Shifted key polynomials

Eric Marberg*1 and Travis Scrimshaw†2

1Department of Mathematics, Hong Kong University of Science and Technology
2Department of Mathematics, Hokkaido University

Abstract. We introduce shifted analogues of key (resp. atom) polynomials that we call $P$- and $Q$-key (resp. atom) polynomials. These families are defined in terms of isobaric divided difference operators applied to dominant symplectic and orthogonal Schubert polynomials. We establish a number of fundamental properties of these functions, formally similar to classical results on key polynomials. For example, we show that our shifted key polynomials are partial versions of Schur $P$- and $Q$-functions in a precise sense. We conjecture that symplectic/orthogonal Schubert polynomials expand positively in terms of $P/Q$-key polynomials. As evidence for this conjecture, we also show that shifted key polynomials are the characters of certain shifted analogues of Demazure crystals.

Keywords: Schur $P/Q$-function, key polynomial, Lie superalgebra, Demazure crystal

1 Introduction

Fix a positive integer $n$. Set $G = \text{GL}_n(\mathbb{C})$ and write $B \subseteq G$ for the Borel subgroup of upper triangular matrices. Let $K$ be either the orthogonal group $\text{O}_n(\mathbb{C})$ or symplectic group $\text{Sp}_n(\mathbb{C})$ (when $n$ is even). For brevity, we omit the rank and field. The (complete) flag variety $G/B$ decomposes into finitely many $B$-orbits indexed by the symmetric group $S_n$. The closures of these orbits give rise to the Schubert classes in $H^*(G/B)$. The cohomology ring $H^*(G/B)$ is naturally a quotient of $\mathbb{Z}[x] = \mathbb{Z}[x_1, x_2, \ldots]$ and the well-known Schubert polynomials $\mathcal{S}_w \in \mathbb{Z}[x]$ for $w \in S_n$ provide representatives for the Schubert classes.

The flag variety $G/B$ also decomposes into finitely many $K$-orbits, indexed by involutions in $S_n$ when $K = \text{O}$ and by fixed-point-free involutions in $S_n$ when $K = \text{Sp}$ and $n$ is even. The closures of the $K$-orbits give rise to cohomology classes in $H^*(G/B)$ that are positive sums of Schubert classes. Polynomial representatives for these classes are provided by the orthogonal and symplectic Schubert polynomials (which we abbreviate as $K$-Schubert polynomials) characterized in [22]. A precise expansion of $K$-Schubert polynomials into usual Schubert polynomials was given in [3]; see also [5, 8].

It is known [15, Ex. 2.2.2] that $\mathcal{S}_w = x^\lambda$ whenever $w \in S_n$ has Rothe diagram equal to the Young diagram of a partition $\lambda = \lambda(w)$. Such $w$ are called dominant and correspond

*emarberg@ust.hk. Partially supported by Hong Kong RGC grant GRF 16306120.
†tcscrims@gmail.com. Partially supported by Grant-in-Aid for JSPS Fellows 21F51028.
to GL dominant weights. There exists a stable limit $F_w$ of $S_w$, known as a Stanley symmetric function [21], and when $w$ is dominant, it holds that $F_w = s_{\lambda(w)}$ is a Schur function. Combining the Billey–Jockusch–Stanley (BJS) formula [2] for $S_w$ with the stable limit shows that if $w \in S_n$ is dominant, then $s_{\lambda(w)}$ is the weight-generating function for the set $RF(w)$ of factorizations of reduced words for $w$ into decreasing subwords. (We refer to elements of $RF(w)$ as reduced factorizations.) Morse and Schilling showed this directly in [19] by constructing a (Kashiwara) crystal [12] on the set $RF(w)$.

The BJS formula for $S_w$ is a sum over a certain class of bounded reduced factorizations $BRF(w) \subset RF(w)$, and so we can restrict the crystal structure on $RF(w)$ to this subset and consider the resulting connected components. These connected components were shown in [1] to be the crystals for $B$-representations called Demazure modules that are constructed as “partial” versions of highest weight GL-representations. The characters of these $\mathfrak{gl}_n$-Demazure crystals are the so-called key polynomials $\kappa_{u\lambda}$, here $u \in S_n$ and $\lambda$ is a partition with at most $n$ parts.

The precise definition of a key polynomial is $\kappa_{u\lambda} = \pi_u S_{\lambda}$ where $\pi_u$ is an isobaric divided difference operator and $w$ is a dominant permutation with $\lambda(w) = \lambda$. For each choice of $K \in \{O, Sp\}$, there is an analogous notion of a $K$-dominant involution $z$. These elements index the $K$-Schubert polynomials that are products of binomials $x_i + x_j$ indexed by positions in the associated Rothe diagram. By considering all expressions of the form $\pi_u S^K_z$ where $z$ is a $K$-dominant involution in $S_n$, we obtain a new family of objects that we refer to as $P$- and $Q$-key polynomials, or collectively as shifted key polynomials.

