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On some Grothendieck expansions

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Abstract. The complete flag variety admits a natural action by both the orthogonal group and the symplectic group. Wyser and Yong defined orthogonal Grothendieck polynomials $\mathcal{G}^{\mathsf{O}}_z$ and symplectic Grothendieck polynomials $\mathcal{G}^{\mathsf{Sp}}_z$ as the K-theory classes of the corresponding orbit closures. There is an explicit formula to expand $\mathcal{G}^{\mathsf{Sp}}_z$ as a nonnegative sum of Grothendieck polynomials $\mathcal{G}^{(\beta)}$, which represent the K-theory classes of Schubert varieties. Although the constructions of $\mathcal{G}^{\mathsf{Sp}}_z$ and $\mathcal{G}^{\mathsf{O}}_z$ are similar, finding the $\mathcal{G}^{(\beta)}$-expansion of $\mathcal{G}^{\mathsf{O}}_z$ or even computing $\mathcal{G}^{\mathsf{O}}_z$ is much harder. When z is vexillary, it has been shown that $\mathcal{G}^{\mathsf{O}}_z$ has a nonnegative $\mathcal{G}^{(\beta)}$-expansion, but the $\mathcal{G}^{(\beta)}$-coefficients are mostly unknown. This paper derives several new formulas for $\mathcal{G}^{\mathsf{O}}_z$ and its $\mathcal{G}^{(\beta)}$-expansion when z is vexillary. In particular, we prove that the latter expansion has a nontrivial stability property when $z(1) = 1$.

Keywords: K-theory, Grothendieck polynomials, matrix Schubert varieties

1 Introduction

This article is concerned with combinatorial formulas for expansions of three different families of *Grothendieck polynomials* related to K-theory classes of Schubert varieties. We first briefly introduce these polynomials in the context of *matrix Schubert varieties*. We will then discuss the central problem of interest and some of our partial solutions.

1.1 Grothendieck polynomials

Let n be a positive integer. Write S_n for the group of permutations of the integers $\mathbb{Z}$ with support in $[n] := \{1, \dots, n\}$. For $w \in S_n$, the *matrix Schubert variety* MX_w is the set of complex $n \times n$ matrices $M \in \mathsf{Mat}_{n\times n}$ whose upper $i \times j$ submatrices $M_{[i][j]}$ all satisfy $\mathrm{rank}(M_{[i][j]}) \le |\{t \in [i] : w(t) \le j\}|$. Results in [8] identify an equivariant K-theory class

$$[MX_w] \in \mathbb{Z}[a_1^{\pm 1}, a_2^{\pm 1}, \dots, a_n^{\pm 1}] \cong K_T(\mathsf{Mat}_{n\times n}).$$

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The *Grothendieck polynomial* $\mathcal{G}^{(\beta)}_w$ introduced in [4] can be formed from $[MX_w]$ by making the variable substitutions $a_i \mapsto 1 + \beta x_i$ for all $i \in [n]$ and dividing by $(-\beta)^{\mathrm{codim}(MX_w)}$. This function always belongs to $\mathbb{Z}_{\geq 0}[\beta][x_1, x_2, \dots, x_n]$ and if $w \in S_\infty := \bigcup_{n\geq 1} S_n$ then the value of $\mathcal{G}^{(\beta)}_w$ does not depend on the choice of n with $w \in S_n$. Moreover, it is well-known [12, Corollary 3.3] that the family $\{\mathcal{G}^{(\beta)}_w : w \in S_\infty\}$ is a $\mathbb{Z}[\beta]$-basis for $\mathbb{Z}[\beta][x_1, x_2, \dots]$.

1.2 Orthogonal Grothendieck polynomials

Let $I_n = \{z \in S_n : z = z^{-1}\}$ and $I_\infty = \{z \in S_\infty : z = z^{-1}\}$. For $z \in I_n$ define

$$\mathsf{Mat}^{\mathsf{O}}_{n\times n} = \left\{ X \in \mathsf{Mat}_{n\times n} : X^\top = X \right\} \quad \text{and} \quad MX^{\mathsf{O}}_z = MX_z \cap \mathsf{Mat}^{\mathsf{O}}_{n\times n}.$$

Results in [11] identify an equivariant K-theory class

$$[MX^{\mathsf{O}}_z] \in \mathbb{Z}[a_1^{\pm 1}, a_2^{\pm 1}, \dots, a_n^{\pm 1}] \cong K_T(\mathsf{Mat}^{\mathsf{O}}_{n\times n}).$$

The *orthogonal Grothendieck polynomial* $\mathcal{G}^{\mathsf{O}}_z$ introduced in [15] can be formed from $[MX^{\mathsf{O}}_z]$ by substituting $a_i \mapsto 1 + \beta x_i$ for all $i \in [n]$ and dividing by $(-\beta)^{\mathrm{codim}(MX^{\mathsf{O}}_z)}$. As with $\mathcal{G}^{(\beta)}_w$, this function always belongs to $\mathbb{Z}_{\geq 0}[\beta][x_1, x_2, \dots, x_n]$ and does not depend on the choice of n with $z \in I_n$.

When $z \in I_\infty$ is *vexillary* in the sense of being 2143-avoiding, it is known [14, Proposition 3.29] that $\mathcal{G}^{\mathsf{O}}_z \in \mathbb{Z}_{\geq 0}[\beta]\text{-span}\{\mathcal{G}^{(\beta)}_w : w \in S_\infty\}$. It is an open problem to describe the $\mathcal{G}^{(\beta)}$-expansion of $\mathcal{G}^{\mathsf{O}}_z$ explicitly. This problem is the focus of this article.

