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Shifted key polynomials

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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 $G = \mathsf{GL}_n(\mathbb{C})$ and write $B \subseteq G$ for the Borel subgroup of upper triangular matrices. Let K be either the orthogonal group $\mathsf{O}_n(\mathbb{C})$ or symplectic group $\mathsf{Sp}_n(\mathbb{C})$ (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 $\mathbb{Z}[\mathbf{x}] = \mathbb{Z}[x_1, x_2, \dots]$ and the well-known *Schubert polynomials* $\mathfrak{S}_w \in \mathbb{Z}[\mathbf{x}]$ 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 $\mathsf{K} = \mathsf{O}$ and by fixed-point-free involutions in S_n when $\mathsf{K} = \mathsf{Sp}$ 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 $\mathfrak{S}_w = \mathbf{x}^\lambda$ 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

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to GL dominant weights. There exists a stable limit F_w of $\mathfrak{S}_w$ 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 $\mathfrak{S}_w$ 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 $\mathrm{RF}(w)$ of factorizations of reduced words for w into decreasing subwords. (We refer to elements of $\mathrm{RF}(w)$ as *reduced factorizations*.) Morse and Schilling showed this directly in [19] by constructing a *(Kashiwara) crystal* [12] on the set $\mathrm{RF}(w)$.

The BJS formula for $\mathfrak{S}_w$ is a sum over a certain class of *bounded reduced factorizations* $\mathrm{BRF}(w) \subset \mathrm{RF}(w)$, and so we can restrict the crystal structure on $\mathrm{RF}(w)$ 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 λ is a partition with at most n parts.

The precise definition of a key polynomial is $\kappa_{u\lambda} = \pi_u \mathfrak{S}_w$ where π_u is an *isobaric divided difference operator* and w is a dominant permutation with $\lambda(w) = \lambda$. For each choice of $\mathsf{K} \in \{\mathsf{O}, \mathsf{Sp}\}$, 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 $\pi_u \mathfrak{S}^{\mathsf{K}}_z$ 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 $\mathfrak{S}^{\mathsf{K}}_z$ 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 $s_\lambda(x_1, x_2, \ldots, x_n) = \kappa_{w_0\lambda}$. 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 $\mathbb{Z}$-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, $[n] = \{1, 2, \dots, n\}$, $\mathbb{N} = \{0, 1, 2, \dots\}$, and $\mathbb{P} = \{1, 2, 3, \dots\}$. Let $\mathbf{x} = (x_1, x_2, \dots)$ be commuting indeterminates.

Define $S_\infty = \langle s_1, s_2, s_3, \dots \rangle$ 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 $i_1 i_2 \dots i_\ell$ 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_∞ acts on the polynomial ring $\mathbb{Z}[\mathbf{x}]$ 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 $\mathrm{RF}(w)$ denote the set of sequences $a = (a^1, a^2, a^3, \cdots)$ 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 $\mathrm{RF}_n(w)$ to be the set of such a with a^i empty for all $i > n$. In examples we express elements of $\mathrm{RF}_n(w)$ as n-tuples rather than as infinite sequences. Let $\mathrm{BRF}_n(w)$ denote the set of reduced factorizations in $\mathrm{RF}_n(w)$ that are *bounded* in the sense that $i \le \min(a^i)$ for all nonempty a^i. Set $\mathrm{BRF}(w) := \bigsqcup_{n=1}^\infty \mathrm{BRF}_n(w)$.

A *weak composition* is a nonnegative integer sequence $\alpha = (\alpha_i \in \mathbb{N})_{i=1}^\infty$ with finite sum $|\alpha| := \sum_{i=1}^\infty \alpha_i$, 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 α, let $\lambda(\alpha)$ be the partition sorting α and define $\mathbf{x}^\alpha = x_1^{\alpha_1} x_2^{\alpha_2} \cdots$. There is a unique $u(\alpha) \in S_\infty$ such that $u(\alpha)\alpha$ is a partition $\lambda(\alpha)$, where the permutation acts on α 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 ∂_i be the *divided difference operator* on $f \in \mathbb{Z}[\mathbf{x}]$ 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 $\overline{\pi}_i := \pi_i - 1$. For $w \in S_\infty$ with reduced word $i_1 \cdots i_\ell$, define $\pi_w = \pi_{i_1} \cdots \pi_{i_\ell}$ and $\overline{\pi}_w = \overline{\pi}_{i_1} \cdots \overline{\pi}_{i_\ell}$; these formulas do not depend on the choice of reduced word. The *key polynomial* of a weak composition α is then $\kappa_\alpha := \pi_{u(\alpha)} \mathbf{x}^{\lambda(\alpha)}$ while the *atom polynomial* of α is $\overline{\kappa}_\alpha = \overline{\pi}_{u(\alpha)} \mathbf{x}^{\lambda(\alpha)}$. It is well-known that $\{\kappa_\alpha : \text{weak compositions } \alpha\}$ is a basis for $\mathbb{Z}[\mathbf{x}]$ and that key polynomials are unitriangular with $\kappa_\alpha = \mathbf{x}^\alpha + (\text{lower order terms})$

