KAZHDAN-LUSZTIG POLYNOMIALS FOR
321-HEXAGON-AVOIDING PERMUTATIONS

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ABSTRACT. In [23], 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 $W = S_n$ (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 ($B_n, F_4, G_2$).

In memory of Rodica Simion

1. INTRODUCTION

In [23], 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 [3, 13]). Introductions to these polynomials can be found in [11, 18, 22].

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 [23], 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) [24], but not for arbitrary Coxeter groups. There has been limited success in finding non-recursive formulas for the Kazhdan-Lusztig polynomials. Brenti [9, 10] has given a non-recursive formula in terms of an alternating sum over paths in the Bruhat graph. Lascoux and Schützenberger [3] 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 [28] extends the results of [3] to twisted vexillary permutations. Finally, Shapiro, Shapiro and Vainshtein [4] and Brenti and Simion [12] find explicit formulas for certain classes of permutations.

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Deodhar [17] 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 $w \in \mathcal{S}_n$. 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 Section 2 and Section 3):

**Theorem 1.** Let $a = s_{i_1} \cdots s_{i_r}$ be a reduced expression for $w \in \mathcal{S}_n$. 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
   \begin{equation}
   P_{x,w} = \sum q^{d(\sigma)}
   \end{equation}
   where $d(\sigma)$ is the defect statistic and the sum is over all masks $\sigma$ on $a$ whose product is $x$.
3. The Poincaré polynomial for the full intersection cohomology group of $X_w$ is
   \begin{equation}
   \sum_i \dim(IH^{2i}(X_w))q^i = (1 + q)^{l(w)}.
   \end{equation}
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. $\text{IH}_*(X_w) \cong H_*(Y)$, where $Y$ is the Bott-Samelson resolution of $X_w$.

**Remark 1.** Equivalence of 2, 4 and 5 is implicit in Deodhar [17].

**Remark 2.** Lusztig [29] and Fan and Green [21] 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 \implies 1 of Theorem 1.

**Remark 3.** For concreteness, this paper refers only to $\mathcal{S}_n$. However, 2 through 6 hold for all Weyl groups. In addition, our combinatorial characterization of 3 \iff 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” \implies “short-braid-hexagon-avoiding”). The characterization in 2 fails to hold for $D_n, E_6, E_7, E_8$ primarily due to failure of Lemma 3. 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 $\mathcal{S}_n$ for which Theorem 1 applies. We do not know a closed form for this sequence.

2. Preliminaries

Let $\mathcal{S}_n$ denote the symmetric group on $n$ letters. Choose the standard presentation $\mathcal{S}_n = \langle s_1, \ldots, s_{n-1} : s_i^2 = 1, s_is_j = s_js_i$ for $|i - j| > 1, and $s_is_{i+1}s_i = s_{i+1}s_is_{i+1}$. Let $S = \{s_i\}_{i \in [1, \ldots, n]}$ denote the generating set for $\mathcal{S}_n$. An expression is any product of generators $s_i$. The length $l(w)$ of an element $w \in \mathcal{S}_n$ is the minimum $r$ for which we have an expression $w = s_i \cdots s_l$. A reduced expression $w = s_i \cdots s_l$ is an expression for which $l(w) = r$. If $v, w, \in \mathcal{S}_n$, then $v \leq w$ will signify that $v$ is below $w$ in the Bruhat-Chevalley order (see, e.g., [23]).

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 $W = \mathcal{S}_n$.

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

\begin{align*}
(3) & \quad T_s T_w = T_{sw} \text{ if } l(sw) > l(w), \\
(4) & \quad T_s^2 = (q - 1)T_s + qT_e
\end{align*}

(where $e$ is the identity element of $W$). This is an algebra over $A = \mathbb{Q}(q^{1/2})$. Following [23], we define an involution on $A$ by $q^{1/2} = q^{-1/2}$. Extend this to an involution on $H$ by setting

\begin{align*}
(5) & \quad \iota \left( \sum_w \alpha_w T_w \right) = \sum_w \bar{\alpha}_w (T_{w^{-1}})^{-1}.
\end{align*}

From [23], we have that the Kazhdan-Lusztig polynomials are determined uniquely by the following:

**Theorem 2** (Theorem 1.1, [23]). For any $w \in W$, there is a unique element $C'_w \in H$ 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 $x \not< w$.

As mentioned above, it is conjectured in [23] that the coefficients of $P_{x,w}$ are non-negative.

Several of the conditions in Theorem 2 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., [8]). $X_w$ will denote the corresponding Schubert variety, $X_w = \cup_{w \leq x} C_x$. For any variety $X$ (such as some $X_w$), we let $IH^i (X)$ denote the $i$-th (middle) intersection cohomology group of $X$. Suppose that $f : Y \rightarrow X$ is a
resolution of singularities of $X$. The map $f$ is said to be a \textit{small resolution} if for every $r > 0$,
\[ \text{codim}\{x \in X : \dim f^{-1}(x) \geq r\} > 2r. \]
A commonly used resolution of the singularities of $X_w$ is the Bott-Samelson resolution (see \cite{15}). Theorem \cite{15} 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 $v$ be a substring of the form $s_{i_1}s_{i_2}\cdots s_{i_k}$ 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 $v = [3, 2, 1]$. It is shown by Billey-Jockusch-Stanley \cite{4} that the 321-avoiding permutations in $\mathfrak{S}_n$ are precisely those for which no reduced expression contains a substring of the form $s_is_{i+1}s_i$. In the context of reduced expressions, 321-avoiding permutations are called \textit{short-braid-avoiding} (terminology due to Zelevinsky, according to \cite{21}). Short-braid-avoiding permutations have been studied by Fan and Stembridge \cite{19, 20, 21, 22}.