Using the fact that each $S^K_z$ is an $\mathbb{N}$-linear combination of Schubert polynomials, we can show that each shifted key polynomial is an $\mathbb{N}$-linear combination of key polynomials (see Theorem 3.4). This suggests that shifted key polynomials may form a combinatorially interesting family. Key polynomials are partial versions of Schur functions, since if $w_0 \in S_n$ denotes the reverse permutation then $s_{\lambda(w)}(x_1, x_2, \ldots, x_n) = \kappa_{w_0\lambda}$. Similarly, we show that $P$- and $Q$-key polynomials are partial versions of the Schur $P$- and $Q$-functions related to the projective representation theory of $S_n$ (see Theorem 3.5).

Classical key polynomials form a $Z$-basis for all polynomials, are uniquely indexed by weak compositions, and decompose every Schubert polynomial with positive coefficients. Shifted key polynomials are not so well-behaved: they are not linearly independent over $\mathbb{Z}$, nor is it clear how to index them uniquely. In spite of this, we conjecture (Conjecture 3.7) that $K$-Schubert polynomials also expand positively for some choice of shifted key polynomials.

In order to classify a good set of linear independent shifted key polynomials, we consider a certain “truncated” crystal structure on a set of bounded reduced factorizations associated to an involution $z$, analogous to constructions in [1, 19]. However, in our case, the crystal will not be for $\mathfrak{gl}_n$ but for the queer Lie superalgebra $\mathfrak{q}_n$ and its extended version $\mathfrak{q}_n^+$ recently introduced in [18]. The full set of reduced factorizations relevant to $K$-Schubert polynomials were given a $\mathfrak{q}_n / \mathfrak{q}_n^+$ crystal structure in [16, 18]. We show in
Theorem 3.8 that when this crystal structure is restricted to its bounded elements for a K-dominant involution, we obtain a connected object whose character is a shifted key polynomial. We conclude by describing a crystal-theoretic generalization of our conjecture that K-Schubert polynomials expand positively into shifted key polynomials. This extended abstract is organized as follows. Section 2 gives some background on key polynomials. Section 3 contains our main results on shifted key polynomials. We have omitted all proofs to save space. Complete arguments can be found in two full-length articles associated to this abstract, this first of which is available as [17].

2 Key polynomials, Schubert calculus, and crystals

Throughout, \( n \) is a positive integer, \( [n] = \{1, 2, \ldots, n\} \), \( \mathbb{N} = \{0, 1, 2, \ldots\} \), and \( \mathbb{P} = \{1, 2, 3, \ldots\} \). Let \( x = (x_1, x_2, \ldots) \) be commuting indeterminates.

Define \( S_\infty = \langle s_1, s_2, s_3, \ldots \rangle \) to be the group permutations of \( \mathbb{P} \) fixing all but finitely many elements, with \( s_i = (i, i + 1) \) denoting a simple transposition. Set \( S_n = \langle s_i : i \in [n - 1] \rangle \subset S_\infty \). A reduced word for \( w \in S_\infty \) a minimal length sequence \( i_1 i_2 \cdots i_\ell \) such that \( w = s_{i_1} s_{i_2} \cdots s_{i_\ell} \), where \( \ell(w) = \ell \) is the length of \( w \). The group \( S_\infty \) acts on the polynomial ring \( \mathbb{Z}[x] \) by permuting variables. The Rothe diagram of \( w \in S_\infty \) is \( D(w) = \{(i, w(j)) : i < j \text{ and } w(i) > w(j)\} \subset \mathbb{P} \times \mathbb{P} \).

A word is a possibly empty sequence of positive integers. For \( w \in S_\infty \), let \( \text{RF}(w) \) denote the set of sequences \( a = (a^1, a^2, a^3, \ldots) \) where each \( a^i \) is a strictly decreasing word such that the concatenation \( a^1 a^2 a^3 \cdots \) is a reduced word for \( w \). We refer to elements of this set as reduced factorizations and define \( \text{RF}_n(w) \) to be the set of such \( a \) with \( a^i \) empty for all \( i > n \). In examples we express elements of \( \text{RF}_n(w) \) as \( n \)-tuples rather than as infinite sequences. Let \( \text{BRF}_n(w) \) denote the set of reduced factorizations in \( \text{RF}_n(w) \) that are bounded in the sense that \( i \leq \min(a^i) \) for all nonempty \( a^i \). Set \( \text{BRF}(w) := \bigsqcup_{n=1}^\infty \text{BRF}_n(w) \).

A weak composition is a nonnegative integer sequence \( \alpha = (a_i \in \mathbb{N})_{i=1}^\infty \) with finite sum \( |\alpha| := \sum_{i=1}^\infty a_i \), and a partition is a weakly decreasing weak composition. We frequently omit the trailing 0’s when writing weak compositions in examples. Given a weak composition \( \alpha \), let \( \lambda(\alpha) \) be the partition sorting \( \alpha \) and define \( x^\alpha := x_1^{a_1} x_2^{a_2} \cdots \). There is a unique \( u(\alpha) \in S_\infty \) such that \( u(\alpha) \alpha \) is a partition \( \lambda(\alpha) \), where the permutation acts on \( \alpha \) by permuting indices; e.g., if \( \alpha = 1021 \), then \( \lambda(\alpha) = 2110 \) and \( u(\alpha) = 3142 = s_2 s_1 s_3 \).

