathrm{lcz}(k), \mathrm{rcz}(k), \mathrm{mcz}(k)\} \ne \emptyset. \tag{20}$$

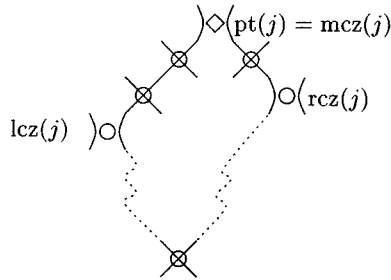In figure 8, we give an example of a heap along with its associated graph G_σ.

Figure 7. Heap showing necessity of existence of 0's on boundary of $\mathrm{Cone}_\wedge(j)$ when $j \in \mathcal{D}(\boldsymbol{\sigma})$.
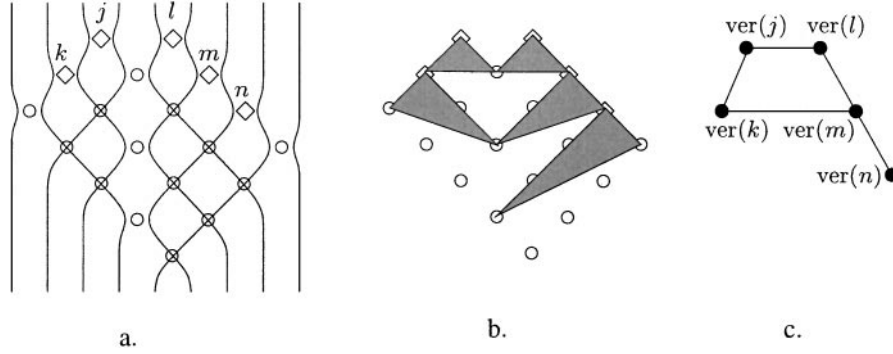
Figure 8. In (a), we depict the permutation $w = [6, 7, 8, 1, 9, 2, 3, 4, 5]$ along with the mask $\sigma = (1, 0, 1, 1,$ $0, 1, 1, 0, 1, 0, 1, 1, 1, 0, 0, 0, 0, 0, 0)$. In (b), G_σ is graphically overlaid on Heap(w). The critical zeros correspond to the corners of the triangles. In (c), we have an abstract realization of the graph.

The key fact we need in the proof of (18) is that G_σ does not contain any cycles. Before proving this fact in Proposition 1, we first introduce some lemmas that illuminate the structure of G_σ. The first two lemmas are easy and stated only for reference. The second and third give criteria for Heap(w) to contain a hexagon.

Lemma 3 *Suppose w is 321-avoiding and $k, l \in \mathcal{D}^0(\sigma)$ with $\mathrm{pt}(l) = \mathrm{lcz}(k)$. Then $\mathrm{pt}(l) + (1, -3) \in$ Heap(w). Similarly, if $\mathrm{pt}(l) = \mathrm{rcz}(k)$, then $\mathrm{pt}(l) - (1, 3) \in$ Heap(w). (See, for example, figure 9(c).)*

Lemma 4 *Let w be a 321-avoiding permutation and $\mathrm{pt}(h), \mathrm{pt}(k) \in$ Heap(w) with $\mathrm{pt}(h) \in$ Cone$_\wedge(\mathrm{pt}(k) - (0, 6))$. If h and k are encountered by a common string, then Heap(w) contains a hexagon. (See, for example, figure 9(c).)*

Lemma 5 *Let $w \in \mathfrak{S}_n$ be 321-avoiding. Heap(w) contains a hexagon if any of the following three situations are met:*
1. *The point $\mathrm{lcz}(r) = \mathrm{pt}(m) = \mathrm{rcz}(l)$ with $m, r, l \in \mathcal{D}^0(\sigma)$. (See figure 9(a).)*
2. *The string γ encounters three distinct strings $\gamma_1, \gamma_2, \gamma_3$ at defects $l, k, m \in \mathcal{D}^0(\sigma)$, respectively. Furthermore, $\mathrm{pt}(m) = \mathrm{rcz}(l)$, $\mathrm{pt}(l) = \mathrm{lcz}(k)$ and $\mathrm{pt}(m)$ is on the boundary of Cone$_\wedge(\mathrm{pt}(k) - (0, 2))$. (See figure 9(b).)*
3. *We have $\mathrm{pt}(l) = \mathrm{lcz}(k)$, $\mathrm{pt}(r) = \mathrm{rcz}(k)$ and $k, l, r \in \mathcal{D}^0(\sigma)$. (See figure 10.)*

Parts 1 and 3 of Lemma 5 tell us that any three defects in a $\vee$-shape or a $\wedge$-shape imply that our heap has a hexagon. Part 2 of Lemma 5 tells us that, under certain conditions, if one string encounters three defects, then we also have a hexagon.

Proof of part 1: A picture is given in figure 9(a). The claim follows immediately from Lateral Convexity by applying Lemma 3 to the pairs $\mathrm{pt}(l), \mathrm{pt}(m)$ and $\mathrm{pt}(r), \mathrm{pt}(m)$.
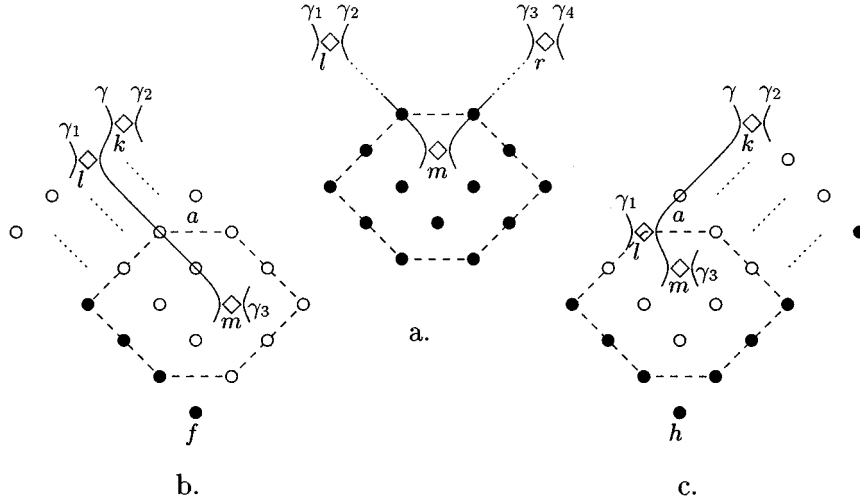
Figure 9. Illustration (a) shows the situation of Lemma 5.1. Illustrations (b, c) refer to Lemma 5.2. In these latter two pictures, it is possible that $pt(a) = pt(k)$.
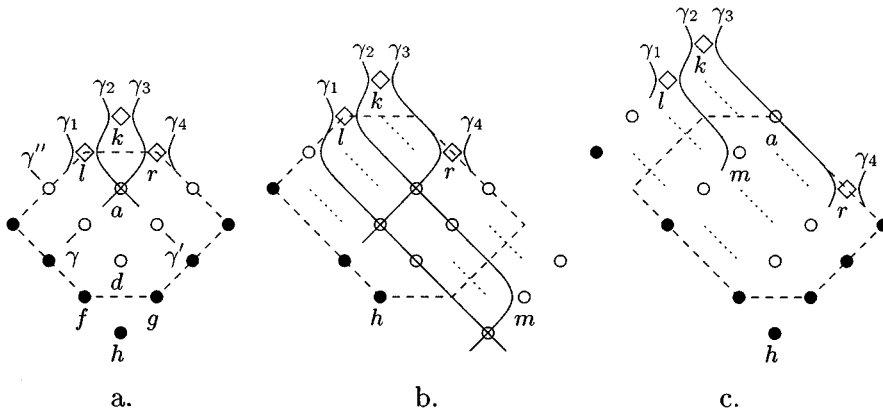