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 $a = s_{i_1} \cdots s_{i_n}$ for $w$. By \cite{13}, all reduced expressions for such a 321-avoiding $w$ are equivalent up to moves of the form $s_is_j \rightarrow s_js_i$ for $|i-j| > 1$. This allows us to associate a well-defined poset to $w$ (rather than just to $a$, see \cite{21}). Let the generators $\{s_i\}_{j=1}^n$ in our reduced expression label the elements of our poset. For an ordering, we take the transitive closure of $s_{i_j} \preceq s_{i_k}$ if $s_{i_{j+1}} \cdots s_{i_k}s_{i_k} = s_{i_k}s_{i_{j+1}} \cdots s_{i_{k-1}}$ and $s_{i_j}s_{i_k} \neq s_{i_k}s_{i_j}$.

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 $(i_j, \text{lvl}(s_{i_j}))$ where $\text{lvl}(s_{i_j})$ measures the maximal length of a chain $s_{i_k} \preceq \ldots \preceq s_{i_j}$ 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 $s_{i_j} \mapsto \text{pt}(j) \overset{\text{def}}{=} (i_j, \text{lvl}(s_{i_j}))$, where we define $\text{lvl}(s_{i_j})$ as follows: Let $k$ be as small as possible in the interval $[1, \ldots, j]$ such that $s_{i_l}$ commutes with $s_{i_j}$ for all $l$ with $k \leq l \leq j$. Now, initially, define a level function by: $\text{lvl}_L(s_{i_j}) = 0$ if $k = 1$ and $\text{lvl}_L(s_{i_j}) = \text{lvl}_L(s_{i_{k-1}}) + 1$ if $k \geq 2$.

For most purposes, $\text{lvl}_L(\cdot)$ gives us what we’d like. However, with $\text{lvl}_L(\cdot)$ as the level function, “connected components” do not necessarily abut. Figure \cite{1} gives an example of the embedding $(i_j, \text{lvl}_L(s_{i_j}))$ 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 $\text{lvl}_L(s_{i_j}) = \text{lvl}_L(s_{i_k})$. We call such elements $\mathfrak{S}_n$-related. The elements $s_{i_1} \cdots s_{i_n}$ in our reduced expression label the elements of our poset. We now define a level function by: $\text{lvl}(s_{i_j}) = \sum\{\text{lvl}(s_{i_l}) : \text{lvl}_L(s_{i_l}) = \text{lvl}_L(s_{i_j}) \}$.
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 \( s_{ij} \mapsto (i_j, \text{lvl}_L(s_{ij})) \). On the right is the result of pushing the “connected components” together.

\[ \text{lvl}_L(s_{ij}) \pm 1 \]

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 \( \text{lvl}(s_{ij}) \) to be this adjustment of the level \( \text{lvl}_L(s_{ij}) \).

We will refer to the realization \( s_{ij} \mapsto (i_j, \text{lvl}(s_{ij})) \) of our poset as Heap(\( w \)). The notion of Heap(\( w \)) is due to Viennot [34], see also the work of Stembridge [31] in the context of fully-commutative elements. Note that \( s_{ij} \) can cover \( s_{ik} \) 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

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

If we set

\[
u = s_3 s_2 s_1 s_5 s_4 s_3 s_2 s_6 s_5 s_4 s_3 s_7 s_6 s_5 \]

then the permutations in (7) correspond to \( u, us_4, s_4u, s_4us_4 \).

Figure 2. Heap(\( u \)) for \( u \) as in (8).

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

\[
u^j = s_{j+3} s_{j+2} s_{j+1} s_j + 5 s_{j+4} s_{j+3} s_{j+2} + 8 s_{j+6} s_{j+5} + 1 s_j + 5 s_{j+4} s_{j+3} s_{j+2} + 8 s_{j+6} s_{j+5} \quad \text{for any } j \geq 0,
\]

\[
s_j s_{j+1} s_j \quad \text{for any } j \geq 1.
\]

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: $\text{Cone}_\lambda(j) = \{(i_j + \alpha, \lambda l s(i_j) - \beta) \in \mathbb{Z}^2 : |\alpha| \leq \beta\}$.

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

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

**Figure 3.** Heap($u$) overlaid with $\text{Cone}_\lambda(6)$ and $\text{Cone}^\vee(6)$. The white nodes are in Heap($u$). The black nodes are in one of the cones, but not in Heap($u$).

The following lemma yields a very nice property of 321-avoiding permutations. In Remark 3 we interpret this result visually in terms of Heap($w$).