For \( i \in \mathbb{P} \), let \( \partial_i \) be the divided difference operator on \( f \in \mathbb{Z}[x] \) defined by \( \partial_i f = (f - s_{i} f) / (x_i - x_{i+1}) \). The isobaric divided difference operators are then given by \( \pi_i f := \partial_i (x_i f) \) and \( \pi_i := \pi_i - 1. \) For \( w \in S_\infty \) with reduced word \( i_1 \cdots i_\ell \), define \( \pi_w = \pi_{i_1} \cdots \pi_{i_\ell} \) and \( \pi_w = \pi_{i_1} \cdots \pi_{i_\ell} \); these formulas do not depend on the choice of reduced word. The key polynomial of a weak composition \( \alpha \) is then \( \kappa_\alpha := \pi_{u(\alpha)} x^{\lambda(\alpha)} \) while the atom polynomial of \( \alpha \) is \( \tau_\alpha = \pi_{u(\alpha)} x^{\lambda(\alpha)} \). It is well-known that \( \{\kappa_\alpha : \text{weak compositions } \alpha \} \) is a basis for \( \mathbb{Z}[x] \) and that key polynomials are unitriangular with \( \kappa_\alpha = x^\alpha + (\text{lower order terms}) \).
with respect to lexicographic order [20, Cor. 7]. Key polynomials are related to atom polynomials by the identity \( \kappa_\alpha = \sum_{\beta \leq \alpha} \kappa_\beta \), where we write \( \alpha \leq \beta \) if \( \lambda(\alpha) = \lambda(\beta) \) and \( u(\alpha) \leq u(\beta) \) in Bruhat order. For more background on key polynomials, see [20].

A permutation \( w \in S_\infty \) is dominant if its Rothe diagram \( D(w) \) is the Young diagram \( D_\lambda = \{ (i, j) \in \mathbb{P} \times \mathbb{P} : j \leq \lambda_i \} \) of a partition \( \lambda = \lambda(w) \). This occurs precisely when \( w \) is 132-avoiding [15, Ex. 2.2.2]. The Schubert polynomial \( w \) is \( 132 \)-avoiding \([15, \text{Ex. 2.2.2}]\). The key polynomials are related to atom polynomials by setting \( S_w = x^{\lambda(w)} \) when \( w \) is dominant and requiring that \( \mathcal{G}_{w_i} = \partial_i \mathcal{G}_w \) for \( w(i) > w(i + 1) \) [13]. For any \( w \in S_\infty \) the Billey–Jockusch–Stanley formula [2] asserts that

\[
\mathcal{G}_w = \sum_{\alpha \in \text{BRF}(w)} x^{\text{wt}(\alpha)}, \quad \text{where } \text{wt}(\alpha) := (\ell(a^1), \ell(a^2), \ldots).
\]  

(2.1)

Key polynomials can be defined in terms of Schubert polynomials, since if \( w \in S_\infty \) is dominant of shape \( \lambda(\alpha) \) then \( \kappa_\alpha = \pi_{u(\alpha)} \mathcal{G}_w \). On the other hand, every Schubert polynomial expands as a positive linear combination of key polynomials with an explicit combinatorial description [20, Thm. 4].

The BJS formula (2.1) can be interpreted as a character formula for certain Demazure crystals which we describe below. A crystal \([12]\) for \( \mathfrak{gl}_n \) is a set \( \mathcal{B} \) with crystal operators \( e_i, f_i : \mathcal{B} \to \mathcal{B} \sqcup \{ \emptyset \} \) for \( i \in [n - 1] \) and a weight function \( \text{wt} : \mathcal{B} \to \mathbb{Z}^n \) that satisfy certain conditions. We can encode this data as a weighted directed graph called a crystal graph with vertices \( \mathcal{B} \) and edges \( b \xrightarrow{i} f_i b \) whenever \( b \in \mathcal{B} \) and \( f_i b \neq 0 \). For each \( w \in S_\infty \), the set \( \text{BRF}(w) \) already has a weight function as used in (2.1). Morse and Schilling [19] identified a natural \( \mathfrak{gl}_n \)-crystal structure on \( \text{RF}_n(w) \), using a certain bracketing rule to describe the crystal operators. See [4, §10] for more information on these crystals.