Figure 10. Situation of Lemma 5.3.

Proof of part 2: First consider the case where $pt(m) = pt(k) + (\delta, -2 - \delta)$ for $\delta \geq 1$. This is illustrated in figure 9(b). By Lemma 3, $pt(f) = pt(m) - (1, 3)$ is in $\text{Heap}(w)$. Since $pt(f) \in \text{Cone}_\wedge(pt(k) + (\delta - 1, -5 - \delta))$, $\text{Heap}(w)$ contains the indicated hexagon by Lemma 4.

Alternatively, we can have $pt(m) = pt(k) - (\delta, 2 + \delta)$ for $\delta \geq 0$. This is illustrated in figure 9(c). Recall that the γ_i are assumed to be distinct. So, starting at $pt(m) - (1, 1)$, γ must move down to the right at least twice (to cross γ_2 and γ_3), and move down to the left at least once (to cross γ_1). Hence, the lowest of the three crossings $\gamma\gamma_i$ must occur in $\text{Cone}_\wedge(pt(h)) = \text{Cone}_\wedge(pt(m) - (0, 4)) = \text{Cone}_\wedge(pt(a) - (\delta, 6 + \delta))$. By Lemma 4, $\text{Heap}(w)$ must therefore contain a hexagon.

Proof of part 3:   By Lemma 3, in order to avoid a hexagon in Heap(w), we need at least one of pt(l), pt(r) to be a distance of exactly $\sqrt{2}$ from pt(k).

Suppose first that both pt(l) = pt(k) − (1, 1) and pt(r) = pt(k) + (1, −1). Then we are in the situation of figure 10(a). Note that if $\sigma_a = 0$ then $a \in \mathcal{D}^0(\sigma)$ and we can appeal to Lemma 5.1. So we can consider only the case where there is a crossing at pt(a). If γ is either γ_1 or γ_3, then it still needs to cross a string currently to its right (either γ_2 or γ_4, respectively). This can only happen in Cone$_\wedge$(f). The only alternative is that $\gamma = \gamma''$. But then $\gamma_1\gamma_2$ cannot cross until Cone$_\wedge$(f). Either way, pt(f) $\in$ Heap(w). Arguing analogously with γ', we see that pt(g) $\in$ Heap(w). So Heap(w) contains a hexagon.

Now suppose that only one of pt(l), pt(r) is a distance of $\sqrt{2}$ away from pt(k). Without loss of generality, we assume that this point is pt(l). We argue depending on whether or not pt(r) $\in$ Cone$^\vee$(pt(m) + (0, 2)) where pt(m) = rcz(l).

Assume first that pt(r) $\in$ Cone$^\vee$(pt(m) + (0, 2)). We are in the situation of figure 10(b). Since pt(r) $\neq$ pt(k)+(1, −1), pt(m) = pt(k)+(δ, −2−δ) for some $\delta \geq 2$. Hence, in order to avoid a hexagon, we must have $\gamma_1\gamma_2$ cross as shown. But then it is easily seen that the crossing $\gamma_3\gamma_4$ must occur in Cone$_\wedge$(h). This ensures that Heap(w) contains the indicated hexagon.

If pt(r) $\notin$ Cone$^\vee$(pt(m) + (0, 2)), then we are in the situation of figure 10(c). Since γ_2 must go left once below pt(m) − (1, 1) (to cross γ_1) and γ_3 must go right once (to cross γ_4), we see that the lowest of the crossings $\gamma\gamma_i$ must occur in Cone$_\wedge$(h). If pt(r) $\neq$ pt(a), then by Lemma 4, Heap(w) contains a hexagon. If pt(r) = pt(a), then we need the additional fact that pt(m) $\neq$ pt(k) − (0, 2) to ensure that pt(h) $\in$ Cone$_\wedge$(pt(k) − (0, 6)). But this follows from the assumption that pt(r) is not at a distance of $\sqrt{2}$ from pt(k).   □

Proposition 1   *If w is 321-hexagon-avoiding and $\sigma \in \mathcal{P}(\mathbf{a})$, then G_σ is a forest.*

Proof: Assume that G_σ is not a forest—i.e., G_σ contains a cycle. We will assume that w is 321-avoiding and show that if G_σ contains a cycle then Heap(w) contains a hexagon. Note that since w is 321-avoiding, Lemma 1 (Lateral Convexity) holds.

Let $V \subset \mathcal{D}^0(\sigma)$ be a minimal subset such that the subgraph G'_σ of G_σ spanned by V is a cycle. Hence, for each $p \in V$, ver(p) $\in G'_\sigma$ has degree at least 2. Choose $C \in Z$ as large as possible such that pt(j) is on the line $y = x + C$ for some $j \in V$. Now choose $l \in V$ to be minimal among such j. By choice of V, pt(m) = rcz(l) must be shared and we must have pt(l) = lcz(k) for some $k \in V$. So our heap looks like figure 11(a).

In the discussion that follows, "shared" should be interpreted in the context of G'_σ.