with respect to lexicographic order [20, Cor. 7]. Key polynomials are related to atom polynomials by the identity $\kappa_\alpha = \sum_{\beta \le \alpha} \overline{\kappa}_\beta$, where we write $\alpha \le \beta$ if $\lambda(\alpha) = \lambda(\beta)$ and $u(\alpha) \le u(\beta)$ 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 $D_\lambda = \{(i,j) \in \mathbb{P} \times \mathbb{P} : j \le \lambda_i\}$ of a partition $\lambda = \lambda(w)$. This occurs precisely when w is 132-avoiding [15, Ex. 2.2.2]. The *Schubert polynomial* of $w \in S_\infty$ is defined recursively by setting $\mathfrak{S}_w = \mathbf{x}^{\lambda(w)}$ when w is dominant and requiring that $\mathfrak{S}_{ws_i} = \partial_i \mathfrak{S}_w$ for $w(i) > w(i+1)$ [13]. For any $w \in S_\infty$ the Billey–Jockusch–Stanley formula [2] asserts that

$$\mathfrak{S}_w = \sum_{a \in \mathrm{BRF}(w)} \mathbf{x}^{\mathrm{wt}(a)}, \qquad \text{where } \mathrm{wt}(a) := (\ell(a^1), \ell(a^2), \dots). \tag{2.1}$$

Key polynomials can be defined in terms of Schubert polynomials, since if $w \in S_\infty$ is dominant of shape $\lambda(\alpha)$ then $\kappa_\alpha = \pi_{u(\alpha)} \mathfrak{S}_w$. 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* $e_i, f_i \colon \mathcal{B} \to \mathcal{B} \sqcup \{\mathbf{0}\}$ for $i \in [n-1]$ and a *weight function* $\mathrm{wt} \colon \mathcal{B} \to \mathbb{Z}^n$ 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 $\mathrm{RF}_n(w)$ already has a weight function as used in (2.1). Morse and Schilling [19] identified a natural $\mathfrak{gl}_n$-crystal structure on $\mathrm{RF}_n(w)$, 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 λ has at most n nonzero parts. Then $\mathrm{RF}_n(w)$ contains a single bounded reduced factorization $b_\lambda \in \mathrm{BRF}_n(w)$. This element has weight λ and is *highest weight* in the sense that $e_i b_\lambda = 0$ for all $i \in [n-1]$. If α is a weak composition with $\lambda = \lambda(\alpha)$ and $u(\alpha) \in S_n$ then we define

$$\mathrm{Dem}_n(\alpha) := \left\{ a \in \mathrm{RF}_n(w) : \begin{array}{l} e_{i_1}^{m_1} e_{i_2}^{m_2} \cdots e_{i_\ell}^{m_\ell} a = b_\lambda \text{ for some reduced word} \\ i_1 i_2 \cdots i_\ell \text{ of } u(\alpha) \text{ and some } m_1, m_2, \dots, m_\ell \in \mathbb{N} \end{array} \right\}. \tag{2.2}$$

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 $\mathrm{RF}_n(w)$. See Figure 1 for an example. The *character* of any finite subset $\mathcal{X}$ of a crystal $\mathcal{B}$ is $\mathrm{ch}(\mathcal{X}) := \sum_{b \in \mathcal{X}} \mathbf{x}^{\mathrm{wt}(b)} \in \mathbb{Z}[\mathbf{x}]$.

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

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

Theorem 2.2 ([1]). *For any $w \in S_\infty$, the set $\mathrm{BRF}_n(w)$ 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 $\mathrm{RF}_n(w)$ induced on $\mathrm{BRF}_n(w)$ to $\mathrm{Dem}_n(\alpha)$ for some α.*

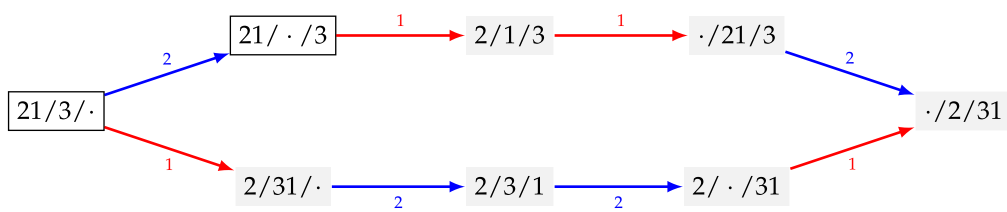

Figure 1: For the dominant $w = 3142 = s_2 s_1 s_3 \in S_\infty$ of shape $\lambda(w) = (2, 1, 0)$, the $\mathfrak{gl}_3$-crystal $\mathrm{RF}_3(w)$. The unique reduced factorization is $b_{\lambda(w)} = (21, 3, \varnothing)$. The elements in the $\mathfrak{gl}_n$-Demazure crystal $\mathrm{Dem}_3(\alpha)$ for $\alpha = (2, 0, 1)$, which are all in $\mathrm{BRF}(w)$, are boxed.