**Lemma (Lateral Convexity).** Label the generators of $S_n$ such that $s_is_j = s_js_i$ if and only if $|i - j| > 2$ (the standard labeling). Then $w \in S_n$ 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.** Lemma 4 can be rephrased as follows. Suppose that $w = s_{i_1} \cdots s_{i_r}$ is 321-avoiding and $\text{pt}(j)$, $\text{pt}(k) \in$ Heap($w$) with $\lambda l s(i_j) < \lambda l s(i_k)$. 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 $(m, \lambda l s(i_m)) \in \text{Cone}_\lambda(s_{i_k}) \cap \text{Cone}^\vee(s_{i_j}) \cap \text{Heap}(w)$ for some $l$, $j \leq l \leq k$. Then the entire diamond $\text{Cone}_\lambda(s_{i_k}) \cap \text{Cone}^\vee(s_{i_j})$ is contained in Heap($w$). This is illustrated in Figure 3. 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 $w \in S_n$ 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 $s_{i \pm 1}$, otherwise our expression would not be reduced. But then our reduced expression looks like $u_1s_1u_2s_1\pm 1u_3s_1u_4$ where $l(w) = 3 + \sum_{j=1}^{4} l(u_j)$. If $s_is_2 = u_2s_i$ and $u_3s_i = s_is_3$, then $w$ has a reduced expression $u_1u_2s_is_{i+1}s_is_{i+4}$. Such a $w$ is not 321-avoiding, which is a contradiction. So either $u_2$ or $u_3$ must contain $s_{i+1}$.
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 \( s_i \) and an \( s_{i+1} \). It is a theorem of Tits [33], 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:

\[
\begin{align*}
C_1 & : \ s_i s_j = s_j s_i, \text{ if } |i - j| > 1, \\
C_2 & : \ s_i s_j s_i = s_j s_i s_j, \text{ if } i = j \pm 1.
\end{align*}
\]

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. \( \square \)

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 [17] (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 \( a = s_{i_1} \cdots s_{i_r} \). To this end, we define a mask \( \sigma \) (associated to \( a \)) to be any binary word \( (\sigma_1, \ldots, \sigma_r) \) in the alphabet \( \{0, 1\} \). Set \( \sigma[j] \overset{\text{def}}{=} (\sigma_1, \ldots, \sigma_j) \) for \( 1 \leq j \leq r \). (So \( \sigma = \sigma[r] \).) We’ll use the notation

\[
\sigma_{i,j} = \begin{cases} 
  s_{i_1}, & \text{if } \sigma_j = 1, \\
  1, & \text{if } \sigma_j = 0.
\end{cases}
\]

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

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

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

Note that \( j \)’s membership in \( \mathcal{D}(\sigma) \) is independent of \( \sigma_k \) for \( k \geq j \). The elements of \( \mathcal{D}(\sigma) \) are simply called defects (of the mask \( \sigma \)).
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 \( w\sigma = w, \sigma^{[9]} = s_3 s_2 s_4 s_3 s_2 s_5 s_4 s_3 \), \( \pi(w\sigma) = s_3 \), and \( D(\sigma) = \{6, 8, 9\} \). If \( x = s_1 s_3 s_5 \), then
\[
\mathcal{P}_x(a) = \{ \sigma' = (0, 0, 1, 0, 0, 1, 0, 1, 0), \sigma'' = (0, 0, 1, 0, 1, 0, 1, 0, 0), \sigma''' = (1, 0, 1, 0, 0, 0, 1, 0, 0), \sigma'''' = (1, 0, 1, 0, 1, 0, 1, 0, 1) \}.
\]
So, \( D(\sigma') = \emptyset, D(\sigma'') = \{9\}, D(\sigma''') = \{5, 9\}, \) and \( D(\sigma''''\sigma'') = \{5\} \).

Deodhar, in [17, 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 \( S \subseteq \mathcal{P}(a) \) that yields the Kazhdan-Lusztig polynomials. This is an amazing result. However, in general, the procedure to find this subset \( S \) is somewhat complicated. But we can restrict our attention to the case where \( S = \mathcal{P}(a) \). 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
\[
\mathcal{P}_x(a) = \sum_{\sigma \in \mathcal{P}_x(a)} q^{\|D(\sigma)\|}.
\]
If \( \deg \mathcal{P}_x(a) \leq \frac{1}{2}(l(w) - l(x) - 1) \) for all \( x \in W \), then \( \mathcal{P}_x(a) \) is the Kazhdan-Lusztig polynomial \( \mathcal{P}_{x.w} \) for all \( x \in W \).

Most of the content of Theorem 3 is that the \( \mathcal{P}_x(a) \) 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 criteria for ensuring that \( |D(\sigma)| \leq \frac{1}{2}(l(w) - l(\pi(w\sigma)) - 1) \) 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 \( D(\sigma) = D^0(\sigma) \cup D^1(\sigma) \) where \( D^0(\sigma) \) consists of those \( j \in D(\sigma) \) for which \( \sigma_j = e \in \{0, 1\} \). Let \( a[j] \) \( \overset{\text{def}}{=} s_{i_1} \cdots s_{i_j} \) for \( 1 \leq j \leq r \). Also, set \( d_j(\sigma) \) \( \overset{\text{def}}{=} |D(\sigma[j])| \), \( d(\sigma) \) \( \overset{\text{def}}{=} |D(\sigma)| \), \( x[j] \) \( \overset{\text{def}}{=} \pi(w\sigma[j]) \) and \( w[j] \) \( \overset{\text{def}}{=} \pi(a[j]) \). Finally, set
\[
\Delta_{\sigma[j]} \overset{\text{def}}{=} \frac{l(w[j]) - l(x[j]) - 1 - |D(\sigma[j])|}{2}.
\]
We write \( \Delta_\sigma \) for \( \sum_{j=1}^r \Delta_{\sigma[j]} \). 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 \( a = s_{i_1} \cdots s_{i_r} \) be a reduced expression for some \( w \in \mathcal{S}_n \). Suppose \( \sigma = (\sigma_1, \ldots, \sigma_r) \in \mathcal{P}(a) \) with \( \pi(w\sigma) \neq w \). Then \( \Delta_\sigma \geq 0 \) if and only if
\[
(\# \text{ of 0's in } \{\sigma_1, \ldots, \sigma_r\}) \geq 2 \cdot |D^0(\sigma)| + 1.
\]