Since V is minimal, either pt(k) = lcz(u) for some $u \in V$, or pt(p) = rcz(k) is shared. In the first case, pt(p) + (1, 1) must be in Heap(w) by Lateral Convexity. Consider the second case—where pt(p) is shared. By Lemma 5.3, $p \notin V$. So pt(p) = lcz(r) for some $r \in V$. So in both cases, we have the following fact which we state for reference.

Fact 1   *If pt(p) = rcz(k), then pt(q) = pt(p) + (1, 1) $\in$ Heap(w).*

Two other simple facts we state for reference are the following.

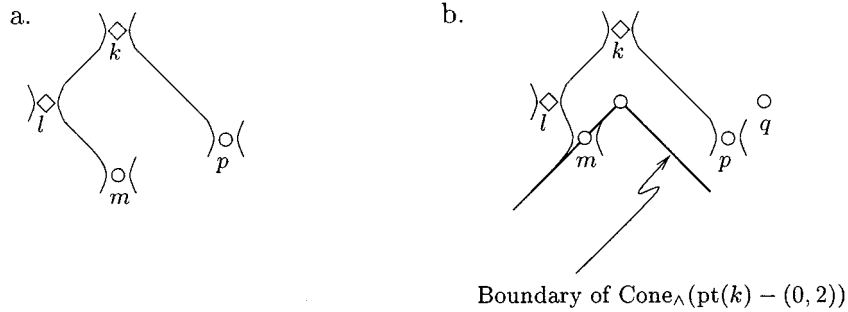a.

b.

Boundary of $\mathrm{Cone}_\wedge(\mathrm{pt}(k) - (0, 2))$

Figure 11. Configuration of Heap(w). Recall that diamond nodes are known defects and white nodes are known to be in Heap(w).

Fact 2 *By Lateral Convexity, any point encountered by a string that still needs to cross below that point must be in the heap (after pushing together connected components). For example, if $j \in \mathcal{D}(\sigma)$, then $pt(j) - (0, 2)$ must be in the heap.*

Fact 3 *Recall that* $\mathrm{pt}(m)$ *is defined as right critical zero of the left critical zero of* $\mathrm{pt}(k)$ *(see figure 11(b)). If* Heap(w) *does not contain a hexagon, then the point m must lie along the boundary of* $\mathrm{Cone}_\wedge(\mathrm{pt}(k) - (0, 2))$.

We now show that, regardless of the characteristics of m (i.e., values of i_m, lvl(m), and whether or not $m \in \mathcal{D}(\sigma)$), Heap($w$) must contain a hexagon. Suppose that $m \in V$. By Lemma 5.2, the only way this can happen is if the other string encountering $\mathrm{pt}(m)$ is γ_3. Since V is minimal, we then need either lcz(m) or rcz(m) shared. Consider figure 12. Suppose $\mathrm{pt}(n) = \mathrm{lcz}(m)$ is shared. By choice of $\mathrm{pt}(k)$ on the line $y = x + C$, this implies that $n \in V$. But then by Lemma 3, $\mathrm{pt}(h) \in$ Heap(w). Then by Lateral Convexity, $\mathrm{pt}(e) \in$ Heap(w). The alternative is that rcz(m) is shared. Again, this implies that $\mathrm{pt}(e) \in$ Heap(w). Since $\mathrm{pt}(q) \in$ Heap(w) by Fact 1, Heap(w) contains a hexagon.
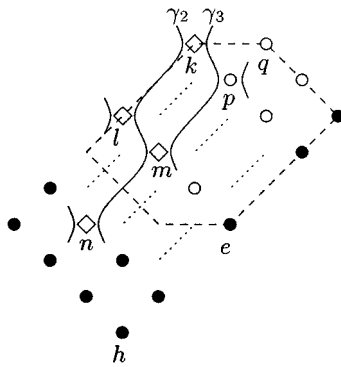
Figure 12. This figure depicts the case where $\mathrm{pt}(m)$ is not the left critical zero of another defect in V.
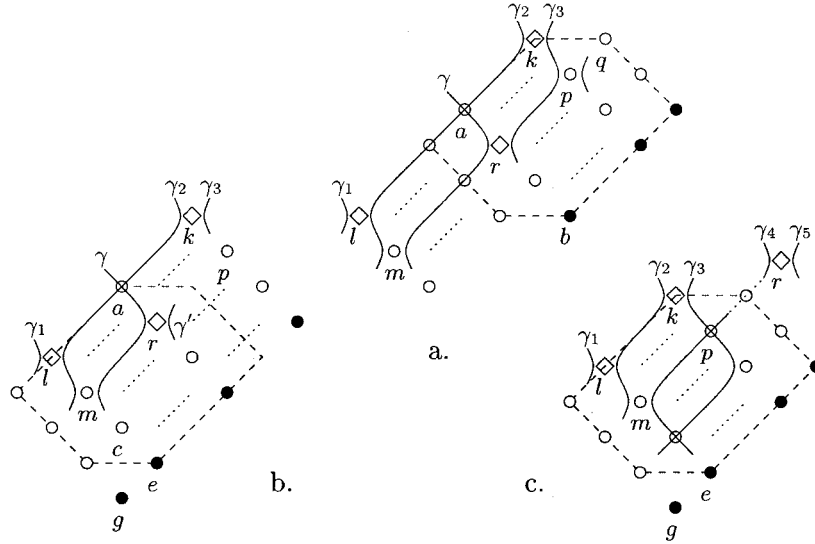
Figure 13.   Case I of proof of Proposition 1.

So we can assume that $m \notin V$. But by choice of l, $\mathrm{pt}(m)$ must be shared. This implies that $\mathrm{pt}(m) = \mathrm{lcz}(r)$ for some $r \in V$. We now argue that $\mathrm{Heap}(w)$ must contain a hexagon according to the position of $\mathrm{pt}(m)$ relative to $\mathrm{pt}(k)$.

Case I: $\mathrm{pt}(m) = \mathrm{pt}(k) - (\delta, 2 + \delta)$ for $\delta \geq 0$. There are three cases to consider. Figure 13(a) depicts the first. Here, γ and γ_3 both encounter $\mathrm{pt}(r)$. Since V is minimal, either $\mathrm{rcz}(r)$ or $\mathrm{pt}(r)$ must be shared. By choice of our line $y = x + C$ and the fact that $p \notin V$, we see that, in fact, $\mathrm{rcz}(r)$ must be shared. But then $\mathrm{pt}(b) \in \mathrm{Heap}(w)$. Since $\mathrm{pt}(q) \in \mathrm{Heap}(w)$, $\mathrm{Heap}(w)$ contains the indicated hexagon.

