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Cluster patterns in Landau and leading singularities via the amplituhedron

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Abstract. We advance the exploration of cluster-algebraic patterns in the building blocks of scattering amplitudes in $\mathcal{N} = 4$ super Yang–Mills theory. In particular, we conjecture that, given a maximal cut of a loop amplitude, Landau singularities and poles of each Yangian invariant appearing in any representation of the corresponding leading singularities can be found together in a cluster. We check these adjacencies for all one-loop amplitudes up to 9 points. Along the way, we also prove that all (rational) N^2MHV Yangian invariants are cluster adjacent, confirming original conjectures.

1. Introduction

Constructing scattering amplitudes from the knowledge of their singularities, i.e., their poles and branch-cut structure, is an approach with a long history [30], which has proven to be particularly effective for scattering amplitudes in $\mathcal{N} = 4$ super Yang–Mills theory (SYM).

Singularities of scattering amplitudes at tree-level are given by multi-particle factorisation channels, which correspond to Mandelstam invariants, and are constructed from subsets of the momenta of the particles in the scattering process, whereas loop amplitudes exhibit more complicated singularities, leading to logarithmic divergences. In cases where loop amplitudes are expressed as (multiple) polylogarithms, the collection of these logarithmic singularities is called the symbol alphabet. When expressed in terms of momentum twistors, many (all for $n \leq 7$, where n is the number of particles) of these are simply polynomials in the Plücker coordinates in $\mathrm{Gr}(4, n)$. Moreover, their vanishing loci correspond to special configurations of momentum twistors in $\mathbb{CP}^3$.

On one side, we have seen the emergence of positive geometries [1] as an overarching framework to geometrise scattering amplitudes and their analytic structure, at tree-level and for loop integrands in several theories, among which is $\mathcal{N} = 4$ SYM.

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In 2013, a full geometric description for tree-level and integrands of loop-level scattering amplitudes in planar $\mathcal{N} = 4$ SYM was proposed in [8] under the name of *amplituhedron*. Other constructions followed a few years later [16, 34].

On the other, we have witnessed an increasing appearance of cluster algebra structures in scattering amplitudes, especially in capturing singularities of (integrated) loop amplitudes in $\mathcal{N} = 4$ SYM. This started in 2013 with the conjecture made by Golden et al. in [33] that the symbol letters of six- and seven-particle loop amplitudes are $\mathcal{A}$-coordinates of the $\mathrm{Gr}(4, n)$ cluster algebra. A few years later, in [24] it was conjectured that these letters satisfy remarkable cluster properties, called *cluster adjacency*. In terms of the symbol, they dictate which letters can appear consecutively. Moreover, shortly after these adjacencies were also observed at tree-level, in connection with symbol entries [25] (see also [43] for a recent work on the cluster adjacency of one-loop amplitudes). The guidance of cluster algebras has unlocked the possibility of developing a powerful bootstrap programme which allowed to perform computations that otherwise would have been beyond reach [14, 15, 18–23, 27, 28]. At the same time, they shed more light on the mathematical structures describing singularities of scattering amplitudes and motivate the existence of a possible geometric origin.

One manifestation of the cluster-algebraic phenomena is an observation that building blocks of a BCFW representation of the tree-level amplitude, which are *Yangian invariants*, are *cluster adjacent* [25]. In other words, all poles of each of them are expressed by a collection of $\mathcal{A}$-coordinates of the $\mathrm{Gr}(4, n)$ cluster algebra that can be found together in a common cluster. Moreover, this conjecture was generalised in [42], for all (rational) Yangian invariants of $\mathcal{N} = 4$ SYM. In geometric terms, poles of (rational) Yangian invariants are codimension-one boundaries of the so-called *generalised triangles* of the amplituhedron [39, 40]. Furthermore, different representations of scattering amplitudes, obtained from identities among Yangian invariants, correspond to different *triangulations* of the same geometric space, i.e., the amplituhedron.

One of the first steps towards an amplituhedronic understanding of cluster phenomena was taken in [39], where a toy model for tree-level cluster adjacency of $\mathcal{N} = 4$ SYM was considered. It was proved that Yangian invariants of the $m = 2$ amplituhedron are cluster adjacent with respect to the well-known $\mathrm{Gr}(2, n) \simeq A_{n-3}$ cluster algebra. The $m = 2$ amplituhedron is often considered as a toy model for the physical $m = 4$ case, moreover it also governs the geometry of one-loop MHV integrands [5] and it has some relevance for the NMHV ones as well [37]. By exploiting the geometry of the $m = 2$ amplituhedron, an explicit expression of all Yangian invariants was provided in [39], where cluster adjacency of their poles is manifest.

The interest in understanding how cluster algebras encode the analytic properties of scattering amplitudes led physicists to explore the connection between cluster algebras and the *positive tropical Grassmannian*, originally introduced in [50]. See for examples [6, 26, 35], for applications in $\mathcal{N} = 4$ SYM. Remarkably, the very same positive tropical Grassmannian has been found to regulate the combinatorics of *triangulations* (and, more generally, subdivisions) of the $m = 2$ amplituhedron [40]. This raises the question of whether there is a deeper connection between the latter object and cluster algebras themselves.

A remarkable instance of how geometry encodes singularities of scattering amplitudes in $\mathcal{N} = 4$ SYM is the fact that all *leading singularities* of the theory, at any loop order, can be computed by a contour integral over the space of k-planes in n dimensions, called *Grassmannian* [3, 44]. Leading singularities are the singularities of the integrand of a loop amplitude with maximal codimension in loop momenta. The geometrisation was pushed even further via [2] and, a year after, the authors of [8] defined the *loop amplituhedron*, whose boundaries encode singularities of the integrand, among which are the leading singularities corresponding to maximal cuts.