Suppose \( w \in S_\infty \) is dominant of shape \( \lambda = \lambda(w) \). Assume \( \lambda \) has at most \( n \) nonzero parts. Then \( \text{RF}_n(w) \) contains a single bounded reduced factorization \( b_\lambda \in \text{BRF}(w) \). This element has weight \( \lambda \) and is highest weight in the sense that \( e_i b_\lambda = 0 \) for all \( i \in [n - 1] \). If \( \alpha \) is a weak composition with \( \lambda = \lambda(\alpha) \) and \( u(\alpha) \in S_n \) then we define

\[
\text{Dem}_n(\alpha) := \left\{ a \in \text{RF}_n(w) : e_{i_1}^{m_{i_1}} e_{i_2}^{m_{i_2}} \cdots e_{i_\ell}^{m_{i_\ell}} a = b_\lambda \text{ for some reduced word } i_1 i_2 \cdots i_\ell \text{ of } u(\alpha) \text{ and some } m_{i_1}, m_{i_2}, \ldots, m_{i_\ell} \in \mathbb{N} \right\}.
\]  

(2.2)

We refer to this subset as a \( \mathfrak{gl}_n \)-Demazure crystal. We identify it with the (connected) subgraph induced from the crystal graph of \( \text{RF}_n(w) \). See Figure 1 for an example. The character of any finite subset \( \mathcal{X} \) of a crystal \( \mathcal{B} \) is \( \text{ch}(\mathcal{X}) := \sum_{b \in \mathcal{X}} x^{\text{wt}(b)} \in \mathbb{Z}[x] \).

**Theorem 2.1** (See [4]). If \( \alpha \) is a weak composition with \( u(\alpha) \in S_n \) such that \( \lambda(\alpha) \) has at most \( n \) parts then \( \text{ch}(\text{Dem}_n(\alpha)) = \kappa_\alpha \).

On the other hand, Assaf and Schilling [1] have shown the following:

**Theorem 2.2** ([1]). For any \( w \in S_\infty \), the set \( \text{BRF}_n(w) \) is a disjoint union of \( \mathfrak{gl}_n \)-Demazure crystals, in the sense that there is a weight-preserving isomorphism from each connected component of the subgraph of the crystal graph of \( \text{RF}_n(w) \) induced on \( \text{BRF}_n(w) \) to \( \text{Dem}_n(\alpha) \) for some \( \alpha \).
Figure 1: For the dominant $w = 3142 = s_2 s_1 s_3 \in S_6$ of shape $\lambda(w) = (2, 1, 0)$, the $\mathfrak{gl}_3$-crystal $\operatorname{RF}_3(w)$. The unique reduced factorization is $b_{\lambda(w)} = (21, 3, \emptyset)$. The elements in the $\mathfrak{gl}_n$-Demazure crystal $\operatorname{Dem}_3(\alpha)$ for $\alpha = (2, 0, 1)$, which are all in $\operatorname{BRF}(w)$, are boxed.

Since $\operatorname{ch}(\operatorname{BRF}_n(w)) = S_w$ if $n$ is sufficiently large, taking characters in this theorem recovers the nontrivial fact noted above that every Schubert polynomial expands as a positive linear combination of key polynomials [20, Thm. 4].

### 3 Shifted key polynomials

In this section, we introduce two shifted analogues of key and atom polynomials. We then present our main results about these polynomials and state a number of conjectures.

A partition $\lambda$ is **strict** if its nonzero parts are all distinct; alternatively, if $\lambda = (\lambda_1 > \cdots > \lambda_\ell > 0)$. We say $\lambda$ is **symmetric** if $\lambda^\top = \lambda$, where $\lambda^\top$ is the conjugate shape. A partition $\lambda$ is **skew-symmetric** if $\lambda^\top = \lambda$ and if $i$ maximal such that $(i, i) \in D_\lambda$, then we cannot add or remove the box $(i, i+1)$ from $D_\lambda$ and still have the diagram of a partition. When $\lambda$ is symmetric, we define its **shifted diagram** to be $S(\lambda) = \{(i,j) \in D_\lambda : i \leq j\}$ and **strict shifted diagram** to be $\hat{S}(\lambda) = \{(i,j) \in D_\lambda : i < j\}$.

Let $H(\lambda)$ (resp. $\hat{H}(\lambda)$) be the (strict) half diagram formed by sliding all boxes to the left of $S(\lambda)$ (resp. $\hat{S}(\lambda)$). This is the diagram of the strict partition $\lambda^H$ (resp. $\lambda^{\hat{H}}$) whose parts count the number of boxes in the distinct rows of $S(\lambda)$ (resp. $\hat{S}(\lambda)$). The map $\lambda \mapsto \lambda^H$ (resp. $\lambda \mapsto \lambda^{\hat{H}}$) is a bijection from symmetric (resp. skew-symmetric) partitions to strict partitions. We say a weak composition $\alpha$ is **(skew-)symmetric** if $\lambda(\alpha)$ is (skew-)symmetric.