The second alternative is that $\mathrm{pt}(r) \in \mathrm{Cone}_\wedge(\mathrm{pt}(k))$ but γ_3 does not encounter γ along any of the nodes between $\mathrm{pt}(m)$. This is depicted in figure 13(b). If $\sigma_c = 0$, then $\gamma_2\gamma_3$ must cross in $\mathrm{Cone}_\wedge(g)$. If $\sigma_c = 1$, then $\gamma\gamma'$ must cross in $\mathrm{Cone}_\wedge(e)$. In either case, $\mathrm{Heap}(w)$ must contain the indicated hexagon.

The third possibility is that $\mathrm{pt}(r) \notin \mathrm{Cone}_\wedge(\mathrm{pt}(k))$ (Figure 13(c)). In fact, this is the only possibility for $\mathrm{pt}(r)$ when $\delta = 0$. Here we see that the path of γ_3 must be as shown in order to avoid $\mathrm{Cone}_\wedge(g)$. But then $\gamma_4\gamma_5$ cannot cross until $\mathrm{Cone}_\wedge(e)$. So we have the indicated hexagon.

Case II: $\mathrm{pt}(m) = \mathrm{pt}(k) + (\delta, -2 - \delta)$ for some $\delta \geq 1$. The situation is depicted in figure 14(a). For both $\gamma_1\gamma_2$ and $\gamma_2\gamma_3$ to cross outside of $\mathrm{Cone}_\wedge(h)$, we need $\gamma_2\gamma_3$ to cross in $\mathrm{Cone}^\vee(m)$. This is shown in figure 14(b). We mention three additional assertions we have made in figure 14(b). First, γ_1 must cross γ_2 as shown in figure 14(b) in order to avoid having $\mathrm{Heap}(w)$ contain a hexagon. Second, $\mathrm{pt}(q) \in \mathrm{Heap}(w)$ by Fact 1. Third, since $\mathrm{rcz}(m)$ must be shared, $\mathrm{pt}(e) \in \mathrm{Heap}(w)$ as shown. So, by Lateral Convexity, $\mathrm{Heap}(w)$ contains the hexagon indicated in figure 14(b). (It is possible that $\mathrm{pt}(a) = \mathrm{pt}(p)$ or $\mathrm{pt}(a) = \mathrm{pt}(k)$, but this does not change our conclusion.)
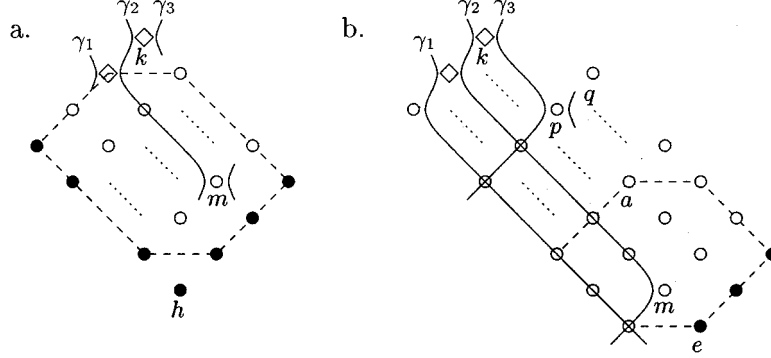
Figure 14. Case II of proof of Proposition 1.

6. Proof of Theorem 1

We present one remaining needed lemma and then the proof of Theorem 1.

In the following lemma, we let $\mathbf{a} = s_{i_1} \cdots s_{i_r}$ be a reduced expression for w and set $s = s_{i_r}$. Then let $\mathbf{a}/s$ denote the truncated reduced expression $s_{i_1} \cdots s_{i_{r-1}}$ for ws.

Lemma 6 *Let $s \in S$, $ws < w$. Then*

$$P_x(\mathbf{a}) = q^{c_s(x)} P_x(\mathbf{a}/s) + q^{1-c_s(x)} P_{xs}(\mathbf{a}/s), \tag{21}$$

$$\text{where } c_s(x) = \begin{cases} 1, & \text{if } xs < x, \\ 0, & \text{if } xs > x. \end{cases} \tag{22}$$

Proof: Partition $\mathcal{P}_x(\mathbf{a}) = \mathcal{P}_x^0(\mathbf{a}) \dot\cup \mathcal{P}_x^1(\mathbf{a})$ where $\mathcal{P}_x^\epsilon(\mathbf{a})$ consists of all masks in $\mathcal{P}_x(\mathbf{a})$ ending in ϵ for $\epsilon \in \{0, 1\}$. There are natural bijections $\mathcal{P}_x^1(\mathbf{a}) \approx \mathcal{P}_{xs}(\mathbf{a}/s)$ and $\mathcal{P}_x^0(\mathbf{a}) \approx \mathcal{P}_x(\mathbf{a}/s)$ given by $\sigma \mapsto \sigma[r-1]$. So, to prove the lemma, we need only compare $|\mathcal{D}(\sigma)|$ to $|\mathcal{D}(\sigma[r-1])|$

If $\sigma \in \mathcal{P}_x^0(\mathbf{a})$, then $\sigma[r-1] \in \mathcal{P}_x(\mathbf{a}/s)$. In this case, if $xs > x$ ($c_s(x) = 0$), then $r \notin \mathcal{D}(\sigma)$, so $|\mathcal{D}(\sigma[r-1])| = |\mathcal{D}(\sigma)|$. Alternatively, if $xs < x$ ($c_s(x) = 1$), then $\mathcal{D}(\sigma) = \mathcal{D}(\sigma[r-1]) \cup \{r\}$ and $|\mathcal{D}(\sigma)| = |\mathcal{D}(\sigma[r-1])| + 1$. This accounts for the first term in (21).

Since $c_s(xs) = 1 - c_s(x)$, proof of the second term in (21) reduces to the above case. $\qquad\square$

Proof of Main Theorem. $1 \Longrightarrow 2$:

Assume w is 321-hexagon-avoiding. We need to show that the $P_x(\mathbf{a})$ are the Kazhdan-Lusztig polynomials.