**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, \( D(\sigma[k]) = \emptyset \). 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. \( j \not\in D(\sigma) \), \( \sigma_j = 1 \). 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. \( j \not\in D(\sigma) \), \( \sigma_j = 0 \). 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. \( j \in D(\sigma) \), \( \sigma_j = 1 \). 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. \( j \in D(\sigma) \), \( \sigma_j = 0 \). 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 \( j > k \),

\[ \Delta_{\sigma[j]} \geq 0 \iff \# \text{ of 0's in } \{\sigma_{k+1}, \ldots, \sigma_j \} \geq 2 \cdot |D^0(\sigma[j])| \]

(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 \( G_\sigma \) whose vertices are in one-to-one correspondence with the defects of \( D^0(\sigma) \). In Lemmas 3, 4, and 5 we develop some technical results relating the shape of \( \text{Heap}(w) \) to the shape of \( G_\sigma \). Then in Proposition 6 we show that \( G_\sigma \) 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 \( G_\sigma \) is a forest, then (18) is satisfied.

The edges of \( G_\sigma \) will depend on how the various defects and zeros in \( \sigma \) are intertwined. To measure this intertwining, we overlay strings on \( \text{Heap}(w) \). 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 5a. If \( \sigma_j = 1 \), then “cross” the strings as in Figure 5b.

In either case, \( \gamma_1 \) and \( \gamma_2 \) are said to meet at \( pt(j) \) and each of \( \gamma_1, \gamma_2 \) 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 5 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...
Figure 6. Heap(w) overlaid with a string diagram for the reduced expression \( a = s_4s_3s_2s_1s_5s_4s_2s_6s_5s_4s_7s_6s_5 \) and \( \sigma = (1,0,1,0,1,0,1,0,0,1,0,0) \). Note that \( \pi(w^{\sigma}) = s_4s_5s_4s_7 \), 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 \( a \)). And \( \gamma_6 \) encounters pt(\( j \)) for \( j \in \{5,6,7,11\} \) (also for \( a \)).

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 6). Formally, there must be \( a, b \) with \( 1 \leq a \not= b < j \) and \( \alpha, \beta > 0 \) such that \((i_j, \text{lvl}(s_{i_j})) = (i_a + \alpha, \text{lvl}(s_{i_a}) + \alpha) = (i_b - \beta, \text{lvl}(s_{i_b}) + \beta) \) where \( \sigma_{i_a} = \sigma_{i_b} = 0 \). Otherwise, the strings meeting at \((i_j, \text{lvl}(s_{i_j}))\) could not have previously crossed.

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

Now, for \( j \in \mathcal{D}(\sigma) \), \{lcz(\( j \)), rcz(\( j \)), 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 mcz(\( j \))). A point pt(\( j \)) is shared if pt(\( j \)) is a critical zero for two separate defects.

Figure 7. Heap showing necessity of existence of 0’s on boundary of Cone(\( j \)) when \( j \in \mathcal{D}(\sigma) \).

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

\[
\{\text{lcz}(j), \text{rcz}(j), \text{mcz}(j)\} \cap \{\text{lcz}(k), \text{rcz}(k), \text{mcz}(k)\} \neq \emptyset.
\]

In Figure 8, we give an example of a heap along with its associated graph \(G_{\sigma}\).

The key fact we need in the proof of (18) is that \(G_{\sigma}\) does not contain any cycles.

Before proving this fact in Proposition 1, we first introduce some lemmas that illuminate the structure of \(G_{\sigma}\). The first two lemmas are easy and stated only for reference. The second and third give criteria for \(\text{Heap}(w)\) to contain a hexagon.

**Lemma 3.** Suppose \(w\) is 321-avoiding and \(k, l \in D_0(\sigma)\) with \(\text{pt}(l) = \text{lcz}(k)\). Then \(\text{pt}(l) + (1, -3) \in \text{Heap}(w)\). Similarly, if \(\text{pt}(l) = \text{rcz}(k)\), then \(\text{pt}(l) - (1, 3) \in \text{Heap}(w)\). (See, for example, Figure 3.c.)

**Lemma 4.** Let \(w\) be a 321-avoiding permutation and \(\text{pt}(h), \text{pt}(k) \in \text{Heap}(w)\) with \(\text{pt}(h) \in \text{Cone}_\gamma(\text{pt}(k) - (0, 6))\). If \(h\) and \(k\) are encountered by a common string, then \(\text{Heap}(w)\) contains a hexagon. (See, for example, Figure 3.c.)