**Definition 3.1.** Let $\alpha$ be a symmetric weak composition, and set $\lambda = \lambda(\alpha)$. Define

$$\kappa_\alpha^Q = \pi_{u(\alpha)} \left( \prod_{(i,j) \in S(\lambda)} (x_i + x_j) \right) \quad \text{and} \quad \kappa_\alpha^Q = \pi_{\hat{u}(\alpha)} \left( \prod_{(i,j) \in \hat{S}(\lambda)} (x_i + x_j) \right).$$

We refer to these functions as **$Q$-key polynomials** and **$Q$-atom polynomials**. Similarly, when
α is skew-symmetric we define
\[ \kappa^P_\alpha = \pi u(\alpha) \left( \prod_{(i,j) \in S(\lambda)} (x_i + x_j) \right) \quad \text{and} \quad \kappa^Q_\alpha = \overline{\pi} u(\alpha) \left( \prod_{(i,j) \in S(\lambda)} (x_i + x_j) \right). \]

We refer to these functions as \textit{P-key polynomials} and \textit{P-atom polynomials}.

The definitions of \( \kappa^P_\alpha \) and \( \kappa^Q_\alpha \) make sense if \( \alpha \) is symmetric but not skew-symmetric, but in this case there is always a skew-symmetric \( \beta \) with \( \kappa^P_\alpha = \kappa^P_\beta \) and \( \kappa^Q_\alpha = \kappa^Q_\beta \).

\textbf{Example 3.2.} If \( \alpha = 3143 \) then \( \lambda(\alpha) = 4211 \) is skew-symmetric with \( \lambda^H = 3100 \) and \( u(\alpha) = 3142 = s_2 s_1 s_3 \), so we have
\[
\kappa^P_{3143} = \pi_2 \pi_1 \pi_3 ((x_1 + x_2)(x_1 + x_3)(x_1 + x_4)(x_2 + x_3)) = \kappa_2 \kappa_0 \kappa_1 + \kappa_0 \kappa_1 \kappa_2 + \kappa_0 \kappa_1 \kappa_2,
\]
\[
\kappa^Q_{3143} = \pi_2 \pi_1 \pi_3 ((x_1 + x_2)(x_1 + x_3)(x_1 + x_4)(x_2 + x_3)) = \kappa_2 \kappa_0 \kappa_1 + \kappa_0 \kappa_1 \kappa_2.
\]

If \( \alpha = 2031 \) then \( \lambda(\alpha) = 3210 \) is symmetric with \( \lambda(\alpha)^H = 3100 \) and \( u(\alpha) = 3142 = s_2 s_1 s_3 \), so
\[
\kappa^Q_{2031} = \pi_2 \pi_1 \pi_3 (4x_1 x_2 (x_1 + x_2)(x_1 + x_3)) = 4\kappa_1 \kappa_2 + 4\kappa_2 \kappa_1 + 4\kappa_0 \kappa_1 \kappa_2 + 4\kappa_0 \kappa_1 \kappa_2,
\]
\[
\kappa^Q_{2031} = \pi_2 \pi_1 \pi_3 (4x_1 x_2 (x_1 + x_2)(x_1 + x_3)) = 0.
\]

We refer to \( \kappa^P_\alpha \) and \( \kappa^Q_\alpha \) collectively as \textit{shifted key polynomials}, and to \( \kappa^P_\alpha \) and \( \kappa^Q_\alpha \) as \textit{shifted atom polynomials}. Shifted atom polynomials are related to shifted key polynomials via the \textit{Bruhat order} \( \leq \) on \( S_\infty \). Recall that \( \beta \leq \alpha \) if \( \lambda(\beta) = \lambda(\alpha) \) and \( u(\beta) \leq u(\alpha) \).

\textbf{Proposition 3.3.} We have \( \kappa^P_\alpha = \sum_{\beta \leq \alpha} \kappa^P_\beta \) and \( \kappa^Q_\alpha = \sum_{\beta \leq \alpha} \kappa^Q_\beta \). Moreover, \( \kappa^Q_\alpha \) and \( \kappa^Q_\alpha \) are divisible by \( 2^\ell \), where \( \ell \) is the length of \( \lambda(\alpha)^H \).

Our first substantial result about shifted key and atom polynomials is the following.

\textbf{Theorem 3.4.} Let \( \alpha \) be a symmetric composition. Then \( \kappa^P_\alpha \) and \( \kappa^Q_\alpha \) (resp. \( \kappa^P_\alpha \) and \( \kappa^Q_\alpha \)) are linear combinations of key (resp. atom) polynomials with nonnegative integer coefficients. Consequently, the polynomials \( \kappa^P_\alpha, \kappa^P_\alpha, \kappa^Q_\alpha, \) and \( \kappa^Q_\alpha \) are all in \( \mathbb{N}[x] \).