Now, every $j \in \mathcal{D}^0(\sigma)$ has three critical zeros. Furthermore, by Lemma 5, no point is a critical zero for 3 distinct defects. So the number of edges in G_σ equals the number of

shared critical zeros. Hence,

$$\text{\# of } 0's \text{ in } \{\sigma_1, \ldots, \sigma_r\} \geq \text{\# of critical zeros in } \{\sigma_1, \ldots, \sigma_r\} \tag{23}$$

$$= 3 \cdot |\mathcal{D}^0(\boldsymbol{\sigma})| - (\text{\# of edges in } G_{\boldsymbol{\sigma}}). \tag{24}$$

Now, by Proposition 1, $G_{\boldsymbol{\sigma}}$ is a forest with $|\mathcal{D}^0(\boldsymbol{\sigma})|$ vertices. Hence, $G_{\boldsymbol{\sigma}}$ has at most $|\mathcal{D}^0(\boldsymbol{\sigma})| - 1$ edges (see, e.g., [4]). Hence,

$$\text{\# of } 0's \text{ in } \{\sigma_1, \ldots, \sigma_r\} \geq 2 \cdot |\mathcal{D}^0(\boldsymbol{\sigma})| + 1. \tag{25}$$

So by Lemma 2, $\Delta_{\boldsymbol{\sigma}} \geq 0$. Therefore the inequality $|\mathcal{D}(\boldsymbol{\sigma})| \leq \frac{1}{2}(l(w) - l(\pi(w^{\sigma}))) - 1)$ holds. Now apply Theorem 3, from which it follows that $P_x(\mathbf{a}) = P_{x,w}$ for all $x \in W$.

$2 \Longrightarrow 1:$

We shall prove (not 1) $\Longrightarrow$ (not 2). Assume w is not 321-avoiding. We can find a reduced expression for w of the form $\mathbf{a} = vs_i s_{i\pm1} s_i v'$ with $l(w) = l(v) + l(v') + 3$. Set

$$\boldsymbol{\sigma} = (\overbrace{1, \ldots, 1}^{l(v)}, 1, 0, 0, \overbrace{1, \ldots, 1}^{l(v')}). \tag{26}$$

Then $|\mathcal{D}^0(\boldsymbol{\sigma})| = 1$ and $|\{j : \sigma_j = 0\}| = 2$. By Lemma 2, $\Delta_{\boldsymbol{\sigma}} < 0$. So $P_x(\mathbf{a})$ does not satisfy the properties of the $P_{x,w}$ listed in Theorem 2.

Now assume w is 321-avoiding but not hexagon avoiding. Then we can write $w = vu^j v'$ where u^j as in Section 2 and $l(w) = l(v) + l(v') + 14$. Set

$$\boldsymbol{\sigma} = (\overbrace{1, \ldots, 1}^{l(v)}, 1, 1, 0, 1, 0, 1, 0, 1, 1, 0, 0, 0, 0, 0, \overbrace{1, \ldots, 1}^{l(v')}). \tag{27}$$

The mask $\boldsymbol{\sigma}$ is depicted graphically in figure 15. Then $|\mathcal{D}^0(\boldsymbol{\sigma})| = 4$ and $|\{j : \sigma_j = 0\}| = 8$. By Lemma 2, $\Delta_{\boldsymbol{\sigma}} < 0$. So $P_x(\mathbf{a})$ does not satisfy the properties of the $P_{x,w}$ listed in Theorem 2.

$2 \Longrightarrow 3:$

We first appeal to a result of Kazhdan and Lusztig relating the intersection Poincaré polynomial of the Schubert variety X_w to the Kazhdan-Lusztig polynomials $P_{x,w}$ (22, [Corollary 4.9]):

$$\sum_i \dim(\text{IH}^{2i}(X_w))q^i = \sum_{x \leq w} q^{l(x)} P_{x,w}(q). \tag{28}$$

Now, we are assuming that $P_x(\mathbf{a}) = P_{x,w}$ for all $x \in \mathfrak{S}_n$. So we need only show that

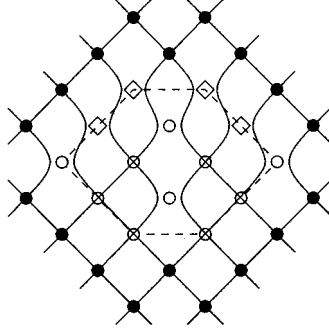$$\sum_{x \leq w} q^{l(x)} P_x(\mathbf{a}) = (1+q)^{l(w)}. \tag{29}$$

Figure 15. Heap view of mask in (27). The black nodes are not known to be in the heap.

We proceed by induction, the result being obvious for $l(w) = 1$. Choose an $s \in S$ such that $ws < w$. From [20, Lemma 7.4], we know that:

$$\text{If } ws < w, \quad \text{then } x \leq w \iff xs \leq w. \tag{30}$$

Using (30), along with Lemma 6, we can write

$$\sum_{x \leq w} q^{l(x)} P_x(\mathbf{a}) = \sum_{x \leq w, \ x < xs} q^{l(x)} P_x(\mathbf{a}) + q^{l(xs)} P_{xs}(\mathbf{a}) \tag{31}$$

$$= (1 + q) \sum_{x \leq w, \ x < xs} q^{l(x)} (P_x(\mathbf{a}/s) + q P_{xs}(\mathbf{a}/s)) \tag{32}$$

$$= (1 + q) \sum_{x \leq w, \ x < xs} q^{l(x)} P_x(\mathbf{a}/s) + q^{l(xs)} P_{xs}(\mathbf{a}/s). \tag{33}$$

If $P_x(\mathbf{a}/s) \neq 0$, then $x \leq ws$, so this becomes

$$= (1 + q) \sum_{x \leq ws} q^{l(x)} P_x(\mathbf{a}/s) \tag{34}$$

$$= (1 + q)(1 + q)^{l(ws)} = (1 + q)^{l(w)}. \tag{35}$$

The last line is by the induction hypothesis.

$$3 \implies 2:$$

Deodhar [15] proves that for any Weyl group W, we can always find a subset $\mathcal{S} \subset \mathcal{P}(\mathbf{a})$ such that

$$\sum_{\substack{\sigma \in \mathcal{S} \\ \pi(w^\sigma) = x}} q^{|\mathcal{D}(\sigma)|} = P_{x,w} \tag{36}$$

for all $x, w \in W$. (More generally, he shows that such an $\mathcal{S}$ exists when the coefficients of

$P_{x,w}$ are already known to be non-negative. Due to their interpretation in terms of dimensions of intersection cohomology groups, this is known for any Weyl group.)