Since $\mathrm{ch}(\mathrm{BRF}_n(w)) = \mathfrak{S}_w$ 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 λ is *strict* if its nonzero parts are all distinct; alternatively, if $\lambda = (\lambda_1 > \cdots > \lambda_\ell > 0)$. We say λ is *symmetric* if $\lambda^\top = \lambda$, where $\lambda^\top$ is the conjugate shape. A partition λ 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_λ and still have the diagram of a partition. When λ is symmetric, we define its *shifted diagram* to be $S(\lambda) = \{(i, j) \in D_\lambda : i \le j\}$ and *strict shifted diagram* to be $\widehat{S}(\lambda) = \{(i, j) \in D_\lambda : i < j\}$.

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

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

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

We refer to these functions as *Q-key polynomials* and *Q-atom polynomials*. Similarly, when

α is skew-symmetric we define

$$\kappa^{\mathsf{P}}_\alpha = \pi_{u(\alpha)}\left(\prod_{(i,j)\in\widehat{S}(\lambda)}(x_i+x_j)\right) \quad\text{and}\quad \overline{\kappa}^{\mathsf{P}}_\alpha = \overline{\pi}_{u(\alpha)}\left(\prod_{(i,j)\in\widehat{S}(\lambda)}(x_i+x_j)\right).$$

We refer to these functions as *P-key polynomials* and *P-atom polynomials*.

The definitions of $\kappa^{\mathsf{P}}_\alpha$ and $\overline{\kappa}^{\mathsf{P}}_\alpha$ make sense if α is symmetric but not skew-symmetric, but in this case there is always a skew-symmetric β with $\kappa^{\mathsf{P}}_\alpha = \kappa^{\mathsf{P}}_\beta$ and $\overline{\kappa}^{\mathsf{P}}_\alpha = \overline{\kappa}^{\mathsf{P}}_\beta$.

Example 3.2. If $\alpha = 3143$ then $\lambda(\alpha) = 4211$ is skew-symmetric with $\lambda^{\widehat{H}} = 3100$ and $u(\alpha) = 3142 = s_2s_1s_3$, so we have

$$\begin{aligned}\kappa^{\mathsf{P}}_{3143} &= \pi_2\pi_1\pi_3\big((x_1+x_2)(x_1+x_3)(x_1+x_4)(x_2+x_3)\big) = \kappa_{0022}+\kappa_{0031}+\kappa_{0112},\\ \overline{\kappa}^{\mathsf{P}}_{3143} &= \overline{\pi}_2\overline{\pi}_1\overline{\pi}_3\big((x_1+x_2)(x_1+x_3)(x_1+x_4)(x_2+x_3)\big) = \overline{\kappa}_{0022}+\overline{\kappa}_{0031}.\end{aligned}$$

If $\alpha = 2031$ then $\lambda(\alpha) = 3210$ is symmetric with $\lambda(\alpha)^H = 3100$ and $u(\alpha) = s_2s_1s_3$, so

$$\begin{aligned}\kappa^{\mathsf{Q}}_{2031} &= \pi_2\pi_1\pi_3\big(4x_1x_2(x_1+x_2)(x_1+x_3)\big) = 4\kappa_{103}+4\kappa_{202}+4\kappa_{1021},\\ \overline{\kappa}^{\mathsf{Q}}_{2031} &= \overline{\pi}_2\overline{\pi}_1\overline{\pi}_3\big(4x_1x_2(x_1+x_2)(x_1+x_3)\big) = 0.\end{aligned}$$

We refer to $\kappa^{\mathsf{P}}_\alpha$ and $\kappa^{\mathsf{Q}}_\alpha$ collectively as *shifted key polynomials*, and to $\overline{\kappa}^{\mathsf{P}}_\alpha$ and $\overline{\kappa}^{\mathsf{Q}}_\alpha$ as *shifted atom polynomials*. Shifted atom polynomials are related to shifted key polynomials via the *Bruhat order* $\leq$ on S_∞. Recall that $\beta \leq \alpha$ if $\lambda(\beta) = \lambda(\alpha)$ and $u(\beta) \leq u(\alpha)$.