Key polynomials are partial Schur functions in the sense that if \( \lambda = (\lambda_1 \geq \lambda_2 \geq \cdots \geq 0) \) is a partition with at most \( n \) nonzero parts then \( \kappa_\alpha = s_\lambda(x_1,x_2,\ldots,x_n) \) for \( \alpha = (\lambda_n, \ldots, \lambda_2, \lambda_1) \) [20, \S2]. Analogously, we can prove that shifted key polynomials are partial \textit{Schur P/Q-functions} (see, [14, \SIII.8] for background on these functions):

\textbf{Theorem 3.5.} If \( \lambda = (\lambda_1 \geq \lambda_2 \geq \cdots \geq 0) \) is a symmetric partition with \( \lambda_1 \leq n \) then
\[ \kappa^P_\alpha = P_\mu(x_1,x_2,\ldots,x_n) \quad \text{and} \quad \kappa^Q_\alpha = Q_\nu(x_1,x_2,\ldots,x_n) \]
for \( \alpha = (\lambda_n, \ldots, \lambda_2, \lambda_1, 0, 0, \ldots) \), \( \mu = \lambda^H \), and \( \nu = \lambda^H \).
We have conjectural formulas for the leading terms of $\kappa^P_\alpha$ and $\kappa^Q_\alpha$. Assume $\alpha$ is a symmetric composition with $\lambda = \lambda(\alpha)$ and $u = u(\alpha)$. Define $D(\alpha) = \{(u(i), u(j)) : (i, j) \in D_\lambda\}$. Let $\rho(\alpha) = (\rho_1, \rho_2, \ldots)$ and $\theta(\alpha) = (\theta_1, \theta_2, \ldots)$ where $\rho_i = |\{(a, b) \in D(\alpha) : i = a \geq b\}|$ and $\theta_i = |\{(a, b) \in D(\alpha) : a \geq b = i\}|$. Also define $\tilde{\rho}(\alpha) = (\tilde{\rho}_1, \tilde{\rho}_2, \ldots)$ and $\tilde{\theta}(\alpha) = (\tilde{\theta}_1, \tilde{\theta}_2, \ldots)$ where $\tilde{\rho}_i = |\{(a, b) \in D(\alpha) : i > a \geq b\}|$ and $\tilde{\theta}_i = |\{(a, b) \in D(\alpha) : a > b = i\}|$. These are the row/column counts of $D(\alpha)$ below the main diagonal.

**Conjecture 3.6.** Suppose $\alpha$ and $\beta$ are symmetric compositions with $\beta$ skew-symmetric. Then

$$\kappa^Q_\alpha \in 2^{\ell(\lambda(\alpha)^H)} \left( x^{\rho(\alpha)} + x^{\theta(\alpha)} + \sum_{\gamma \neq \rho(\alpha)} N x^\gamma \right) \quad \text{and} \quad \kappa^P_\beta \in x^{\tilde{\rho}(\beta)} + x^{\tilde{\theta}(\beta)} + \sum_{\gamma \neq \tilde{\rho}(\beta)} N x^\gamma.$$  

Moreover, $x^{\rho(\alpha)}$ and $x^{\tilde{\theta}(\beta)}$ are the leading terms of $\kappa^Q_\alpha$ and $\kappa^P_\beta$ in lexicographic order.

We can prove that if $\alpha$ and $\beta$ are as above then $D(\alpha)$ (hence, also $\alpha$) is uniquely determined by $\rho(\alpha)$ and $\theta(\alpha)$, while $D(\beta)$ (hence, also $\beta$) is uniquely determined by $\tilde{\rho}(\beta)$ and $\tilde{\theta}(\beta)$. This does not hold for general symmetric subsets of $\mathbb{P} \times \mathbb{P}$. Shifted key/atom polynomials are not as well-behaved as their classical analogues in a few other ways:

- Shifted atom polynomials are zero for some indices $\alpha$. They can also coincide for different indices. For example, $\kappa^Q_{30023} = \kappa^Q_{21014} \neq 0$ and $\kappa^P_{402402} = \kappa^P_{313501} \neq 0$.

- $P$-key polynomials are not uniquely indexed by skew-symmetric compositions: for example, $\kappa^P_{4313} = \kappa^P_{4133} \neq 0$.

- However, we have not yet been able to find a pair of distinct symmetric compositions $\alpha \neq \beta$ such that $\kappa^Q_\alpha = \kappa^Q_\beta$. It is possible that the $Q$-key polynomials are uniquely indexed by symmetric compositions.

- Even if this is the case, the $Q$-key polynomials are still not linearly independent. For example, we have $\kappa^Q_{123} + \kappa^Q_{0321} = \kappa^Q_{132} + \kappa^Q_{0231}$.

Shifted key polynomials are closely related to certain “orthogonal” and “symplectic” versions of type A Schubert polynomials. Let $I^Q_\infty = \{z \in S_\infty : z = z^{-1}\}$ and let $I^{Sp}_\infty$ be the $S_\infty$-conjugacy class of $1_{fpf} = (1 \ 2) (3 \ 4) (5 \ 6) \cdots$. If $\lambda$ is a symmetric partition, then the unique dominant element of $S_\infty$ of shape $\lambda$ already belongs to $I^Q_\infty$. If $\lambda$ is a skew-symmetric partition, then there is a unique $z \in I^{Sp}_\infty$ with $\{(i, j) \in D(z) : i \neq j\} = \{(i, j) \in D_\lambda : i \neq j\}$, which we call the **dominant** element of $I^{Sp}_\infty$ with shape $\lambda$.