Hence, for such an $\mathcal{S}$, we have the following string of equalities:

$$(1+q)^{l(w)} = \sum_i \dim(\mathrm{IH}^{2i}(X_w))q^i = \sum_{x \leq w} q^{l(x)} P_{x,w} = \sum_{\substack{\sigma \in \mathcal{S} \\ \pi(w^\sigma)=x}} q^{l(x)} q^{|\mathcal{D}(\sigma)|}. \qquad (37)$$

Setting $q = 1$, we find that $2^{l(w)} = |\mathcal{S}|$. But then $S = \mathcal{P}(\mathbf{a})$. So $P_x(\mathbf{a}) = P_{x,w}$ for all $x, w \in \mathfrak{S}_n$.

$2 \Longleftrightarrow 4$:

This follows from Deodhar [15, Proposition 3.5 and Corollary 4.8].

$3 \Longrightarrow 5$:

This is the content of Deodhar [15, Proposition 3.9].

$5 \Longrightarrow 6$:

This is a standard result on small resolutions. See, for example, [23, Section 6.5].

$6 \Longrightarrow 3$:

Recall that Y denotes the Bott-Samelson resolution of X_w (corresponding to some reduced expression $\mathbf{a}$). By [5, Proposition 4.2],

$$\sum_i \dim(H^{2i}(Y))q^i = (1+q)^{l(w)}. \qquad (38)$$

We are assuming that $H_*(Y) \cong \mathrm{IH}_*(X_w)$. By Poincaré duality, we know that $H^{2i}(Y) \cong \mathrm{IH}^{2i}(X_w)$. Combining (30) with this isomorphism yields

$$\sum_i \dim(\mathrm{IH}^{2i}(X_w))q^i = (1+q)^{l(w)} \qquad (39)$$

as desired.

This completes the proof of the Theorem 1.   □

Corollary 1   *If $w = s_{i_1} \cdots s_{i_r}$ with $i_1, \ldots, i_r$ all distinct, then $P_{x,w} = 1$ for all $x \leq w$.*

7.   A conjecture of Haiman and a generalization

Define q-Fibonacci numbers by $F_n(q) = F_{n-1}(q) + q F_{n-2}(q)$ where $F_n(q) = 0$ if $n < 0$ and $F_0(q) = F_1(q) = 1$. Theorem 1 gives us a simple proof of the following conjecture of Haiman ([9, Conjecture 7.18]):

Corollary 2 *Let $w_{k,l} \in \mathfrak{S}_n$ have reduced expression*

$$\mathbf{a} = s_k s_{k-1} s_{k+1} s_k \cdots s_l s_{l-1} \in \mathfrak{S}_n, \ 2 \leq k < l < n. \tag{40}$$

Then $P_{e,w_{k,l}} = F_{l-k+1}(q)$.

Recently, Brenti-Simion [10] have independently proved this conjecture and generalized it to a class of elements that are not 321-hexagon-avoiding. In fact, the corollary can be generalized to apply to any 321-hexagon-avoiding element for which no generator appears more than twice.

Proof: As a permutation,

$$w = [1, 2, \ldots, k-2, k+1, \ldots, l+1, k-1, k, l+2, \ldots, n]. \tag{41}$$

This is easily seen to be 321-hexagon-avoiding. So by Theorem 1, $P_e(\mathbf{a}) = P_{e,w_{k,l}}$.

The claim is true for $l = k$. The proof is by induction. The situation of the general case is illustrated in figure 16 for some $\sigma \in \mathcal{P}_e(\mathbf{a})$. Let $r = l(w)$. In figure 16(b), no new defect is introduced by γ, so $|\mathcal{D}(\sigma)| = |\mathcal{D}(\sigma[r-2])|$. In figure 16(c), we have $|\mathcal{D}(\sigma)| = |\mathcal{D}(\sigma[r-4])| + 1$. The claim follows by the induction hypothesis. $\square$

We give below the generalization where Heap(w) is a $3 \times (l-k+1)$ diamond rather than a $2 \times (l-k+1)$ diamond.

Theorem 4 *Suppose $v_{k,l} \in \mathfrak{S}_n$ has reduced expression*

$$\mathbf{a} = s_l s_{l+1} s_{l+2} s_{l-1} s_l s_{l+1} \cdots s_k s_{k+1} s_{k+2} \tag{42}$$
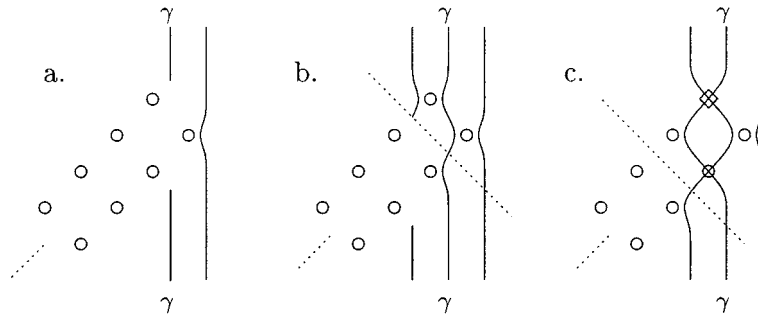

Figure 16. It is clear that γ must remain in its column in order for $\pi(w^\sigma) = e$. This is shown in (a). Diagrams (b) and (c) show the only two possibilities for the path of γ.
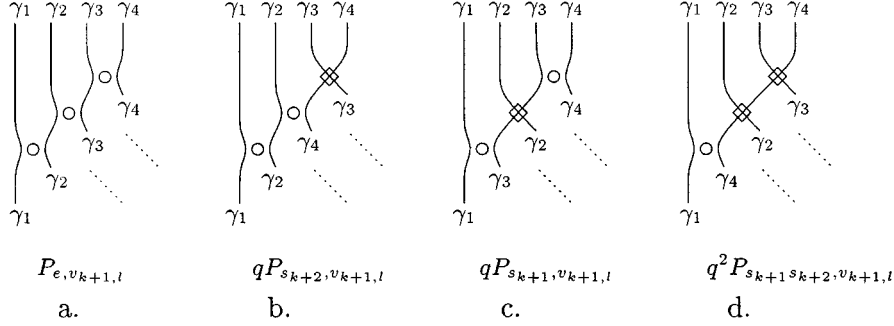
$$P_{e,v_{k+1,l}} \qquad qP_{s_{k+2},v_{k+1,l}} \qquad qP_{s_{k+1},v_{k+1,l}} \qquad q^2 P_{s_{k+1}s_{k+2},v_{k+1,l}}$$

a.   b.   c.   d.