1.3 Symplectic Grothendieck polynomials

It is instructive to contrast this open problem with what is known about the formally similar *symplectic Grothendieck polynomials*. Let I^{fpf}_n be the set of fixed-point-free involutions of $\mathbb{Z}$ sending $i \mapsto i - 1$ for all even integers $i \notin [n]$. For $z \in I^{\mathsf{fpf}}_n$ define

$$\mathsf{Mat}^{\mathsf{Sp}}_{n\times n} = \left\{ X \in \mathsf{Mat}_{n\times n} : X^\top = -X \right\} \quad \text{and} \quad MX^{\mathsf{Sp}}_z = MX_z \cap \mathsf{Mat}^{\mathsf{Sp}}_{n\times n}.$$

Just as in the previous two cases, there is an equivariant K-theory class [11]

$$[MX^{\mathsf{Sp}}_z] \in \mathbb{Z}[a_1^{\pm 1}, a_2^{\pm 1}, \dots, a_n^{\pm 1}] \cong K_T(\mathsf{Mat}^{\mathsf{Sp}}_{n\times n}).$$

The *symplectic Grothendieck polynomial* $\mathcal{G}^{\mathsf{Sp}}_z$ introduced in [15] can be formed from $[MX^{\mathsf{Sp}}_z]$ by substituting $a_i \mapsto 1 + \beta x_i$ for all $i \in [n]$ and dividing by $(-\beta)^{\mathrm{codim}(MX^{\mathsf{Sp}}_z)}$. Once again $\mathcal{G}^{\mathsf{Sp}}_z \in \mathbb{Z}_{\geq 0}[\beta][x_1, x_2, \dots]$ and if $z \in I^{\mathsf{fpf}}_\infty := \bigcup_{n\geq 1} I^{\mathsf{fpf}}_n$ then $\mathcal{G}^{\mathsf{Sp}}_z$ does not depend on the choice of n with $z \in I^{\mathsf{fpf}}_n$.

Like $\mathcal{G}^{\mathsf{O}}_z$ (at least for vexillary z), there is a positive $\mathcal{G}^{(\beta)}$-expansion of each $\mathcal{G}^{\mathsf{Sp}}_z$. Unlike $\mathcal{G}^{\mathsf{O}}_z$, this expansion can be explicitly computed in the following way.

Write $w_i = w(i)$ for $w \in S_\infty$ and $i \in \mathbb{Z}$. Let $\approx$ be the transitive closure of the relation on S_∞ that has $v^{-1} \approx w^{-1}$ if there is an even index $i \in 2\mathbb{Z}_{\geq 0}$ and integers $a < b < c < d$ such that $v_{i+1}v_{i+2}v_{i+3}v_{i+4}$ and $w_{i+1}w_{i+2}w_{i+3}w_{i+4}$ are both in $\{adbc, bcad, bdac\}$, while $v_j = w_j$ for all $j \notin \{i+1, i+2, i+3, i+4\}$. For example, in one-line notation, we have

$$(\,15\underline{2634}\,)^{-1} \approx (\,15\underline{3624}\,)^{-1} \approx (\,\overline{15\underline{34}}\underline{26}\,)^{-1} \approx (\,\overline{3415}26\,)^{-1} \approx (\,\overline{3514}26\,)^{-1}.$$

Given $z \in I^{\mathsf{fpf}}_\infty$ let $a_1 < a_2 < a_3 < \dots$ be the integers with $0 < a_i < b_i := z(a_i)$ and define $\alpha_{\mathsf{fpf}}(z)$ to be inverse of the one-line permutation $a_1b_1a_2b_2a_3b_3\cdots$. Then [11, Theorem 3.12]

$$\mathcal{G}^{\mathsf{Sp}}_z = \textstyle\sum_{w \approx \alpha_{\mathsf{fpf}}(z)} \beta^{\ell(w) - \ell(\alpha_{\mathsf{fpf}}(z))} \mathcal{G}^{(\beta)}_w.$$

1.4 Grothendieck expansions

For each $z \in I_\infty$ there exists a *orthogonal Grothendieck coefficient function* $\mathrm{GC}^{\mathsf{O}}_z : S_\infty \to \mathbb{Z}$ such that $\mathcal{G}^{\mathsf{O}}_z = \sum_{w \in S_\infty} \mathrm{GC}^{\mathsf{O}}_z(w) \cdot \beta^{\ell(w) - \ell_{\mathsf{inv}}(z)} \cdot \mathcal{G}^{(\beta)}_w$. The support $\mathrm{supp}(\mathrm{GC}^{\mathsf{O}}_z) := \{w \in S_\infty : \mathrm{GC}^{\mathsf{O}}_z(w) \neq 0\}$ must be a finite set of permutations. As noted earlier, when $z \in I_\infty$ is vexillary, it is known that $\mathrm{GC}^{\mathsf{O}}_z : S_\infty \to \mathbb{Z}_{\geq 0}$ takes all nonnegative values, but otherwise little is known about this function in the literature to date.

We mention that if one sets $\beta = 0$ then $\mathcal{G}^{(\beta)}_w$, $\mathcal{G}^{\mathsf{O}}_y$, and $\mathcal{G}^{\mathsf{Sp}}_z$ turn into the *(involution) Schubert polynomials* $\mathfrak{S}_w$, $\hat{\mathfrak{S}}_y$, and $\hat{\mathfrak{S}}^{\mathsf{fpf}}_z$ studied in [6, 10], for which the relevant expansions are all much simpler: both $\hat{\mathfrak{S}}_y$ and $\hat{\mathfrak{S}}^{\mathsf{fpf}}_z$ are equal to a constant (which is 1 in the second case) times a multiplicity-free sum of $\mathfrak{S}_w$'s. Moreover, the terms that appear are predicted by a general formula of Brion [1] and are described combinatorially in [3].

This work contains the first explicit results about the coefficient functions $\mathrm{GC}^{\mathsf{O}}_z$. Our main theorems can be summarized as follows. In Sections 3 and 4 we derive an exact, though not obviously positive formula for $\mathrm{GC}^{\mathsf{O}}_z$ when z is any *quasi-dominant* involution (see Theorem 4.3). Then we explain a new formula for $\mathcal{G}^{\mathsf{O}}_z$ when z is any vexillary involution, which shows that $\mathrm{GC}^{\mathsf{O}}_z$ is *shift invariant* whenever $z(1) = 1$ (see Theorems 5.4 and 5.5). These results lead to a new proof of the existence of *stable limits* of orthogonal Grothendieck polynomials. Finally, we compute $\mathrm{GC}^{\mathsf{O}}_z$ in some special cases in Section 6.

2 Product formulas and divided difference operators

So far we have not discussed any method of computing $\mathcal{G}^{(\beta)}_w$ or $\mathcal{G}^{\mathsf{O}}_z$ as polynomials, let alone the expansion of the latter in terms of the former. This section quickly reviews an algebraic method to compute $\mathcal{G}^{(\beta)}_w$, which can be adapted to $\mathcal{G}^{\mathsf{O}}_z$ when z is vexillary.