Let $K \in \{Sp, O\}$. By results in [22], there are unique polynomials $\{\mathcal{G}^K_z\}_{z \in I^K_\infty}$ with $\mathcal{G}^K_z = \kappa^P_\lambda$ when $K = Sp$ (resp. $\mathcal{G}^K_z = \kappa^Q_\alpha$ when $K = O$) and $z \in I^K_\infty$ is dominant of shape $\lambda$, ...
and which satisfy
\[
\partial_i \mathcal{S}^p_z = \begin{cases} 
0 & \text{if } z(i) < z(i+1), \\
0 & \text{if } z(i) = i + 1, \\
\mathcal{S}^p_{z_i 2z_i} & \text{otherwise,}
\end{cases}
\quad \text{and} \quad
\partial_i \mathcal{S}^o_z = \begin{cases} 
0 & \text{if } z(i) < z(i+1), \\
2\mathcal{S}^o_{z_i} & \text{if } z(i) = i + 1, \\
\mathcal{S}^o_{z_i 2z_i} & \text{otherwise,}
\end{cases}
\]
for all \( z \in l^K_\infty \) and \( i \in \mathbb{P} \). We refer to the \( \mathcal{S}^K_z \)'s as \textit{K-Schubert polynomials}. These elements, called \textit{involution Schubert polynomials} in [9, 10, 11], represent cohomology classes of the closures of the \( \mathcal{S}^p_\cdot \text{ and } \mathcal{O} \)-orbits in the complete flag variety [22]. The following conjecture is one of our primary motivations for studying shifted key polynomials:

\textbf{Conjecture 3.7.} Each polynomial \( \mathcal{S}^p_z \) for \( z \in l^K_\infty \) (resp. \( \mathcal{S}^o_z \) for \( z \in l^K_\infty \)) is an \( \mathbb{N} \)-linear combination of \( P \)-key polynomials (resp. \( Q \)-key polynomials).

This conjecture is supported by many computational examples and closely parallels the classical case. Below, we will outline a shifted analogue of Theorem 2.1 that also provides some heuristic support for the conjecture.

Like ordinary Schubert polynomials, K-Schubert polynomials can be expressed via a BJS-type formula as \( \mathcal{S}^K_z = \sum_{a \in BRF^K(z)} x^{\text{wt}(a)} \) for an analogue \( BRF^K(z) \) of the set \( BRF(z) \) [9]. For each choice of \( K \), \( BRF^K(z) \) consists of the bounded elements in a larger set of \( K \)-\textit{reduced factorizations} \( RF^K(z) \). If \( K = \mathcal{S}^p \) then \( RF^K(z) \) is explicitly given as the disjoint union of \( RF(w) \) over all minimal length \( w \in S_\infty \) with \( z = w^{-1} f_{\text{pf}} w \). The definition of \( RF^O(z) \) for \( z \in l^K_\infty \) is more involved: this is formed by taking another disjoint union of sets \( RF(w) \) for certain \( w \in S_\infty \), and then optionally annotating some letters in each reduced factorization by primes; see [18] for the precise details.

Define \( BRF^p_n(z) \subseteq RF^p_n(z) \) to be the respective subsets of \( BRF^K(z) \subseteq RF^K(z) \) consisting of the tuples \( a = (a^1, a^2, \ldots) \) with \( a^i \) empty for \( i > n \). Like \( RF_n(w) \), the sets \( RF^p_n(z) \) have natural crystal structures. Results in [16] identify a crystal structure on \( RF^p_n(z) \) corresponding to the \textit{queer Lie superalgebra} \( q_n \) (as described axiomatically in [7]), extending the \( gl_n \) crystal in [19]. The set \( RF^O_n(z) \) similarly is the prototypical example of what is called an \textit{extended queer supercrystal} or \( q_n^+ \)-crystal in [18].

Crystals for \( q_n \) are \( gl_n \) crystals with \textit{odd crystal operators} \( e_\bar{i}, f_\bar{i} \) for \( \bar{i} \in \{1, \ldots, n-\bar{1}\} := \{\bar{1}, \ldots, n-\bar{1}\} \) satisfying certain axioms. It is sufficient to define \( e_\bar{i}, f_\bar{i} \) as the other odd crystal operators come from inductively twisting the root system [6, Lemma 2.2]:

\[
e_\bar{i} = s_{i-1} s_i e_{\bar{i} - \bar{1}} s_i s_{i-1} \quad \text{and} \quad f_\bar{i} = s_{i-1} s_i f_{\bar{i} - \bar{1}} s_i s_{i-1}. \tag{3.1}
\]