Figure 17. Terms contributing to $p_e, v_{k,l}$.

for some $1 \le k \le l < n - 2$. Then $P_{e,v_{k,l}} \in \mathbb{Z}[q]$ is given by the coefficient of z^{l-k+1} in the generating function

$$G_e(z) = \frac{-1 + q^2 z^2 + q^3 z^3}{(1 + qz + q^2 z^2)(-1 + z + qz + qz^2 + q^2 z^2 + q^2 z^3 - q^4 z^4)}.$$

Proof: We only sketch the proof. We see that $v_{k,l}$ is clearly 321-hexagon-avoiding, so by Theorem 1, $P_{x,w} = P_{x(\mathbf{a})}$. The idea is to use recursion on $n = l - k$. From figure 17, it is easy to see that $P_{e,v_{k,l}} = P_{e,v_{k+1,l}} + q P_{s_{k+1},v_{k+1,l}} + q P_{s_{k+2},v_{k+1,l}} + q^2 P_{s_{k+1}s_{k+2},v_{k+1,l}}$. Similar recurrences can be found for $P_{x,v_{k,l}}$ where $x \in \mathfrak{S}_4$. Solving these recurrences for $P_{e,v_{k,l}}$ yields (4). □

8. Singular loci of 321-hexagon-avoiding elements

The Schubert variety X_w is said to be *singular* at a point $x \le w$ (or, more properly, on the Schubert cell $C_x \subset X_w$) if the Zariski tangent space to X_w at x has dimension strictly greater than $l(w)$. The set of singular points forms a lower order ideal in the Bruhat-Chevalley order ([3]). We define X_w^{sing} to consist of the maximal elements (under this Bruhat-Chevalley order) of the set $\{x \in \mathfrak{S}_n : x \le w \text{ and } x \text{ singular}\}$.

The following theorem gives a complete description of X_w^{sing} when w is 321-hexagon-avoiding. In fact, this proves a conjecture of Lakshmibai and Sandhya [25] in this special case.

Theorem 5 *Let $w \in \mathfrak{S}_n$ be 321-hexagon-avoiding (hence $\mathrm{Heap}(w)$ is well-defined). Then every diamond with vertices (x, y), $(x - \alpha, y - \alpha)$, $(x + \beta, y - \beta)$, $(x - \alpha + \beta, y - \alpha - \beta)$, $\alpha, \beta > 0$ in the heap determines an element in X_w^{sing}. More explicitly, let*

$$
\begin{aligned}
T = \{(j, k, l) \in \mathbb{Z}^3 : 1 &\le j, k, l \le r, \ \mathrm{pt}(j) = \mathrm{pt}(k) - (\alpha, \alpha), \\
\mathrm{pt}(l) &= \mathrm{pt}(k) + (\beta, -\beta) \text{ for some } \alpha, \beta > 0, \\
\text{and } &\mathrm{Cone}_\wedge(j) \cap \mathrm{Cone}_\wedge(l) \cap \mathrm{Heap}(w) \ne \emptyset\}
\end{aligned}
\tag{43}
$$

and

$$\Sigma = \{\sigma \in \mathcal{P}(\mathbf{a}) : (j, k, l) \in T, \ \sigma_j = \sigma_k = \sigma_l = 0,$$
$$\text{and } \sigma_m = 1 \text{ for } m \neq j, k, l\}. \tag{44}$$

Then the maximal singular locus X_w^{sing} of X_w is given by $X_w^{\text{sing}} = \{\pi(\sigma) : \sigma \in \Sigma\}$.

Proof: It has been proved by Deodhar [14] that for $W = \mathfrak{S}_n$ and $v \leq w$, X_w is smooth on the Schubert cell C_v if and only if $P_{v,w} = 1$. By Theorem 1, $\mathcal{P}_x(\mathbf{a}) = P_{x,w}$ for every $x \in \mathfrak{S}_n$. So to show that X_w is singular, we need only show that $\mathcal{P}(\mathbf{a})$ contains a mask of positive defect.

Let $\sigma \in \Sigma$ correspond to $(j, k, l) \in T$. Since every defect must have two critical zeros (in addition to the defect itself), $l(w) - l(\pi(\sigma)) = 3$. Lateral Convexity tells us that if $l(w) - l(\pi(\sigma)) < 3$ for some other $\sigma \in \mathcal{P}(\mathbf{a})$, then $|\mathcal{D}(\sigma)| = 0$. So for $\sigma \in \Sigma$, if X_w is singular at $C_{\pi(\sigma)}$, $\pi(\sigma)$ is maximally singular. Now, the conditions in (43) imply that $k \in \mathcal{D}(\sigma)$. By Theorem 1, this implies that $P_{\pi(\sigma),w} \neq 1$. So $\{\pi(\sigma) : \sigma \in \Sigma\} \subseteq X_w^{\text{sing}}$.

The only fact that remains to be checked is that if y is a singular point of X_w, then $y \leq \pi(\sigma)$ for some $\sigma \in \Sigma$. So pick some $\sigma \in \mathcal{P}_y(\mathbf{a})$ with $|\mathcal{D}(\sigma)| \geq 1$. Choose $b \in \mathcal{D}(\sigma)$ and suppose $\text{pt}(a) = \text{lcz}(b)$ and $\text{pt}(c) = \text{rcz}(b)$. Now define a mask σ' by setting

$$\sigma'_m = \begin{cases} 1, & m \notin \{a, b, c\}, \\ 0, & m \in \{a, b, c\}. \end{cases} \tag{45}$$

Using the characterization of Bruhat-Chevalley order in terms of subexpressions (see, e.g., [20]), it is easily checked that $\pi(\sigma) \leq \pi(\sigma')$. Since σ' is in Σ, we are done. □

Corollary 3 *For w 321-hexagon-avoiding, each element of X_w^{sing} has codimension 3 in X_w.*

Example 2 Here we give an example of calculating the singular locus as in Theorem 5. We have set $w = s_2 s_1 s_5 s_4 s_3 s_2 s_6 s_5 s_4 s_3$. Figure 18 illustrates the eight different points in the maximal singular locus of X_w. Namely,

$$X_w^{\text{sing}} = \{[3, 1, 6, 2, 7, 4, 5], [1, 6, 3, 2, 7, 4, 5], [3, 1, 6, 4, 2, 7, 5],$$
$$[3, 1, 6, 5, 2, 4, 7], [1, 3, 7, 2, 6, 4, 5], [3, 2, 6, 1, 4, 7, 5],$$
$$[3, 2, 6, 1, 5, 4, 7], [3, 4, 6, 1, 2, 5, 7]\}.$$

Example 3 For $v_{1,4}$ as in Theorem 4, $|X_w^{sing}| = 18$.