**Lemma 5.** Let \(w \in S_n\) be 321-avoiding. \(\text{Heap}(w)\) contains a hexagon if any of the following three situations are met:

1. The point \(\text{lcz}(r) = \text{pt}(m) = \text{rcz}(l)\) with \(m, r, l \in D_0(\sigma)\). (See Figure 4.a.)
2. The string \(\gamma\) encounters three distinct strings \(\gamma_1, \gamma_2, \gamma_3\) at defects \(l, k, m \in D_0(\sigma)\), respectively. Furthermore, \(\text{pt}(m) = \text{rcz}(l), \text{pt}(l) = \text{lcz}(k)\) and \(\text{pt}(m)\) is on the boundary of \(\text{Cone}_\gamma(\text{pt}(k) - (0, 2))\). (See Figure 4.b.)
3. We have \(\text{pt}(l) = \text{lcz}(k), \text{pt}(r) = \text{rcz}(k)\) and \(k, l, r \in D_0(\sigma)\). (See Figure 4.c.)

Parts 1 and 3 of Lemma 5 tell us that any three defects in a \(\lor\)-shape or a \(\land\)-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 4.a. The claim follows immediately from Lateral Convexity by applying Lemma 3 to the pairs \(\text{pt}(l), \text{pt}(m)\) and \(\text{pt}(r), \text{pt}(m)\).
Proof of part 2. First consider the case where pt(m) = pt(k) + (δ, −2 − δ) for δ ≥ 1. This is illustrated in Figure 9b. By Lemma 3, pt(m) = (1, 3) is in Heap(w). Since pt(f) ∈ Cone(δ)(pt(k) + (δ − 1, −5 − δ)), Heap(w) contains the indicated hexagon by Lemma 4.

Alternatively, we can have pt(m) = pt(k) − (δ, 2 + δ) for δ ≥ 0. This is illustrated in Figure 9c. 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 γγ_i must occur in Cone(δ)(pt(h)) = Cone(δ)(pt(m) − (0, 4)) = Cone(δ)(pt(a) − (δ, 6 + δ)). By Lemma 4, 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 $a_0 = 0$ then $a \in D^0(\sigma)$ and we can appeal to Lemma 3.1. So we can consider only the case where there is a crossing at pt($a$). If $\gamma$ is either $\gamma_1$ or $\gamma_3$, then it still needs to cross a string currently to its right (either $\gamma_2$ or $\gamma_4$, respectively). This can only happen in Cone$_\lambda(f)$. The only alternative is that $\gamma = \gamma''$. But then $\gamma_1\gamma_2$ cannot cross until Cone$_\lambda(f)$. Either way, pt($f$) $\in$ Heap($w$). Arguing analogously with $\gamma'$, 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$_\lambda(pt(m) + (0, 2))$ where pt($m$) = rcz($l$).

Assume first that pt($r$) $\in$ Cone$_\lambda(pt(m) + (0, 2))$. We are in the situation of Figure 10.b. Since pt($r$) $\neq$ pt($k$) + (1, −1), pt($m$) = pt($k$) + ($\delta$, −2 − $\delta$) 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$_\lambda(h)$. This ensures that Heap($w$) contains the indicated hexagon.

If pt($r$) $\not\in$ Cone$_\lambda(pt(m) + (0, 2))$, then we are in the situation of Figure 10.c. Since $\gamma_2$ must go left once below pt($m$) − (1, 1) (to cross $\gamma_1$) and $\gamma_3$ must go right once (to cross $\gamma_4$), we see that the lowest of the crossings $\gamma_3\gamma_4$ must occur in Cone$_\lambda(h)$. If pt($r$) $\neq$ pt($a$), then by Lemma 3, 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$_\lambda(pt(k) − (0, 6))$. But this follows from the assumption that pt($r$) is not at a distance of $\sqrt{2}$ from pt($k$). \hfill \Box

**Proposition 1.** If $w$ is 321-hexagon-avoiding and $\sigma \in P(a)$, then $G_\sigma$ is a forest.

**Proof.** Assume that $G_\sigma$ is not a forest — i.e., $G_\sigma$ contains a cycle. We will assume that $w$ is 321-avoiding and show that if $G_\sigma$ contains a cycle then Heap($w$) contains a hexagon. Note that since $w$ is 321-avoiding, Lemma 3 (Lateral Convexity) holds.

Let $V \subset D^0(\sigma)$ be a minimal subset such that the subgraph $G'_\sigma$ of $G_\sigma$ 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 $G'_\sigma$.

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 3.3, $p \notin V$. 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.
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 \( j \in D(\sigma) \), then \( pt(j) - (0, 2) \) must be in the heap.

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

We now show that, regardless of the characteristics of \( m \) (i.e., values of \( i_m \), \( \text{lvl}(m) \), and whether or not \( m \in D(\sigma) \)), \( \text{Heap}(w) \) 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 \( pt(m) \) is \( \gamma_3 \). Since \( V \) is minimal, we then need either \( \text{lcz}(m) \) or \( \text{rcz}(m) \) shared. Consider Figure 12. Suppose \( pt(n) = \text{lcz}(m) \) is shared. By choice of \( pt(k) \) on the line \( y = x + C \), this implies that \( n \in V \). But then by Lemma 2, \( pt(h) \in \text{Heap}(w) \). Then by Lateral Convexity, \( pt(e) \in \text{Heap}(w) \). The alternative is that \( \text{rcz}(m) \) is shared. Again, this implies that \( pt(e) \in \text{Heap}(w) \). Since \( pt(q) \in \text{Heap}(w) \) by Fact 1, \( \text{Heap}(w) \) contains a hexagon.