The group S_∞ acts on $\mathbb{Z}[\beta][x_1, x_2, \dots]$ by permuting the x_i variables. For each $i \in \mathbb{Z}_{>0}$ the *divided difference operators* ∂_i and $\partial_i^{(\beta)}$ act on $\mathbb{Z}[\beta][x_1, x_2, \dots]$ by the formulas

$$\partial_i f = \tfrac{f - s_i f}{x_i - x_{i+1}} \quad \text{and} \quad \partial_i^{(\beta)} f = \partial_i\big((1+\beta x_{i+1}) f\big) = -\beta f + (1+\beta x_i)\partial_i f. \tag{2.1}$$

These operators satisfy the Coxeter braid relations for S_∞ along with $\partial_i^{(\beta)}\partial_i^{(\beta)} = -\beta\partial_i^{(\beta)}$.

The *Rothe diagram* of $w \in S_\infty$ is the set $D(w)$ of positive integer pairs (i,j) satisfying both $i < w^{-1}(j)$ and $j < w(i)$. A permutation $w \in S_\infty$ is *dominant* if there is a partition λ such that $D(w)$ coincides with the *Young diagram* $\mathsf{D}_\lambda := \{(i,j) : 1 \le j \le \lambda_i\}$. In this case we say that w is of shape λ.

There is a unique dominant $w \in S_\infty$ of each partition shape λ, and for this permutation $\mathcal{G}_w^{(\beta)} = \prod_{(i,j)\in \mathsf{D}_\lambda} x_i$ [4]. Moreover, for any $w \in S_\infty$, one has $\partial_i^{(\beta)}\mathcal{G}_w^{(\beta)} = \mathcal{G}_{ws_i}^{(\beta)}$ if $i \in \mathrm{Des}_R(w) := \{i \in \mathbb{Z} : w(i) > w(i+1)\}$ [4]. These formulas determine $\mathcal{G}_w^{(\beta)}$ for all w.

Suppose $z \in I_\infty$ is dominant of shape λ. Then z is also vexillary and $\lambda = \lambda^\top$ is necessarily a *symmetric* partition since $D(z) = D(z^{-1}) = D(z)^\top$, and one has $i < z(i)$ if and only if $(i,i) \in \mathsf{D}_\lambda$. For dominant involutions, one again has a product formula

$$\mathcal{G}_z^{\mathsf{O}} = \prod_{\substack{(i,j)\in\mathsf{D}_\lambda \\ i \le j}} x_i \oplus x_j \quad \text{where } x \oplus y := x + y + \beta xy \text{ [11, Theorem 3.8]}. \tag{2.2}$$

Moreover, if $z \in I_\infty$ is vexillary and $i \in \mathrm{Des}_R(z)$ is such that $s_i z s_i \neq z$ is also vexillary, then the formula $\partial_i^{(\beta)}\mathcal{G}_z^{\mathsf{O}} = \mathcal{G}_{s_i z s_i}^{\mathsf{O}}$ also holds [11, Proposition 3.23]. This recurrence, combined with the product formula (2.2) can be used to calculate $\mathcal{G}_z^{\mathsf{O}}$ for any vexillary $z \in I_\infty$.

For involutions $z \in I_\infty$ that are not vexillary, no simple algebraic formula is known for computing $\mathcal{G}_z^{\mathsf{O}}$. In particular, these polynomials cannot be expressed using $\partial_i^{(\beta)}$'s. We mention that by contrast, the polynomials $\mathcal{G}_z^{\mathsf{Sp}}$ are completely determined by a product formula and a divided difference recurrence; see [11, Theorem 3.8 and Proposition 3.11].

3 Involution Grothendieck polynomials

There is another family of polynomials indexed by involutions $z \in I_\infty$ that share several favorable algebraic properties with $\mathcal{G}_z^{\mathsf{Sp}}$, and will turn out to be closely related to $\mathcal{G}_z^{\mathsf{O}}$.

Write $\ell : S_\infty \to \mathbb{Z}_{\ge 0}$ for the usual Coxeter length function counting the number of inversions of a permutation. The *Demazure product* is the unique associative operation $\circ : S_\infty \times S_\infty \to S_\infty$ with $u \circ v = uv$ if and only if $\ell(uv) = \ell(u) + \ell(v)$, and with $s_i \circ s_i = s_i$ for simple transpositions $s_i := (i, i+1) \in S_\infty$. The formula $w \mapsto w^{-1} \circ w$ is a surjective map $S_\infty \to I_\infty$, so the set $\mathcal{B}_{\mathsf{inv}}(z) := \{w \in S_\infty : w^{-1} \circ w = z\}$ is nonempty for $z \in I_\infty$. Define the *involution Grothendieck polynomial* of z to be

$$\widehat{\mathcal{G}}_z := \sum_{w \in \mathcal{B}_{\mathsf{inv}}(z)} \beta^{\ell(w) - \ell_{\mathsf{inv}}(z)} \mathcal{G}_w^{(\beta)} \quad \text{where } \ell_{\mathsf{inv}}(z) := \min\{\ell(w) : w \in \mathcal{B}_{\mathsf{inv}}(z)\}. \tag{3.1}$$

The set $\mathcal{B}_{\mathsf{inv}}(z)$ was extensively studied in [5] and can be generated using a certain equivalence relation. Let $\sim$ be the transitive closure of the relation on S_∞ that has $v^{-1} \sim w^{-1}$ if there is an index $i \in \mathbb{Z}_{>0}$ and integers $a < b < c$ such that $v_i v_{i+1} v_{i+2}$ and $w_i w_{i+1} w_{i+2}$ are both in $\{cba, cab, bca\}$, while $v_j = w_j$ for all $j \notin \{i, i+1, i+2\}$.

For $z \in I_\infty$ let $a_1 < a_2 < \dots$ be the positive integers with $a_i \leq b_i := z(a_i)$. Define $\alpha_{\mathsf{inv}}(z)$ to be inverse of the permutation whose one-line notation is formed by removing the repeated letters from $b_1 a_1 b_2 a_2 b_3 a_3 \cdots$. Then by [5, Section 6.1] and [6, Section 3] we have

$$\mathcal{B}_{\mathsf{inv}}(z) = \{w \in S_\infty : w \sim \alpha_{\mathsf{inv}}(z)\} \quad \text{and} \quad \ell_{\mathsf{inv}}(z) = \ell(\alpha_{\mathsf{inv}}(z)). \tag{3.2}$$

For example, $\mathcal{B}_{\mathsf{inv}}(45312) = \{\alpha_{\mathsf{inv}} = 24513,\ 25413,\ 25314,\ 35214,\ 35124\}$. The polynomials $\widehat{\mathcal{G}}_z$ were previously considered in [13, Section 4], but the following theorem is new.