Proposition 3.3. *We have* $\kappa^{\mathsf{P}}_\alpha = \sum_{\beta\leq\alpha}\overline{\kappa}^{\mathsf{P}}_\beta$ *and* $\kappa^{\mathsf{Q}}_\alpha = \sum_{\beta\leq\alpha}\overline{\kappa}^{\mathsf{Q}}_\beta$*. Moreover,* $\kappa^{\mathsf{Q}}_\alpha$ *and* $\overline{\kappa}^{\mathsf{Q}}_\alpha$ *are divisible by* 2^ℓ*, where* ℓ *is the length of* $\lambda(\alpha)^H$*.*

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

Theorem 3.4. *Let* α *be a symmetric composition. Then* $\kappa^{\mathsf{P}}_\alpha$ *and* $\kappa^{\mathsf{Q}}_\alpha$ *(resp.* $\overline{\kappa}^{\mathsf{P}}_\alpha$ *and* $\overline{\kappa}^{\mathsf{Q}}_\alpha$*) are linear combinations of key (resp. atom) polynomials with nonnegative integer coefficients. Consequently, the polynomials* $\kappa^{\mathsf{P}}_\alpha$*,* $\overline{\kappa}^{\mathsf{P}}_\alpha$*,* $\kappa^{\mathsf{Q}}_\alpha$*, and* $\overline{\kappa}^{\mathsf{Q}}_\alpha$ *are all in* $\mathbb{N}[\mathbf{x}]$*.*

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 $\kappa_\alpha = s_\lambda(x_1, x_2, \dots, x_n)$ for $\alpha = (\lambda_n, \dots, \lambda_2, \lambda_1)$ [20, §2]. Analogously, we can prove that shifted key polynomials are partial *Schur P/Q-functions* (see, [14, §III.8] for background on these functions):

Theorem 3.5. *If* $\lambda = (\lambda_1 \geq \lambda_2 \geq \cdots \geq 0)$ *is a symmetric partition with* $\lambda_1 \leq n$ *then*

$$\kappa^{\mathsf{P}}_\alpha = P_\mu(x_1, x_2, \dots, x_n) \quad\textit{and}\quad \kappa^{\mathsf{Q}}_\alpha = Q_\nu(x_1, x_2, \dots, x_n)$$

for $\alpha = (\lambda_n, \dots, \lambda_2, \lambda_1, 0, 0, \dots)$*,* $\mu = \lambda^{\widehat{H}}$*, and* $\nu = \lambda^H$*.*

We have conjectural formulas for the leading terms of $\kappa^{\mathsf{P}}_\alpha$ and $\kappa^{\mathsf{Q}}_\alpha$. Assume α 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 $\rho(\alpha) = (\rho_1, \rho_2, \dots)$ and $\theta(\alpha) = (\theta_1, \theta_2, \dots)$ 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 $\widetilde{\rho}(\alpha) = (\widetilde{\rho}_1, \widetilde{\rho}_2, \dots)$ and $\widetilde{\theta}(\alpha) = (\widetilde{\theta}_1, \widetilde{\theta}_2, \dots)$ where $\widetilde{\rho}_i = |\{(a,b) \in D(\alpha) : i = a > b\}|$ and $\widetilde{\theta}_j = |\{(a,b) \in D(\alpha) : a > b = i\}|$. These are the row/column counts of $D(\alpha)$ below the main diagonal.

Conjecture 3.6. *Suppose α and β are symmetric compositions with β skew-symmetric. Then*

$$\kappa^{\mathsf{Q}}_\alpha \in 2^{\ell(\lambda(\alpha)^H)} \left(\mathbf{x}^{\rho(\alpha)} + \mathbf{x}^{\theta(\alpha)} + \sum_{\gamma \neq \rho(\alpha)} \mathbb{N}\mathbf{x}^\gamma \right) \quad \textit{and} \quad \kappa^{\mathsf{P}}_\beta \in \mathbf{x}^{\widetilde{\rho}(\beta)} + \mathbf{x}^{\widetilde{\theta}(\beta)} + \sum_{\gamma \neq \widetilde{\rho}(\beta)} \mathbb{N}\mathbf{x}^\gamma.$$

Moreover, $\mathbf{x}^{\rho(\alpha)}$ and $\mathbf{x}^{\widetilde{\rho}(\beta)}$ are the leading terms of $\kappa^{\mathsf{Q}}_\alpha$ and $\kappa^{\mathsf{P}}_\beta$ in lexicographic order.