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

Figure 12. This figure depicts the case where \( pt(m) \) is not the left critical zero of another defect in \( V \).
So we can assume that \( m \notin V \). But by choice of \( l \), \( \text{pt}(m) \) must be shared. This implies that \( \text{pt}(m) = \text{lcz}(r) \) for some \( r \in V \). We now argue that \( \text{Heap}(w) \) must contain a hexagon according to the position of \( \text{pt}(m) \) relative to \( \text{pt}(k) \).

**Case I:** \( \text{pt}(m) = \text{pt}(k) - (\delta, 2 + \delta) \) for \( \delta \geq 0 \). There are three cases to consider. Figure 13.a. depicts the first. Here, \( \gamma \) and \( \gamma_3 \) both encounter \( \text{pt}(r) \). Since \( V \) is minimal, either \( \text{rcz}(r) \) or \( \text{pt}(r) \) must be shared. By choice of our line \( y = x + C \) and the fact that \( p \notin V \), we see that, in fact, \( \text{rcz}(r) \) must be shared. But then \( \text{pt}(b) \in \text{Heap}(w) \). Since \( \text{pt}(q) \in \text{Heap}(w) \), \( \text{Heap}(w) \) contains the indicated hexagon.

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

The third possibility is that \( \text{pt}(r) \notin \text{Cone}_\lambda(\text{pt}(k)) \) (Figure 13.c). In fact, this is the only possibility for \( \text{pt}(r) \) when \( \delta = 0 \). Here we see that the path of \( \gamma_3 \) must be as shown in order to avoid \( \text{Cone}_\lambda(g) \). But then \( \gamma_4 \gamma_5 \) cannot cross until \( \text{Cone}_\lambda(e) \). So we have the indicated hexagon.

**Case II:** \( \text{pt}(m) = \text{pt}(k) + (\delta, -2 - \delta) \) 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 \( \text{Cone}_\lambda(h) \), we need \( \gamma_2 \gamma_3 \) to cross in \( \text{Cone}_\lambda'(m) \). This is shown in Figure 14.b. We mention three additional assertions we have made in Figure 14.b. First, \( \gamma_1 \) must cross \( \gamma_2 \) as shown in Figure 14.b in order to avoid having \( \text{Heap}(w) \) contain a hexagon. Second, \( \text{pt}(q) \in \text{Heap}(w) \) by Fact 4. Third, since \( \text{rcz}(m) \) must be shared, \( \text{pt}(e) \in \text{Heap}(w) \) as shown. So, by Lateral Convexity, \( \text{Heap}(w) \) contains the hexagon indicated in Figure 14.b. (It is possible that \( \text{pt}(a) = \text{pt}(p) \) or \( \text{pt}(a) = \text{pt}(k) \), but this does not change our conclusion.)
6. Proof of Theorem \[1\]

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

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

Lemma 6. Let \(s \in S\), \(ws < w\). Then

\[
P_x(a) = q^{c_s(x)}P_x(a/s) + q^{1-c_s(x)}P_x(as/s),
\]

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

Proof. Partition \(P_x(a) = P_0^x(a) \cup P_1^x(a)\) where \(P_0^x(a)\) consists of all masks in \(P_x(a)\) ending in \(\epsilon\) for \(\epsilon \in \{0, 1\}\). There are natural bijections \(P_0^x(a) \approx P_x(as/s)\) and \(P_1^x(a) \approx P_x(a/s)\) given by \(\sigma \mapsto \sigma[r-1]\). So, to prove the lemma, we need only compare \(|D(\sigma)|\) to \(|D(\sigma[r-1])|\).

If \(\sigma \in P_0^x(a)\), then \(\sigma[r-1] \in P_x(a/s)\). In this case, if \(xs > x\) \((c_s(x) = 0)\), then \(r \notin D(\sigma)\), so \(|D(\sigma[r-1])| = |D(\sigma)|\). Alternatively, if \(xs < x\) \((c_s(x) = 1)\), then \(D(\sigma) = D(\sigma[r-1]) \cup \{r\}\) and \(|D(\sigma)| = |D(\sigma[r-1])| + 1\). 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. \(\square\)

Proof of Theorem \[1\] \(\implies\) \[2\].

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

Now, every \(j \in D^0(\sigma)\) has three critical zeros. Furthermore, by Lemma \[3\], no point is a critical zero for 3 distinct defects. So the number of edges in \(G_\sigma\) equals the number of shared critical zeros. Hence,

\[
\# \text{ of 0's in } \{\sigma_1, \ldots, \sigma_r\} \geq \# \text{ of critical zeros in } \{\sigma_1, \ldots, \sigma_r\}
\]

\[
= 3 \cdot |D^0(\sigma)| - (\# \text{ of edges in } G_\sigma).
\]
Now, by Proposition 1, $G_\sigma$ is a forest with $|D^0(\sigma)|$ vertices. Hence, $G_\sigma$ has at most $|D^0(\sigma)| - 1$ edges (see, e.g., [3]). Hence,

\begin{equation}
\text{# of 0's in } \{\sigma_1, \ldots, \sigma_r\} \geq 2 \cdot |D^0(\sigma)| + 1.
\end{equation}

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

We shall prove (not 1) $\Rightarrow$ (not 2). Assume $w$ is not 321-avoiding. We can find a reduced expression for $w$ of the form $a = vs_i\pm s_is_i v'$ with $l(w) = l(v) + l(v') + 3$. Set

\begin{equation}
\sigma = (1, \ldots, 1, 1, 0, 1, \ldots, 1).
\end{equation}

Then $|D^0(\sigma)| = 1$ and $|\{j : \sigma_j = 0\}| = 2$. By Lemma 2, $\Delta_\sigma < 0$. So $P_x(a)$ does not satisfy the properties of the $P_{x,w}$ listed in Theorem 3.