Remark 8 Let $w = [w(1), \ldots, w(n)]$. A result of Lakshmibai and Sandhya [25, Theorem 1] is that X_w is nonsingular if an only if w avoids [3 4 12] and [4 2 31]. It is shown in [12] that X_w is non-singular precisely when $P_{e,w} = 1$. So from Theorem 1 and Corollary 1, we see that if w is 321-hexagon-avoiding and X_w is singular, then we must be able to find a [3 4 12]-sequence in w.
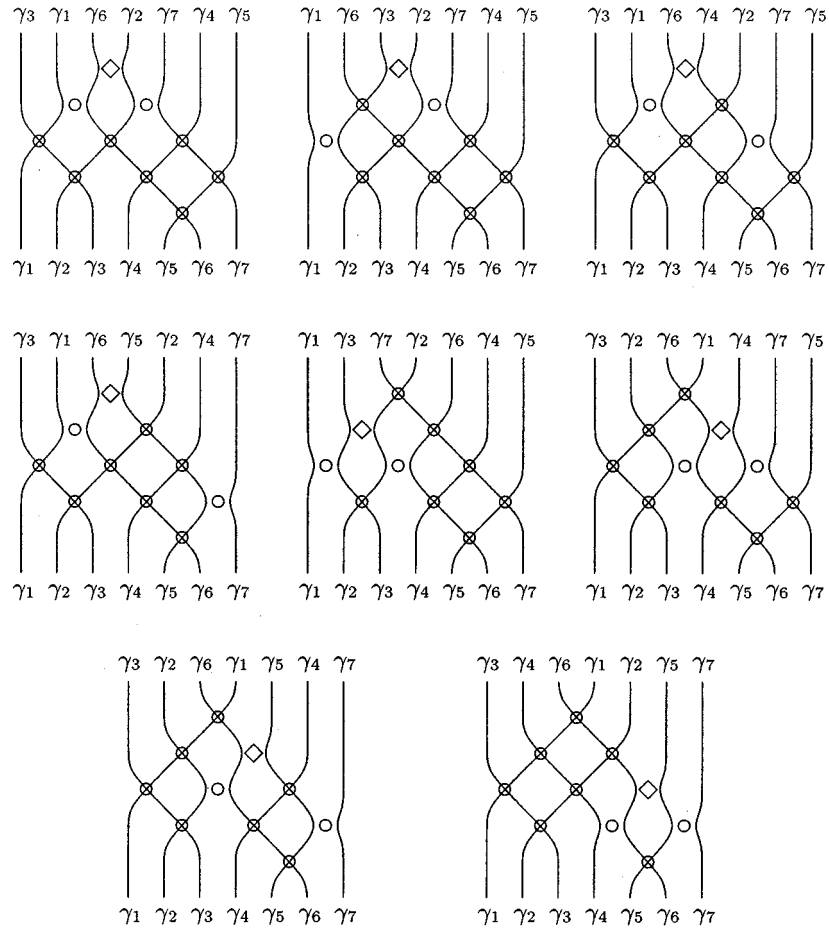
Figure 18.   Description of X_w^{sing} for example 2.

9.   Example and enumeration of 321-hexagon-avoiding elements

Table 1 lists both the number of 321-avoiding elements in $\mathfrak{S}_n$ and the number of 321-hexagon-avoiding elements in $\mathfrak{S}_n$ for $7 \leq n \leq 13$ (these numbers are equal for $n \leq 7$). The number of 321-hexagon-avoiding elements has been calculated by computer. The number of 321-avoiding elements is well-known to be given by the Catalan numbers (see, e.g., [2, 24, 29]).

Below we give an example showing the use of Theorem 1 for calculating $P_{x,w}$.

Example 4   Here we calculate $P_{x,w}$ for $w = s_2 s_1 s_3 s_2 s_4 s_3$. As a permutation, w is [3 4 5 1 2], which is clearly 321-hexagon-avoiding. (Note that $w = w_{2,4}$ in the sense of Corollary 2.) It is a result of Deodhar that for each $x \leq w$, there exists a unique mask in $\mathcal{P}_x(\mathbf{a})$ of defect 0. Table 2 lists all of the $\sigma \in \mathcal{P}(\mathbf{a})$ for which $|\mathcal{D}(\sigma)| > 0$. For this w, all of these

Table 1.   Number of 321-hexagon-avoiding elements in $\mathfrak{S}_n$.

n	7	8	9	10	11	12	13
321-avoiding	429	1430	4862	16796	58786	208012	742900
321-hexagon-avoiding	429	1426	4806	16329	55740	190787	654044

Table 2.   Computing $P_{x,w}$ using the defect statistic.

$s_2s_1s_3s_2s_4s_3$	$\pi(w^\sigma)$	$s_2s_1s_3s_2s_4s_3$	$\pi(w^\sigma)$
0 0 1 0 0 1	e	1 1 1 0 0 1	s_2s_1
1 0 0 1 0 0	e	1 0 0 0 0 1	s_2s_3
0 1 1 0 0 1	s_1	1 0 1 0 0 0	s_2s_3
1 0 1 0 0 1	s_2	1 0 1 1 0 1	s_3s_2
1 0 0 0 0 0	s_2	1 0 0 1 1 1	s_4s_3
1 0 0 1 0 1	s_3	1 0 0 0 1 0	s_2s_4
0 0 1 0 0 0	s_3	1 0 0 0 1 1	$s_2s_4s_3$
1 0 0 1 1 0	s_4	1 0 1 1 0 0	$s_2s_3s_2$
0 1 1 0 0 0	s_1s_3	1 1 1 0 0 0	$s_2s_1s_3$

masks happen to have $|\mathcal{D}(\sigma)| = 1$. Hence, we see that for $x \leq w$,

$$
P_{x,w} = \begin{cases}
1 + 2q, & \text{if } x \in \{e, s_2, s_3, s_2s_3\}, \\
1 + q, & \text{if } x \in \{s_1, s_4, s_1s_3, s_2s_1, s_3s_2, s_4s_3, \\
& \qquad s_2s_4, s_2s_4s_3, s_2s_3s_2, s_2s_1s_3\}, \\
1, & \text{otherwise.}
\end{cases}
\tag{46}
$$

Acknowledgments

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