Theorem 3.1. Suppose $z \in I_\infty$. Then for any $i \in \mathbb{Z}_{>0}$ it holds that

$$\partial_i^{(\beta)} \widehat{\mathcal{G}}_z = \begin{cases} \widehat{\mathcal{G}}_{zs_i} & \text{if } i \in \mathrm{Des}_R(z) \text{ and } z(i) = i+1 \\ \widehat{\mathcal{G}}_{s_i z s_i} & \text{if } i \in \mathrm{Des}_R(z) \text{ and } z(i) \neq i+1 \\ -\beta \widehat{\mathcal{G}}_z & \text{if } i \notin \mathrm{Des}_R(z). \end{cases}$$

Moreover, if z is dominant of shape λ then $\widehat{\mathcal{G}}_z = \prod_{\substack{(i,j) \in \mathsf{D}_\lambda \\ i=j}} x_i \prod_{\substack{(i,j) \in \mathsf{D}_\lambda \\ i<j}} x_i \oplus x_j$.

Example 3.2. If $z = 45312 = (1,4)(2,5) \in I_\infty$ then z is dominant of shape $(3,3,2)$ and

$$\widehat{\mathcal{G}}_z = \mathcal{G}^{(\beta)}_{24513} + \beta \mathcal{G}^{(\beta)}_{25413} + \mathcal{G}^{(\beta)}_{25314} + \beta \mathcal{G}^{(\beta)}_{35214} + \mathcal{G}^{(\beta)}_{35124} = x_1 x_2 (x_1 \oplus x_2)(x_1 \oplus x_3)(x_2 \oplus x_3).$$

4 Grothendieck expansions in the quasi-dominant case

We now explain how to leverage the $\mathcal{G}^{(\beta)}$-expansion of $\widehat{\mathcal{G}}_z$ to get information about $\mathcal{G}^{\mathsf{O}}_z$. Let I^{vex}_∞ be the set of vexillary (i.e., 2143-avoiding) involutions in I_∞. An element $z \in I^{\mathsf{vex}}_\infty$ is *quasi-dominant* if $i-1 < z(i-1)$ whenever $1 < i < z(i)$. Every dominant involution is quasi-dominant. Define $k(z) := \min\{i \in \mathbb{Z}_{\geq 0} : (j,j) \notin D(z) \text{ for all } j > i\}$ for $z \in I_\infty$.

Theorem 4.1. If $z \in I^{\mathsf{vex}}_\infty$ is quasi-dominant with $k = k(z)$ then $\mathcal{G}^{\mathsf{O}}_z = \widehat{\mathcal{G}}_z \prod_{i=1}^k (2 + \beta x_i)$.

We can turn this theorem into an exact, though not manifestly positive, formula for the coefficient function $\mathrm{GC}^{\mathsf{O}}_z : S_\infty \to \mathbb{Z}_{\geq 0}$ with $\mathcal{G}^{\mathsf{O}}_z = \sum_{w \in S_\infty} \mathrm{GC}^{\mathsf{O}}_z(w) \cdot \beta^{\ell(w) - \ell_{\mathsf{inv}}(z)} \cdot \mathcal{G}^{(\beta)}_w$.

Following the notation in [9], we write $v \xrightarrow{(a,b)} w$ for $v, w \in S_\infty$ and positive integers $a < b$ to indicate that $w = v(a,b)$ and $\ell(w) = \ell(v) + 1$, meaning that w covers v in the

Bruhat order on S_∞. The length condition holds precisely when $v(a) < v(b)$ and no i with $a < i < b$ has $v(a) < v(i) < v(b)$. Fix a positive integer k. The *k-Bruhat order* on S_∞ is transitive closure of the relation with $v <_k w$ whenever $v \xrightarrow{(a,b)} w$ and $a \leq k < b$.

Definition 4.2. An *unmarked k-Pieri chain* between from $v \in S_\infty$ to $w \in S_\infty$ is a saturated chain in k-Bruhat order of the form $v = v_0 \xrightarrow{(a_1,b_1)} v_1 \xrightarrow{(a_2,b_2)} \cdots \xrightarrow{(a_q,b_q)} v_q = w$ satisfying $b_1 \geq b_2 \geq \cdots \geq b_q$ and $b_i > b_{i+1}$ if $a_j = a_i > a_{i+1}$ for some $1 \leq j < i < q$.

We write $v \xrightarrow{c(k)} w$ if such a chain exists. An essential and non-obvious property of this definition is that for any permutations $v, w \in S_\infty$ at most one unmarked k-Pieri chain exists from v to w. See [9, Theorem 2.2], which also explains how to construct this chain.

Suppose $v = v_0 \xrightarrow{(a_1,b_1)} v_1 \xrightarrow{(a_2,b_2)} \cdots \xrightarrow{(a_q,b_q)} v_q = w$ is the unique unmarked k-Pieri chain from $v \in S_\infty$ to $w \in S_\infty$. Define $\mathsf{F}_k(v, w)$ to be the number of indices $i \in [q]$ such that either $b_1 = \cdots = b_i$ and $a_1 > \cdots > a_i$, or $b_i = b_{i+1}$ and $a_i > a_{i+1}$. Also let $\mathsf{P}_k(v, w)$ be the number of indices $i \in [q]$ such that $a_j = a_i$ for some $1 \leq j < i$.

Now, for $v = w$ set $\epsilon_k(v, w) = 1$ and $\rho_k(v, w) = 2^k$, and for $v \xrightarrow{c(k)} w \neq v$ define

$$\epsilon_k(v, w) = (-1)^{1+\mathsf{F}_k(v,w)} \quad \text{and} \quad \rho_k(v, w) = 2^{k+\ell(v)-\ell(w)+\mathsf{P}_k(v,w)}. \tag{4.1}$$

Set $\epsilon_k(v, w) = \rho_k(v, w) = 0$ when we do not have $v \xrightarrow{c(k)} w$.