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

\begin{equation}
\sigma = (1, \ldots, 1, 1, 1, 0, 1, 0, 1, 0, 1, 0, 0, 1, \ldots, 1).
\end{equation}

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

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

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 $P_{x,w}$ ([24, Corollary 4.9]):

\begin{equation}
\sum_i \dim(IH_i(X_w))q^i = \sum_{x \leq w} q^{l(x)} P_{x,w}(q).
\end{equation}
Now, we are assuming that \( P_x(a) = P_{x,w} \) for all \( x \in \mathfrak{S}_n \). So we need only show that
\[
\sum_{x \leq w} q^{l(x)} P_x(a) = (1 + q)^{l(w)}.
\]

We proceed by induction, the result being obvious for \( l(w) = 1 \). Choose an \( s \in S \) such that \( ws < w \). From [22, Lemma 7.4], we know that:
\[
\text{If } ws < w, \text{ then } x \leq w \iff xs \leq w.
\]

Using (30), along with Lemma 6, we can write
\[
\sum_{x \leq w} q^{l(x)} P_x(a) = \sum_{x \leq w, x < xs} q^{l(x)} P_x(a) + q^{l(xs)} P_{xs}(a)
\]
\[
= (1 + q) \sum_{x \leq w, x < xs} q^{l(x)} (P_x(a/s) + qP_{xs}(a/s))
\]
\[
= (1 + q) \sum_{x \leq w, x < xs} q^{l(x)} P_x(a/s) + q^{l(xs)} P_{xs}(a/s).
\]

If \( P_x(a/s) \neq 0 \), then \( x \leq ws \), so this becomes
\[
= (1 + q) \sum_{x \leq ws} q^{l(x)} P_x(a/s)
\]
\[
= (1 + q)(1 + q)^{l(ws)} = (1 + q)^{l(w)}.
\]

The last line is by the induction hypothesis.

Deodhar [17] proves that for any Weyl group \( W \), we can always find a subset \( S \subset \mathcal{P}(a) \) such that
\[
\sum_{\sigma \in S} q^{\lambda_D(\sigma)} = P_{x,w}
\]
for all \( x, w \in W \). (More generally, he shows that such an \( S \) 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 \( S \), we have the following string of equalities:
\[
(1 + q)^{l(w)} = \sum_i \dim(\text{IH}^2(X_w)) q^i = \sum_{x \leq w} q^{l(x)} P_{x,w}
\]
\[
= \sum_{\sigma \in S} q^{l(x)} q^{\lambda_D(\sigma)}.
\]

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

This follows from Deodhar [17, Proposition 3.5 and Corollary 4.8].

This is the content of Deodhar [17, Proposition 3.9].

This is a standard result on small resolutions. See, for example, [23, Section 6.5].
Recall that $Y$ denotes the Bott-Samelson resolution of $X_w$ (corresponding to some reduced expression $a$). By [7, Proposition 4.2],

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

We are assuming that $H_*(Y) \cong IH_*(X_w)$. By Poincaré duality, we know that $H^2_*(Y) \cong IH^2_*(X_w)$. Combining (38) with this isomorphism yields

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

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 $F_n(q) = F_{n-1}(q) + qF_{n-2}(q)$ 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 ([11, Conjecture 7.18]):

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

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

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

Recently, Brenti-Simion [12] 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.

![Figure 16](image)

**Figure 16.** It is clear that $\gamma$ 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 $\gamma$. 


Proof. As a permutation,
\begin{equation}
(41) \quad w = [1, 2, \ldots, k-2, k+1, \ldots, l+1, k-1, l+2, \ldots, n].
\end{equation}

This is easily seen to be 321-hexagon-avoiding. So by Theorem 4, \( P_e(a) = P_{e,w_{k,l}} \).

The claim is true for \( l = k \). The proof is by induction. The situation of the general case is illustrated in Figure 17. From Figure 16.b, no new defect is introduced by \( \gamma \), so by Theorem 1, we have \( |D(\gamma)| = |D(\sigma[r - 4])| + 1 \). The claim follows by the induction hypothesis.