We can prove that if α and β are as above then $D(\alpha)$ (hence, also α) is uniquely determined by $\rho(\alpha)$ and $\theta(\alpha)$, while $D(\beta)$ (hence, also β) is uniquely determined by $\widetilde{\rho}(\beta)$ and $\widetilde{\theta}(\beta)$. 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 α. They can also coincide for different indices. For example, $\overline{\kappa}^{\mathsf{Q}}_{30023} = \overline{\kappa}^{\mathsf{Q}}_{21014} \neq 0$ and $\overline{\kappa}^{\mathsf{P}}_{402402} = \overline{\kappa}^{\mathsf{P}}_{313501} \neq 0$.
- P-key polynomials are not uniquely indexed by skew-symmetric compositions: for example, $\kappa^{\mathsf{P}}_{4313} = \kappa^{\mathsf{P}}_{4133} \neq 0$.
- However, we have not yet been able to find a pair of distinct symmetric compositions $\alpha \neq \beta$ such that $\kappa^{\mathsf{Q}}_\alpha = \kappa^{\mathsf{Q}}_\beta$. 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 $\kappa^{\mathsf{Q}}_{123} + \kappa^{\mathsf{Q}}_{0321} = \kappa^{\mathsf{Q}}_{132} + \kappa^{\mathsf{Q}}_{0231}$.

Shifted key polynomials are closely related to certain "orthogonal" and "symplectic" versions of type A Schubert polynomials. Let $I^{\mathsf{O}}_\infty = \{z \in S_\infty : z = z^{-1}\}$ and let I^{Sp}_∞ be the S_∞-conjugacy class of $1_{\mathsf{fpf}} = (1\ 2)(3\ 4)(5\ 6)\cdots$. If λ is a symmetric partition, then the unique dominant element of S_∞ of shape λ already belongs to I^{O}_∞. If λ is a skew-symmetric partition, then there is a unique $z \in I^{\mathsf{Sp}}_\infty$ 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}_∞ with shape λ.

Let $\mathsf{K} \in \{\mathsf{Sp}, \mathsf{O}\}$. By results in [22], there are unique polynomials $\{\mathfrak{S}^{\mathsf{K}}_z\}_{z \in I^{\mathsf{K}}_\infty}$ with $\mathfrak{S}^{\mathsf{K}}_z = \kappa^{\mathsf{P}}_\lambda$ when $\mathsf{K} = \mathsf{Sp}$ (resp. $\mathfrak{S}^{\mathsf{K}}_z = \kappa^{\mathsf{Q}}_\lambda$ when $\mathsf{K} = \mathsf{O}$) and $z \in I^{\mathsf{K}}_\infty$ is dominant of shape λ, and which satisfy

$$\partial_i \mathfrak{S}^{\mathsf{Sp}}_z = \begin{cases} 0 & \text{if } z(i) < z(i+1), \\ 0 & \text{if } z(i) = i+1, \\ \mathfrak{S}^{\mathsf{Sp}}_{s_i z s_i} & \text{otherwise,} \end{cases} \quad \text{and} \quad \partial_i \mathfrak{S}^{\mathsf{O}}_z = \begin{cases} 0 & \text{if } z(i) < z(i+1), \\ 2\mathfrak{S}^{\mathsf{O}}_{z s_i} & \text{if } z(i) = i+1, \\ \mathfrak{S}^{\mathsf{O}}_{s_i z s_i} & \text{otherwise,} \end{cases}$$

for all $z \in I^{\mathsf{K}}_\infty$ and $i \in \mathbb{P}$. We refer to the $\mathfrak{S}^{\mathsf{K}}_z$'s as *$\mathsf{K}$-Schubert polynomials*. These elements, called *involution Schubert polynomials* in [9, 10, 11], represent cohomology classes of the closures of the Sp- and O-orbits in the complete flag variety [22]. The following conjecture is one of our primary motivations for studying shifted key polynomials:

Conjecture 3.7. *Each polynomial $\mathfrak{S}^{\mathsf{Sp}}_z$ for $z \in I^{\mathsf{Sp}}_\infty$ (resp. $\mathfrak{S}^{\mathsf{O}}_z$ for $z \in I^{\mathsf{O}}_\infty$) 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 $\mathfrak{S}^{\mathsf{K}}_z = \sum_{a \in \mathrm{BRF}^{\mathsf{K}}(z)} \mathbf{x}^{\mathrm{wt}(a)}$ for an analogue $\mathrm{BRF}^{\mathsf{K}}(z)$ of the set $\mathrm{BRF}(z)$ [9]. For each choice of K, $\mathrm{BRF}^{\mathsf{K}}(z)$ consists of the bounded elements in a larger set of *K-reduced factorizations* $\mathrm{RF}^{\mathsf{K}}(z)$. If $\mathsf{K} = \mathsf{Sp}$ then $\mathrm{RF}^{\mathsf{K}}(z)$ is explicitly given as the disjoint union of $\mathrm{RF}(w)$ over all minimal length $w \in S_\infty$ with $z = w^{-1} 1_{\mathsf{fpf}} w$. The definition of $\mathrm{RF}^{\mathsf{O}}(z)$ for $z \in I^{\mathsf{O}}_\infty$ is more involved: this is formed by taking another disjoint union of sets $\mathrm{RF}(w)$ 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 $\mathrm{BRF}^{\mathsf{K}}_n(z) \subseteq \mathrm{RF}^{\mathsf{K}}_n(z)$ to be the respective subsets of $\mathrm{BRF}^{\mathsf{K}}(z) \subseteq \mathrm{RF}^{\mathsf{K}}(z)$ consisting of the tuples $a = (a^1, a^2, \dots)$ with a^i empty for $i > n$. Like $\mathrm{RF}_n(w)$, the sets $\mathrm{RF}^{\mathsf{K}}_n(z)$ have natural crystal structures. Results in [16] identify a crystal structure on $\mathrm{RF}^{\mathsf{Sp}}_n(z)$ corresponding to the *queer Lie superalgebra* $\mathfrak{q}_n$ (as described axiomatically in [7]), extending the $\mathfrak{gl}_n$ crystal in [19]. The set $\mathrm{RF}^{\mathsf{O}}_n(z)$ similarly is the prototypical example of what is called an *extended queer supercrystal* or *$\mathfrak{q}^+_n$-crystal* in [18].

Crystals for $\mathfrak{q}_n$ are $\mathfrak{gl}_n$ crystals with *odd crystal operators* $e_{\bar{\imath}}, f_{\bar{\imath}}$ for $\bar{\imath} \in [\overline{n-1}] := \{\bar{1}, \dots, \overline{n-1}\}$ satisfying certain axioms. It is sufficient to define $e_{\bar{1}}, f_{\bar{1}}$ as the other odd crystal operators come from inductively twisting the root system [6, Lemma 2.2]:

$$e_{\bar{\imath}} = s_{i-1} s_i e_{\overline{i-1}} s_i s_{i-1} \quad \text{and} \quad f_{\bar{\imath}} = s_{i-1} s_i f_{\overline{i-1}} s_i s_{i-1}. \tag{3.1}$$

Here s_i acts as the crystal operator that reverses each *i-string*. We remark that $e_{\bar{1}}$ is not defined by a usual bracketing rule but by a weight condition. For $\mathfrak{q}^+_n$ crystals, there are additional crystal operators e_0, f_0. Similar to $\mathfrak{gl}_n$ crystals, we encode $\mathfrak{q}_n / \mathfrak{q}^+_n$ crystals as crystal graphs. In view of (3.1), we omit $\bar{2}, \bar{3}, \dots$ when drawing the crystal graphs.