Theorem 4.3. Suppose $z \in I_\infty^{\mathsf{vex}}$ is quasi-dominant and $k = k(z)$. Then

$$\mathrm{GC}^{\mathsf{O}}_z(w) = \textstyle\sum_{v \in \mathcal{B}_{\mathsf{inv}}(z)} \epsilon_k(v, w)\rho_k(v, w) \geq 0 \quad \text{for all } w \in S_\infty.$$

Fix $1 \neq z \in I_\infty$, define $k = k(z) = \min\{i \in \mathbb{Z}_{\geq 0} : (j, j) \notin D(z) \text{ for all } j > i\}$ as above, and let $j = j(z)$ be the largest integer with $z(i) = i$ for all $1 \leq i \leq j$. For $v, w \in S_\infty$ we write $v \xrightarrow{[z]} w$ if there exists an unmarked k-Pieri chain as in Definition 4.2 that has $j \leq a_i \leq k < b_i$ and also either $a_i < z(a_i)$ or $z(b_i) < b_i$ for each $i \in [q]$. Finally, let

$$\mathcal{B}^+_{\mathsf{inv}}(z) := \left\{ w \in S_\infty : v \xrightarrow{[z]} w \text{ for some } v \in \mathcal{B}_{\mathsf{inv}}(z) \right\}. \tag{4.2}$$

Also define $\mathcal{B}^+_{\mathsf{inv}}(1) = \mathcal{B}_{\mathsf{inv}}(1) = \{1\}$. Based on computations and the preceding theorem, the set $\mathcal{B}^+_{\mathsf{inv}}(z)$ appears to give a good approximation for $\mathrm{supp}(\mathrm{GC}^{\mathsf{O}}_z)$. In particular:

Corollary 4.4. If $z \in I_\infty^{\mathsf{vex}}$ is quasi-dominant and $k = k(z)$ then

$$\mathrm{supp}(\mathrm{GC}^{\mathsf{O}}_z) \subseteq \mathcal{B}^+_{\mathsf{inv}}(z) = \left\{ w \in S_\infty : v \xrightarrow{c(k)} w \text{ for some } v \in \mathcal{B}_{\mathsf{inv}}(z) \right\}.$$

We have used a computer to verify the following for all vexillary $z \in I_{11}$:

Conjecture 4.5. If $z \in I_\infty^{\mathsf{vex}}$ then $\mathcal{B}_{\mathsf{inv}}(z) \subseteq \mathrm{supp}(\mathrm{GC}^{\mathsf{O}}_z) \subseteq \mathcal{B}^+_{\mathsf{inv}}(z)$.

Both containments in this conjecture can be strict, but in some notable cases we actually have equality $\mathrm{supp}(\mathrm{GC}^{\mathsf{O}}_z) = \mathcal{B}^+_{\mathsf{inv}}(z)$. Below are some relevant examples.

Example 4.6. Suppose $t = t_n := (1,n) \in I_n$ is a transposition. Then t is dominant of shape $\lambda = (n-1, 1^{n-2})$ and $\mathcal{B}_{\mathsf{inv}}(t)$ consists of the permutations in S_n whose **inverses** in one-line notation are the shuffles of $n1$ and $234\cdots(n-1)$ with at most one letter between n and 1. The larger set $\mathcal{B}^+_{\mathsf{inv}}(t)$ consists of the permutations in S_{n+1} whose **inverses** in one-line notation are the shuffles of the words $n1$ and $234\cdots(n-1)(n+1)$ with at most two letters between n and 1, excluding the inverse of $234\cdots(n-1)(n+1)n1$. In this case it can be proved that $\mathrm{supp}(\mathrm{GC}^{\mathsf{O}}_t) = \mathcal{B}^+_{\mathsf{inv}}(t)$.

It is useful to represent $\mathcal{B}^+_{\mathsf{inv}}(z)$ as the following directed graph. For $v, w \in S_\infty$ we write $v \lessdot_L w$ when $\ell(w) = \ell(v) + 1$ and $w = s_i v$ for some $i \in \mathbb{Z}_{>0}$. We then turn $\mathcal{B}^+_{\mathsf{inv}}(z)$ into a directed graph by adding edges $v \to w$ whenever $v \lessdot_L w$. Figure 1 shows some instances of this graph corresponding to the previous and next two examples.

Example 4.7. Suppose $g = g_n := (1, n+1)(2, n+2)\cdots(n, 2n) \in I_{2n}$. Then g is dominant of shape $\lambda = (n^n)$ and the set $\mathcal{B}_{\mathsf{inv}}(g)$ consists of the single element whose **inverse** is $(n+1)1(n+2)2\cdots(2n)n \in S_{2n}$. The larger set $\mathcal{B}^+_{\mathsf{inv}}(g_{1,n})$ consists of the 2^n permutations whose **inverses** have the form $(n+1)a_1b_1a_2b_2\cdots a_nb_n \in S_{2n+1}$ where $\{a_i, b_i\} = \{i, n+1+i\}$ for each $i \in [n]$. It again can be proved that $\mathrm{supp}(\mathrm{GC}^{\mathsf{O}}_g) = \mathcal{B}^+_{\mathsf{inv}}(g)$.

Example 4.8. Finally let $w_0 = n\cdots321 \in I_n$ be the longest element of S_n. Then w_0 is dominant of shape $\lambda = (n-1, \dots, 3, 2, 1)$. The set $\mathcal{B}_{\mathsf{inv}}(w_0)$ does not have any description simpler than (3.2). One can show that $\mathcal{B}^+_{\mathsf{inv}}(w_0)$ is the set of the permutations in S_{n+1} whose **inverses** in one-line notation have the form $u_1\cdots u_i(n+1)u_{i+1}\cdots u_n$ where $u = u_1u_2\dots u_n$ is the **inverse** of an element of $\mathcal{B}_{\mathsf{inv}}(w_0)$ and $i \in [n]$ has $n \geq 2u_j$ for each $i < j \leq n$. We conjecture, but do not know how to prove, that $\mathrm{supp}(\mathrm{GC}^{\mathsf{O}}_{w_0}) = \mathcal{B}^+_{\mathsf{inv}}(w_0)$ for all n. This has been checked by computer for $n \leq 11$.