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

**Theorem 4.** Suppose \( v_{k,l} \in S_n \) has reduced expression
\begin{equation}
(42) \quad a = s_t s_{t+1} s_{t+2} s_{t+1} s_{t+2} \cdots s_k s_{k+1} s_{k+2}
\end{equation}
for some \( 1 \leq k \leq l < n - 2 \). Then \( P_{e,v_{k,l}} \in \mathbb{Z}[q] \) is given by the coefficient of \( z^{l-k+1} \) in the generating function
\begin{equation}
G_e(z) = \frac{-1 + q^2 z^2 + q^3 z^3}{(1 + q z + q^2 z^2)(-1 + z + qz + q^2z^2 + q^2z^2 + q^2z^3 - q^3 z^4)}.
\end{equation}

**Figure 17.**

Proof. We only sketch the proof. We see that \( v_{k,l} \) is certainly 321-hexagon-avoiding, so by Theorem 4, \( P_{e,v_{k,l}} = P_{e,a} \). The idea is to use recursion on \( n = l - k \). From Figure 17 it is easy to see that \( P_{e,v_{k,l}} = P_{e,v_{k+1,l}} + qP_{e,v_{k+1,l}^1} + qP_{e,v_{k+1,l}^2} + qP_{e,v_{k+1,l}^3} \). Similar recurrences can be found for \( P_{x,v_{k,l}} \) where \( x \in S_4 \). Solving these recurrences yields \( P_{e,v_{k,l}} \).

8. **Singular Loci of 321-hexagon-avoiding Elements**

The Schubert variety \( X_w \) is said to be singular at a point \( x \leq w \) (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 \( l(x) \). The set of singular points forms a lower order ideal in the Bruhat-Chevalley order. We define \( X_w^{\text{sing}} \) to consist of the maximal elements (under this Bruhat-Chevalley order) of the set \( \{ x \in S_n : x \leq w \text{ and } x \text{ singular} \} \).
The following theorem gives a complete description of $X_w^{\text{sing}}$ when $w$ is 321-hexagon-avoiding. In fact, this proves a conjecture of Lakshmibai and Sandhya in this special case.

**Theorem 5.** Let $w \in \mathfrak{S}_n$ be 321-hexagon-avoiding (hence $\text{Heap}(w)$ 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 $X_w^{\text{sing}}$. More explicitly, let

$$T = \{(j, k, l) \in \mathbb{Z}^3 : 1 \leq j, k, l \leq r, \ pt(j) = pt(k) - (\alpha, \alpha), \ pt(l) = pt(k) + (\beta, -\beta) \text{ for some } \alpha, \beta > 0,$$

and $\text{Cone}_\alpha(j) \cap \text{Cone}_\beta(l) \cap \text{Heap}(w) \neq \emptyset \}$

and

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

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

**Proof.** It has been proved by Deodhar 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, $P_{\pi(\sigma), w} = 1$ for every $x \in \mathfrak{S}_n$. So to show that $X_w$ is singular, we need only show that $\mathcal{P}(a)$ 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 $\sigma \in \mathcal{P}(a)$, 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 $\sigma \in \mathcal{P}(a)$ with $|\mathcal{D}(\sigma)| \geq 1$. Choose $b \in \mathcal{D}(\sigma)$ and suppose $pt(a) = \text{lcz}(b)$ and $pt(c) = \text{rcz}(b)$. Now define a mask $\sigma'$ by setting

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

Using the characterization of Bruhat-Chevalley order in terms of subexpressions (see, e.g., [22]), it is easily checked that $\pi(\sigma) \leq \pi(\sigma')$. Since $\sigma'$ is in $\Sigma$, we are done.

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

**Example 2.** Here we give an example of calculating the singular locus as in Theorem 2. We have set $w = s_8s_4s_2s_6s_5s_4s_3$. Figure 14 illustrates the eight different points in the maximal singular locus of $X_w$. Namely,

$$X_w^{\text{sing}} = \{3, 1, 6, 2, 4, 5, 3, 1, 6, 4, 2, 7, 5, 3, 1, 6, 5, 2, 4, 7, 1, 3, 7, 2, 6, 4, 5, 3, 2, 6, 1, 4, 7, 5, 3, 2, 6, 1, 5, 4, 7, 3, 4, 6, 1, 2, 5, 7\}.$$
Example 3. For $v_{1,4}$ as in Theorem 4, $|X_w^{\text{sing}}| = 18$.

Remark 8. Let $w = [w(1), \ldots, w(n)]$. A result of Lakshmibai and Sandhya [27, Theorem 1] is that $X_w$ is nonsingular if and only if $w$ avoids $[3,4,1,2]$ and $[4,2,3,1]$. It is shown in [4] 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 $[3,4,1,2]$-sequence in $w$.

9. Example and Enumeration of 321-hexagon-avoiding Elements

The following table 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 $n \leq 6$). 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., [4, 26, 30]).

Below we give an example showing the use of Theorem 1 for calculating $P_{x,w}$.
KAZHDAN-LUSZTIG POLYNOMIALS FOR 321-HEXAGON-AVOIDING PERMUTATIONS

| 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 1. Number of 321-hexagon-avoiding elements in $S_n$.

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 4.) It is a result of Deodhar that for each $x \leq w$, there exists a unique mask in $\mathcal{P}_x(a)$ of defect 0. The following table lists all of the $\sigma \in \mathcal{P}_x(a)$ for which $|D(\sigma)| > 0$. For this $w$, all of these masks happen to have $|D(\sigma)| = 1$.

Hence, we see that for $x \leq w$,

$$
P_{x,w} = \begin{cases} 
1 + 2q, & \text{if } x \in \{e, s_2, s_3, s_2 s_3\}, \\
1 + q, & \text{if } x \in \{s_1, s_4, s_1 s_3, s_2 s_1, s_3 s_2, s_4 s_3, s_2 s_4, s_2 s_4 s_3, s_2 s_3 s_2, s_2 s_1 s_3\}, \\
1, & \text{otherwise}. 
\end{cases}
$$

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

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