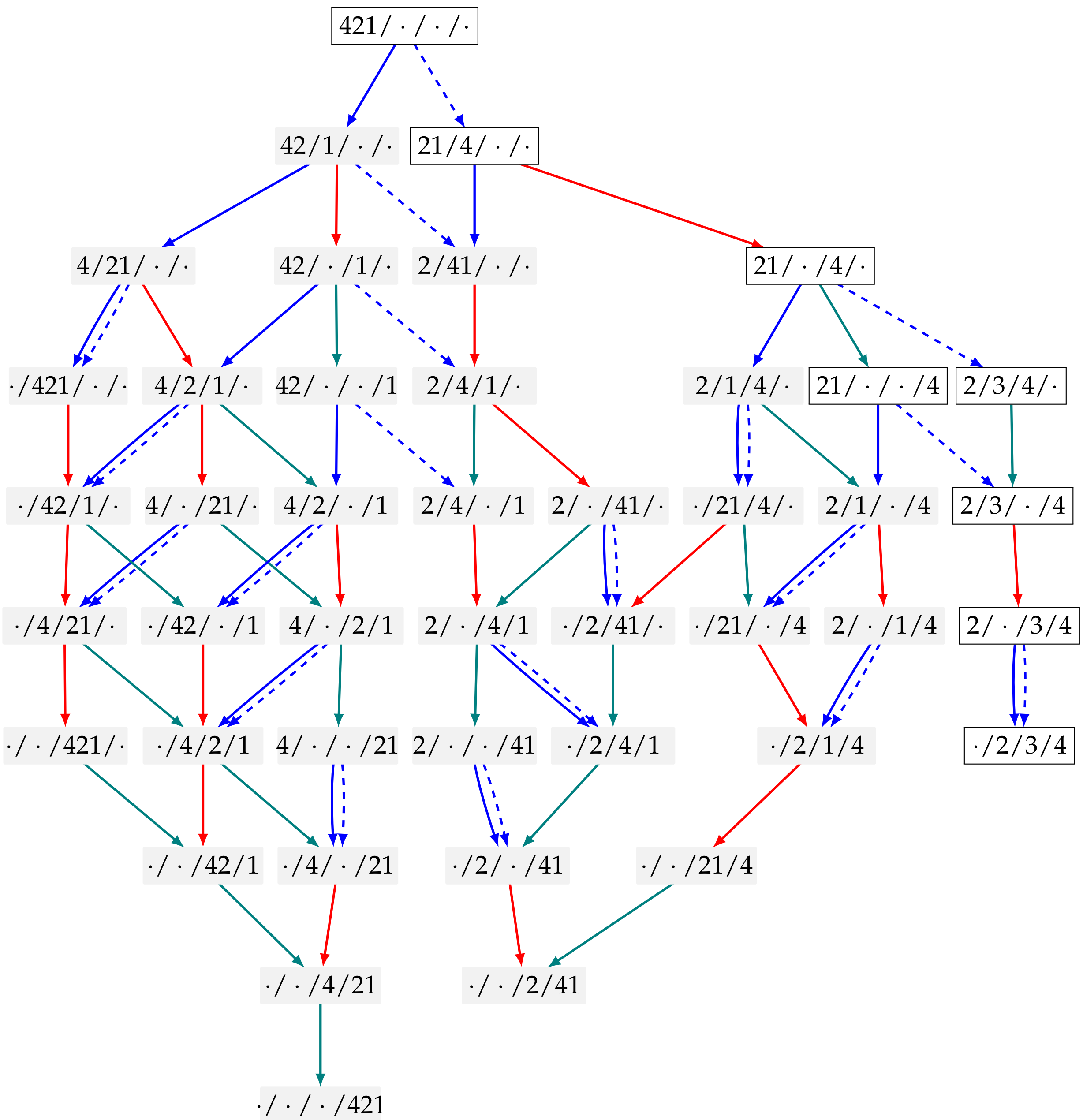

Figure 2: The $\mathfrak{q}_4$-crystal on $\mathrm{RF}^{\mathsf{Sp}}(z)$ corresponding to $\kappa^{\mathsf{P}}_\lambda$ for $z = s_1 s_2 s_4 \cdot 1_{\mathsf{fpf}} \cdot s_4 s_2 s_1$ and $\lambda = (4, 1, 1, 1)$. The boxed elements are in $\mathrm{BRF}^{\mathsf{Sp}}(z)$. Solid blue, red, and green arrows indicate 1-, 2-, and 3-edges, respectively, while dashed blue arrows are $\overline{1}$-edges.