Extending this example, let $w_{ij} := (i,j)(i+1, j-1)(i+2, j-2)\cdots(i+k, j-k) \in I_\infty^{\mathsf{vex}}$ for any integers $1 \leq i < j$ where $k = \lfloor \frac{j-i-1}{2} \rfloor$. Computations support the following:

Conjecture 4.9. It holds that $\mathrm{supp}(\mathrm{GC}^{\mathsf{O}}_{w_{ij}}) = \mathcal{B}^+_{\mathsf{inv}}(w_{ij})$ if and only if $i = 1$ or $j - i$ is odd.

5 Shift invariance and stable limits

This section contains a new formula for $\mathcal{G}^{\mathsf{O}}_z$ that holds for all vexillary $z \in I_\infty^{\mathsf{vex}}$ and which will lead to a nontrivial shift invariance property of the coefficient function $\mathrm{GC}^{\mathsf{O}}_z$.

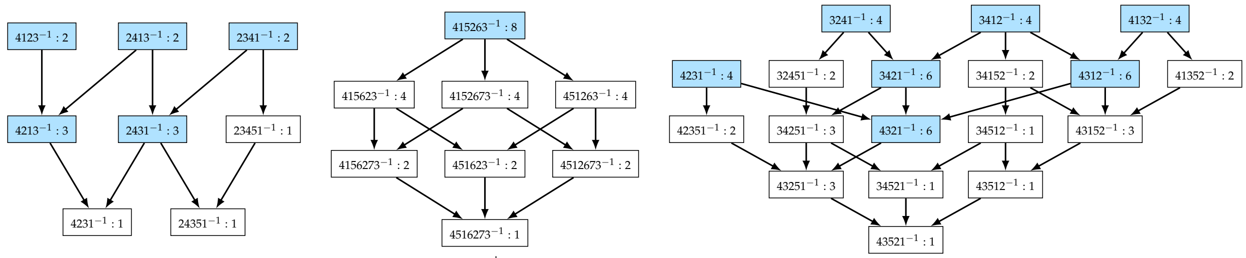


Figure 1: The directed graphs $\mathcal{B}^{+}_{\mathsf{inv}}(z)$ when z is $t_4 = (1,4)$ (left), $g_3 = (1,4)(2,5)(3,6)$ (middle), or $w_0 = 4321$ (right). The data in each box is $\boxed{w : \mathrm{GC}^{\mathsf{O}}_z(w)}$, with w given in (inverse) one-line notation. The blue vertices correspond to elements of $\mathcal{B}_{\mathsf{inv}}(z)$.

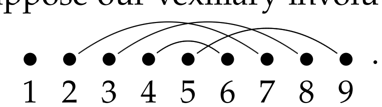
A generic vexillary involution $z \in I^{\mathsf{vex}}_\infty := \{z \in I_\infty : z \text{ is 2143-avoiding}\}$ has cycle notation $z = (a_1, b_1)(a_2, b_2)\cdots(a_q, b_q)$ where $1 \le a_1 < a_2 < \cdots < a_q < \min\{b_1, b_2, \dots, b_q\}$. We refer to the numbers a_i as *left endpoints*, to the numbers b_i as *right endpoints*, and to the ordered pairs (a_i, b_i) as *cycles*.

The *left segments* of z are the maximal subsets of consecutive left endpoints, that is, the equivalence classes in $\{a_1, a_2, \dots, a_q\}$ under the transitive closure of the relation with $a_i \sim a_j$ if $|a_j - a_i| \le 1$. There is at most one left segment containing 1, which we refer to as the *immobile segment*. All other left segments are *mobile*.

Suppose L is a mobile left segment of z and define $c_0 = \min(L) - 1$. Notice that we must have $c_0 = z(c_0) \in \mathbb{Z}_{>0}$. Now, for any subset $S \subseteq \{a_1, a_2, \dots, a_q\}$ define $\sigma_{S,L} \in S_\infty$ to be the cyclic permutation $\sigma_{S,L} = (c_0, c_1, c_2, \dots, c_k)$ where $S \cap L = \{c_1 < c_2 < \cdots < c_k\}$. This is the identity element when $S \cap L$ is empty. Also define $\sigma_S = \prod_L \sigma_{S,L}$ where the product is over all mobile left segments of z in any order.

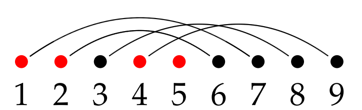
Example 5.1. We often draw $z \in I_n$ as an *arc diagram*, that is, as the graph with vertex set $[n]$ having edges $\{i, z(i)\}$ for $i \in \mathrm{supp}(z)$. Suppose our vexillary involution is

$$z = (2,7)(3,8)(4,6)(5,9) =$$



This involution has a unique left segment $L = \{2,3,4,5\}$, which is mobile. For the subset $S = \{2,4,5\}$ we have $\sigma_{S,L} = (1,2,4,5)$ and

$$(\sigma_{S,L})^{-1} \cdot z \cdot \sigma_{S,L} = (1,7)(2,6)(3,8)(4,9) =$$



Suppose a_i and a_j are left endpoints of z in the same left segment with $i < j$. We say that a_j is a *crossing bound* of a_i if $\{i\} = \{t : i \le t < j \text{ and } b_t < b_j\}$. Now, given a subset $S \subseteq \{a_1, a_2, \dots, a_q\}$ we define $\varpi_{z,S} = \prod_{i \in [q]} \varpi^{(a_i)}_{z,S}$ where

$$\varpi^{(a)}_{z,S} = \begin{cases} -1 & \text{if } S \text{ contains any crossing bound of } a \\ 2 + \beta x_a & \text{if } a \notin S \\ 1 + \beta x_a & \text{otherwise.} \end{cases} \tag{5.1}$$

Example 5.2. If $z = (2,7)(3,8)(4,6)(5,9)$ is as in Example 5.1 then

$$\begin{aligned} \varpi_{z,\varnothing} &= (2+\beta x_2)(2+\beta x_3)(2+\beta x_4)(2+\beta x_5), \\ \varpi_{z,\{2,4,5\}} &= -(1+\beta x_2)(2+\beta x_3)(1+\beta x_5). \end{aligned}$$

Finally, we define $S \subseteq \{a_1, a_2, \dots, a_q\}$ to be *shiftable* if (1) no element of S is in the left segment of z containing 1, if this exists, and (2) if some $a_i \notin S$ then S does not contain any crossing bound of a_i. Given such a subset, write $\widehat{\mathcal{G}}_{z,S} = \widehat{\mathcal{G}}_v$ where $v = (\sigma_S)^{-1} \cdot z \cdot \sigma_S$.