Here \( s_i \) acts as the crystal operator that reverses each \( i \)-\textit{string}. We remark that \( e_{\bar{i}} \) is not defined by a usual bracketing rule but by a weight condition. For \( q_n^+ \) crystals, there are additional crystal operators \( e_0, f_0 \). Similar to \( gl_n \) crystals, we encode \( q_n / q_n^+ \) crystals as crystal graphs. In view of (3.1), we omit \( \bar{2}, \bar{3}, \ldots \) when drawing the crystal graphs.
Figure 2: The $q_4$-crystal on $\mathrm{RP}^{Sp}(z)$ corresponding to $\kappa^p_\lambda$ for $z = s_1 s_2 s_4 \cdot 1_{\text{fif}} \cdot s_4 s_2 s_1$ and $\lambda = (4, 1, 1, 1)$. The boxed elements are in $\mathrm{BRP}^{Sp}(z)$. Solid blue, red, and green arrows indicate 1-, 2-, and 3-edges, respectively, while dashed blue arrows are $\overline{1}$-edges.
Figure 3: The $q^+_{\lambda}$-crystal on $RF^O(z)$ corresponding to $\kappa_{\lambda}^Q$ for $z = (1,3)(2,4)$ and $\lambda = (3,3,3)$. The boxed elements are in $\text{BRF}^O(z)$. Solid blue, solid red, dotted green, and dashed blue arrows are $i$-edges for $i = 1,2,0,\bar{1}$, respectively.

Now suppose $z \in \mathcal{I}_K^\infty$ is dominant with (skew-)symmetric shape $\lambda$ having $\lambda_1 \leq n$. In general, the set $\text{BRF}_n^K(z)$ contains more than one element in $RF_n^K(z)$. Nevertheless, there is an interesting shifted analogue of the $\mathfrak{gl}_n$-Demazure crystal (2.2). Fix a (skew-)symmetric composition $\alpha$ with $\lambda = \lambda(\alpha)$ and $u(\alpha) \in S_n$. Then define

$$\text{Dem}_n^K(\alpha) := \left\{ a \in RF_n^K(z) : \begin{array}{c} e_{i_1}^{m_1} e_{i_2}^{m_2} \cdots e_{i_\ell}^{m_\ell} a \in \text{BRF}_n^K(z) \text{ for some reduced word} \\ i_1 i_2 \cdots i_\ell \text{ for } u(\alpha) \text{ and some } m_1, m_2, \ldots, m_\ell \in \mathbb{N} \end{array} \right\}.$$ 

We refer to this subset as a $K$-Demazure crystal; see Figures 2 and 3 for examples. We identify $\text{Dem}_n^K(\alpha)$ with the subgraph that it induces in the extended $q_n/q_n^+$-crystal graph of $RF_n^K(z)$ (formed by drawing arrows corresponding to all even and odd crystal operators). This directed subgraph is connected, although this is not at all obvious:
**Theorem 3.8.** Assume $u(\alpha) \in S_n$ and $\lambda(\alpha)$ has at most $n$ parts. Then the $K$-Demazure crystal $\text{Dem}_n^K(\alpha)$ is connected with character equal to $\kappa^K_\alpha$ when $K = \text{Sp}$ and to $\kappa^K_\alpha$ when $K = O$.

Our second main conjecture is the following analogue of Theorem 2.2:

**Conjecture 3.9.** If $z \in I^K_n$ then $\text{BRF}_n^K(z)$ is a disjoint union of $K$-Demazure crystals, in the sense that there is a weight-preserving isomorphism from each connected component of the subgraph of the extended crystal graph of $\text{RF}_n^K(z)$ induced on $\text{BRF}_n^K(z)$ to $\text{Dem}_n^K(\alpha)$ for some $\alpha$.

As $\text{ch}(\text{BRF}_n^K(z)) = \mathcal{E}_z^K$ if $n \gg 0$, Conjecture 3.7 would follow from this conjecture on taking characters. This conjecture is again supported by extensive computer calculations. Conjectures 3.7 and 3.9 also have more refined versions involving $K$-reduced factorizations that are bounded by arbitrary flags, which would generalize [20, Thm. 21].

An interesting discrepancy with the classical case is that the subsets $\text{Dem}_n^K(\alpha)$ are not closed under $e_i$ for all $i \in [n-1]$. Contrast this with the situation for $\text{gl}_n$-Demazure crystals: if $b_\beta$ is the unique element of weight $\beta \leq \alpha$ in a $\text{gl}_n$-Demazure crystal, then while we cannot obtain all elements from $b_\alpha$ through applying $\{e_i : i \in [n-1]\}$, we can obtain everything by applying these operators to the closure of $\{b_\beta : \beta \leq \alpha\}$.

**Example 3.10.** Consider the $q_4$-crystal $\text{RF}_n^K(z)$ in Figure 2. For $b = (2/3/4/\cdot) \in \text{BRF}_n^K(z)$, we have $e_2(2/3/4/\cdot) = s_1s_2e_1s_2s_1(2/3/4/\cdot) = s_1s_2(21/\cdot/4/\cdot) = s_1(21/4/\cdot/\cdot) = (2/41/\cdot/\cdot) \not\in \text{BRF}_n^K(z)$.

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**References**