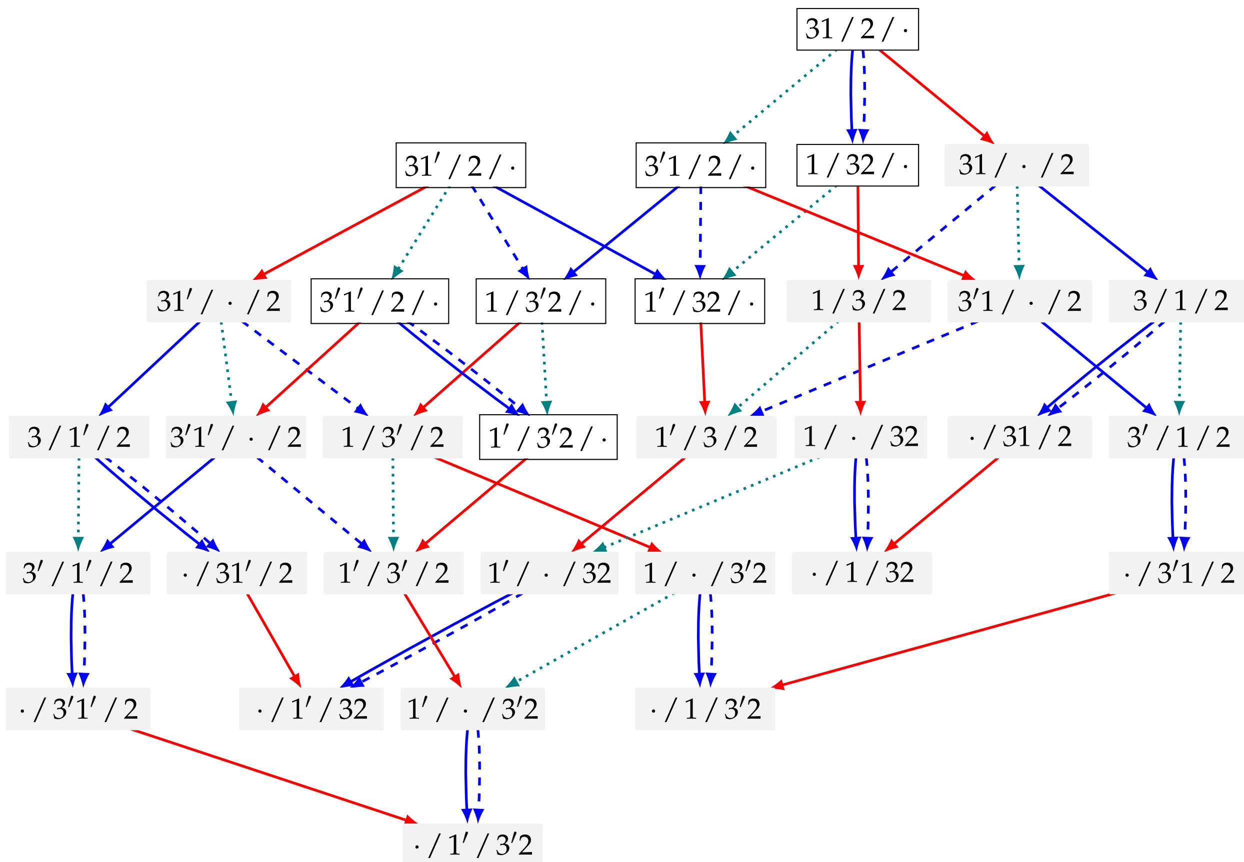

Figure 3: The $\mathfrak{q}_3^+$-crystal on $\mathrm{RF}^{\mathsf{O}}(z)$ corresponding to $\kappa_\lambda^{\mathsf{Q}}$ for $z = (1\ 3)(2\ 4)$ and $\lambda = (3,3,3)$. The boxed elements are in $\mathrm{BRF}^{\mathsf{O}}(z)$. Solid blue, solid red, dotted green, and dashed blue arrows are i-edges for $i = 1, 2, 0, \overline{1}$, respectively.

Now suppose $z \in I_\infty^{\mathsf{K}}$ is dominant with (skew-)symmetric shape λ having $\lambda_1 \leq n$. In general, the set $\mathrm{BRF}_n^{\mathsf{K}}(z)$ contains more than one element in $\mathrm{RF}_n^{\mathsf{K}}(z)$. Nevertheless, there is an interesting shifted analogue of the $\mathfrak{gl}_n$-Demazure crystal (2.2).

Fix a (skew-)symmetric composition α with $\lambda = \lambda(\alpha)$ and $u(\alpha) \in S_n$. Then define

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

We refer to this subset as a K-*Demazure crystal*; see Figures 2 and 3 for examples. We identify $\mathrm{Dem}_n^{\mathsf{K}}(\alpha)$ with the subgraph that it induces in the *extended* $\mathfrak{q}_n/\mathfrak{q}_n^+$*-crystal graph* of $\mathrm{RF}_n^{\mathsf{K}}(z)$ (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* $\mathrm{Dem}_n^{\mathsf{K}}(\alpha)$ *is connected with character equal to $\kappa_\alpha^{\mathsf{P}}$ when $\mathsf{K} = \mathsf{Sp}$ and to $\kappa_\alpha^{\mathsf{Q}}$ when $\mathsf{K} = \mathsf{O}$.*

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

Conjecture 3.9. *If $z \in I_\infty^{\mathsf{K}}$ then $\mathrm{BRF}_n^{\mathsf{K}}(z)$ 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 $\mathrm{RF}_n^{\mathsf{K}}(z)$ induced on $\mathrm{BRF}_n^{\mathsf{K}}(z)$ to $\mathrm{Dem}_n^{\mathsf{K}}(\alpha)$ for some α.*

As $\mathrm{ch}(\mathrm{BRF}_n^{\mathsf{K}}(z)) = \mathfrak{S}_z^{\mathsf{K}}$ 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 $\mathrm{Dem}_n^{\mathsf{K}}(\alpha)$ are not closed under $e_{\bar{\imath}}$ for all $\bar{\imath} \in \overline{[n-1]}$. Contrast this with the situation for $\mathfrak{gl}_n$-Demazure crystals: if b_β is the unique element of weight $\beta \leq \alpha$ in a $\mathfrak{gl}_n$-Demazure crystal, then while we cannot obtain all elements from b_α 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 $\mathfrak{q}_4$-crystal $\mathrm{RF}^{\mathsf{Sp}}(z)$ in Figure 2. For $b = (2/3/4/\cdot) \in \mathrm{BRF}^{\mathsf{Sp}}(z)$, we have $e_{\bar{2}}(2/3/4/\cdot) = s_1 s_2 e_{\bar{1}} s_2 s_1 (2/3/4/\cdot) = s_1 s_2 e_{\bar{1}}(2/3/4/\cdot) = s_1 s_2 (21/\cdot/4/\cdot) = s_1(21/4/\cdot/\cdot) = (2/41/\cdot/\cdot) \notin \mathrm{BRF}^{\mathsf{Sp}}(z)$.

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