Example 5.3. When $z = (2,7)(3,8)(4,6)(5,9)$ there are 9 shiftable subsets of left endpoints, given by $\varnothing$, $\{2\}$, $\{4\}$, $\{2,3\}$, $\{2,4\}$, $\{4,5\}$, $\{2,3,4\}$, $\{2,4,5\}$, and $\{2,3,4,5\}$.

The following theorem significantly generalizes Theorem 4.1:

Theorem 5.4. If $z \in I_\infty^{\mathsf{vex}}$ is any vexillary involution then $\mathcal{G}_z^{\mathsf{O}} = \sum_S \beta^{|S|} \cdot \varpi_{z,S} \cdot \widehat{\mathcal{G}}_{z,S}$ where the sum is over all shiftable subsets of left endpoints of z.

Recall that our permutations $w \in S_\infty$ are maps $w : \mathbb{Z} \to \mathbb{Z}$ with $w(i) = i$ for $i \leq 0$. Given any integer $n \in \mathbb{Z}$, define $w \downarrow n$ to be the permutation of $\mathbb{Z}$ with the formula

$$(w \downarrow n)(i) = w(i+n) - n \quad \text{for } i \in \mathbb{Z}. \tag{5.2}$$

Notice that if $n \leq 0$ then $w \downarrow n \in S_\infty$, but if $w(m) \neq m$ then $w \downarrow n \notin S_\infty$ for all $n \geq m$. Define $1^n \times w := w \downarrow (-n)$ for $n \in \mathbb{Z}_{\geq 0}$.

Now for $z \in I_\infty$ we extend the domain of the Grothendieck coefficient function $\mathrm{GC}_z^{\mathsf{O}}$ by setting $\mathrm{GC}_z^{\mathsf{O}}(w) = 0$ if $w \notin S_\infty$. Our main application of Theorem 5.4 is the following:

Theorem 5.5. Suppose $n \in \mathbb{Z}_{\geq 0}$ and $z \in I_\infty^{\mathsf{vex}}$.

(a) If $z(1) = 1$ then $GC_{1^n \times z}(w) = \mathrm{GC}_z^{\mathsf{O}}(w \downarrow n)$ for all $w \in S_\infty$.

(b) If $z \downarrow n \in S_\infty$ then $\mathrm{GC}_{z\downarrow n}^{\mathsf{O}}(w) = \mathrm{GC}_z^{\mathsf{O}}(1^n \times w)$ for all $w \in S_\infty$.

The hypothesis $z(1) = 1$ is necessary for the first identity. For example, $\mathcal{G}_{(1,2)}^{\mathsf{O}} = 2\mathcal{G}_{21}^{(\beta)} + \beta \mathcal{G}_{312}^{(\beta)}$ but the $\mathcal{G}^{(\beta)}$-expansion of $\mathcal{G}_{(n+1,n+2)}^{(\beta)} = \mathcal{G}_{1^n \times (1,2)}^{(\beta)}$ has 4 terms if $n > 0$.

Corollary 5.6. If $z \in I_\infty^{\mathsf{vex}}$ then $\mathrm{GC}_z^{\mathsf{O}}(w) = \mathrm{GC}_{1^n \times z}^{\mathsf{O}}(1^n \times w)$ for all $n \in \mathbb{Z}_{\geq 0}$ and $w \in S_\infty$.

These shift invariance properties of $\mathrm{GC}_z^{\mathsf{O}}$ are consistent with Conjecture 4.5 since one can show that if $n \in \mathbb{Z}$ and $z \in I_\infty^{\mathsf{vex}}$ are such that $z(1) = 1$ and $1^n \times z \in S_\infty$ then

$$\mathcal{B}_{\mathsf{inv}}(1^n \times z) = \{w \in S_\infty : w \downarrow n \in \mathcal{B}_{\mathsf{inv}}(z)\}, \ \mathcal{B}_{\mathsf{inv}}^+(1^n \times z) = \left\{w \in S_\infty : w \downarrow n \in \mathcal{B}_{\mathsf{inv}}^+(z)\right\}.$$

Theorem 5.5 has an application concerning the *stable limit* of $\mathcal{G}_z^{\mathsf{O}}$. The *symmetric Grothendieck function* of $w \in S_\infty$ is $G_w := \lim_{n\to\infty} \mathcal{G}_{1^n \times w}^{(\beta)}$ where the limit is taken in the sense of formal power series. This means the limit exists precisely when the coefficients of any fixed monomial in $\mathcal{G}^{(\beta)}_{1^n\times w}$ is eventually a constant sequence. It is known [2] that G_w always exists and is a formal power series that is symmetric in the x_i variables.

For $z \in I_\infty$ let $GQ_z := \lim_{n\to\infty} \mathcal{G}^{\mathsf{O}}_{1^n\times z}$. When $z \in I^{\mathsf{vex}}_\infty$, it is known that GQ_z also exists and is a symmetric formal power series; in fact, it is equal to the *K-theoretic Schur Q-function* of Ikeda and Naruse [7] indexed by the *involution shape* of z [11, Theorem 4.11].

This was proved in [11] by a difficult geometric argument. Theorem 5.5 leads to a much simpler derivation of the fact that GQ_z is a symmetric formal power series. We also get a new formula relating the G-expansion of GQ_z to the $\mathcal{G}^{(\beta)}$-expansion of $\mathcal{G}^{\mathsf{O}}_z$:

Corollary 5.7. If $z \in I^{\mathsf{vex}}_\infty$ has $z(1) = 1$ then $GQ_z = \sum_{w\in S_\infty} \mathrm{GC}^{\mathsf{O}}_z(w) \cdot \beta^{\ell(w)-\ell_{\mathsf{inv}}(z)} \cdot G_w$.

6 Special cases

We can compute $\mathrm{GC}^{\mathsf{O}}_z$ explicitly in a few special cases—namely, when z is any transposition $t_{ij} = (i,j)$ or the element $g_{ij} := (i,j+1)(i+1,j+2)(i+3,j+4)\cdots(j,2j-i+1)$ where i and j are any positive integers with $i < j$. These involutions are always vexillary, and in the notation of Example 4.6 and 4.7 we have $t_n = t_{1,n}$ and $g_n = g_{1,n}$.

Define $t^+_n := t_{2,n}$ and $g^+_n := g_{2,n}$. By Theorem 5.5, to compute $\mathrm{GC}^{\mathsf{O}}_{t_{ij}}$ and $\mathrm{GC}^{\mathsf{O}}_{g_{ij}}$ for all positive integers $i < j$, it suffices just to determine $\mathrm{GC}^{\mathsf{O}}_z$ when z is t^+_n and g^+_n. We explain these calculations in the following sections.

6.1 Transpositions

Let $\mathsf{Sh}(n)$ denote the set of words obtained by shuffling

$$n2 \quad \text{and} \quad 1345\cdots(n-3)(n-2)(n-1)(n+1).$$

Define $\mathcal{X}(n)$ to be the subset of words in $\mathsf{Sh}(n)$ for which

- the first letter is 1 while the last letter is $n+1$; and
- at most one letter appears between n and 2.

Define $\mathcal{Y}(n) \subset \mathsf{Sh}(n)$ be the set of words with exactly one or exactly two letters between n and 2. The sets $\mathcal{X}(n)$ and $\mathcal{Y}(n)$ are not disjoint, but the following holds:

Proposition 6.1. Let $z = t^+_n = (2,n)$. Then $\mathcal{B}_{\mathsf{inv}}(z) = \left\{w^{-1} : w \in \mathcal{X}(n)\right\}$. Define $c \in S_n$ to be the cycle $c = (1,2,5,4)$ when $n \leq 4$ and $c = (1,2,5,6,7,\cdots,n)$ if $n \geq 5$. Then

$$\mathcal{B}^+_{\mathsf{inv}}(z) = \left\{w^{-1} : w \in \mathcal{X}(n) \cup \mathcal{Y}(n)\right\} \sqcup \begin{cases} \varnothing & \text{if } n \leq 3 \\ \{c\} & \text{if } n \geq 4. \end{cases}$$

Finally, one has $\mathcal{G}^{\mathsf{O}}_z = 2\sum_{w^{-1}\in\mathcal{X}(n)} \beta^{w(2)-w(n)-1}\mathcal{G}^{(\beta)}_w + \sum_{w^{-1}\in\mathcal{Y}(n)} \beta^{w(2)-w(n)-1}\mathcal{G}^{(\beta)}_w$.

See Figure 2 for an illustration of this proposition.

6.2 Vexillary involutions that are fully commutative

The involutions g_{ij} are the only elements of I_∞ that are both 2143- and 321-avoiding [6, Theorem 3.35 and Corollary 3.36], that is, both vexillary and *fully commutative*.

Proposition 6.2. Let $z = g_n^+ = (2, n+1)(3, n+2)\cdots(n, 2n-1)$ where $n > 2$. Then:

(a) $\mathcal{B}_{\mathsf{inv}}(z)$ consists of the **inverse** of $1(n+1)2(n+2)3\cdots(2n-1)n(2n) \in S_{2n-1}$.

(b) $\mathcal{B}^+_{\mathsf{inv}}(z)$ consists of the 2^n permutations whose **inverses** in one-line notation have the form $a_1b_1a_2b_2\cdots a_nb_n \in S_{2n}$ where $\{a_i, b_i\} = \{i, n+i\}$ for each $i \in [n]$.

(c) If we define $\mathrm{ODes}_L(w) = \{i \in \mathrm{Des}_R(w^{-1}) : i \text{ is odd}\}$ then

$$\mathcal{G}^{\mathsf{O}}_z = \textstyle\sum_{w\in\mathcal{B}^+_{\mathsf{inv}}(z)} 2^{n-1-|\mathrm{ODes}_L(w)|}\beta^{|\mathrm{ODes}_L(w)|}\mathcal{G}^{(\beta)}_w + \tfrac{1}{2}(-\beta)^n\mathcal{G}^{(\beta)}_{w_{\max}}$$

where $w_{\max} \in \mathcal{B}^+_{\mathsf{inv}}(z)$ is the **inverse** of $(n+1)1(n+2)2\cdots(2n)n$.

See Figure 2 for an illustration of this proposition.

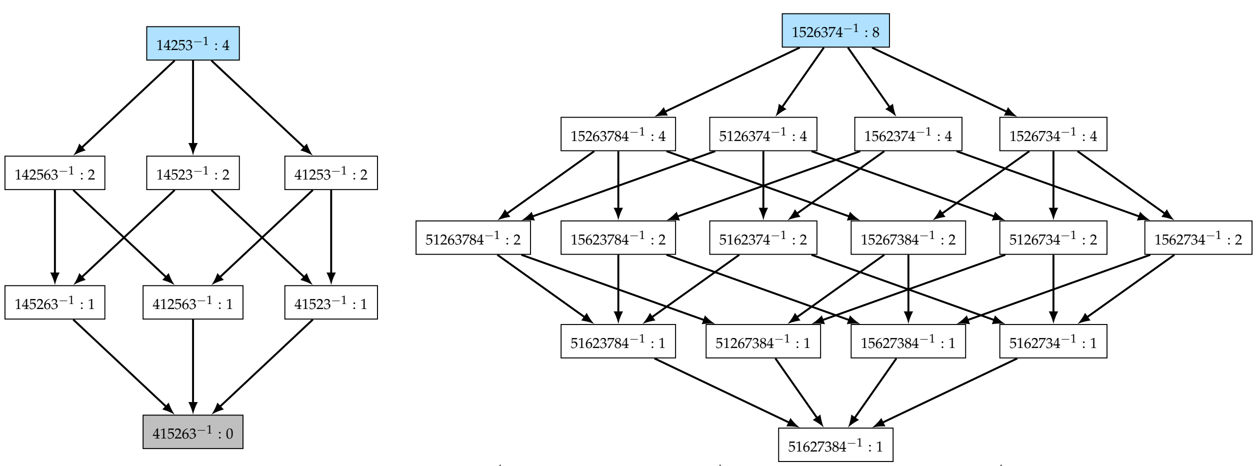


Figure 2: The directed graphs $\mathcal{B}^+_{\mathsf{inv}}(z)$ when z is $t_5^+ = (2,5)$ (left) and $g_3^+ = (2,4)(3,5)$ (right), presented using the conventions as in Figure 1. Here the grey boxes indicate the (in these cases, unique) elements of $\mathcal{B}^+_{\mathsf{inv}}(z)$ that are not in $\mathrm{supp}(\mathrm{GC}^{\mathsf{O}}_z)$.

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