The application of this geometric approach to *Landau singularities* [17, 47, 48] is another example of its utility to obtain a better understanding of the structure of singularities of scattering amplitudes. The Landau analysis allows to connect singularities of the *integrand*, described geometrically from boundaries of loop amplituhedra, to the ones of the *integrated* amplitudes. Among all Landau singularities, there are in general many spurious ones coming from summing over Feynman diagrams. On the other hand, the amplituhedron can tell which are the true singularities of the integrand, and therefore select the true Landau singularities of the loop amplitude.

In this work, using an amplituhedron-based approach to encode building blocks of scattering amplitudes in $\mathcal{N} = 4$ SYM, i.e., Yangian invariants and leading singularities, we explore cluster patterns between the latter and Landau singularities.

We first review the preliminary concepts appearing in our work in Section 2. In particular, we review the notion of *cluster adjacency* in Section 2.1 and state its known various incarnations; then, in Section 2.2, we introduce the concepts of *leading singularities* and the *(loop) amplituhedron*, and how one can obtain the former from special boundaries of the latter; in Section 2.3, we present the definition of *Landau singularities* and how the loop amplituhedron can select the non-spurious ones; for both leading and Landau singularities we present in the respective sections examples at one-loop which will be relevant for our work.

In Section 3, we will prove *cluster adjacency for all (rational) N^2MHV Yangian invariants*. In particular, we introduce the geometric method used to determine the actual poles of Yangian invariants in terms of cluster variables, and we present the results in Section 3.1; finally, in Section 3.2, we prove that Yangian invariants of the four-mass box type violate cluster adjacency.

In Section 4, we present the main conjecture of our paper: *cluster adjacency between leading and Landau singularities*, which we abbreviate as "LL-cluster adjacency". We first introduce how to find all Yangian invariants which can be used to represent a given leading singularity from the geometry of the loop amplituhedron. We then present our checks and proofs about these adjacencies in Sections 4.1 and 4.2 for all one-loop amplitudes up to 9 points for the NMHV and N^2MHV cases, respectively. In Section 4.1.5, we show the one-loop NMHV 7-point amplitude in a representation which is uniquely fixed by LL-cluster adjacency. Finally, in Section 5, we end with conclusions and directions for future works.

2. Cluster algebras, singularities and geometry

2.1. Cluster adjacency

We begin by reviewing the notion of cluster adjacency for singularities of scattering amplitudes in planar $\mathcal{N} = 4$ SYM. These are observations about the appearance of singularities of the amplitudes in relation to how they are encoded in a corresponding $\mathrm{Gr}(4,n)$ cluster algebra.

The mathematics literature on cluster algebras, e.g., [31,32,49], provides an excellent introduction to the concept. Aspects of cluster algebras of Grassmannian-type in the context of scattering amplitudes have been explained in detail in [24, 25, 33]. We will therefore introduce only the cluster-terminology which will be employed in stating our results.

One way of representing clusters of $\mathrm{Gr}(4,n)$ cluster algebras are quiver diagrams. These have $3(n-5)$ distinct nodes, called $\mathcal{A}$-*coordinates*, that are in general polynomials in the Plücker coordinates of $\mathrm{Gr}(4,n)$. When n is greater than 8, there are infinitely-many clusters and therefore infinitely-many $\mathcal{A}$-coordinates. Remarkably, all known *rational* singularities of BDS-like normalised amplitudes are $\mathcal{A}$-coordinates of $\mathrm{Gr}(4,n)$ cluster algebras [33].

Each cluster in a given cluster algebra can be obtained from any other cluster by (sequences of) *mutations*. A mutation, expressed in terms of $\mathcal{A}$-coordinates, is an operation which replaces a chosen node of the quiver with a new value, as well as locally changing the connectivity of the quiver diagram. Two $\mathcal{A}$-coordinates are said to be *cluster adjacent* if there exists a cluster in which they appear together.

As a toy model, one can consider $\mathrm{Gr}(2,n)$ cluster algebra where clusters correspond to triangulations of an n-gon and the $\mathcal{A}$-coordinates correspond to the chords of this triangulation. Mutations act as flipping the chord inside the quadrilateral that they are the diagonal of. In this case, cluster adjacent coordinates correspond to non-crossing chords. Two coordinates are not cluster adjacent if and only if the corresponding chords cross, i.e., they mutate into each other.

The $\mathrm{Gr}(4,n)$ cluster algebras are more complicated and allows for other adjacency situations. In particular, pairs of $\mathrm{Gr}(4,n)$ $\mathcal{A}$-coordinates can never appear in a cluster together even though there is no mutation that relates to them. Therefore there is no known simple geometric picture from which one can infer (collective) adjacencies of sets of these variables.

There are various different but related cluster adjacency statements for scattering amplitudes in $\mathcal{N} = 4$ SYM.

Adjacency of symbol letters. Two $\mathcal{A}$-coordinates appear next to each other in the symbol of a BDS-like normalised amplitude only if there is a cluster that contains both of them [24]. For all known integrable words with physical initial entries, this requirement appears to be equivalent to the extended Steinmann conditions of [13, 45].

Poles of tree BCFW amplitudes. In [25], it is conjectured that BCFW representations of tree amplitudes in $\mathcal{N} = 4$ SYM are linear combinations of terms whose poles are mutually cluster adjacent in a strict sense. Moreover, it was observed in several examples that it is possible to find a cluster in the relevant cluster algebra which contains all poles of each BCFW term.

The simplest case of this statement is for NMHV tree amplitudes,[1] which are sums of R-invariants,

$$\mathcal{A}_{n,1} = \sum_{1<i<j<n} R_{1\,i\,i+1\,j+1}.$$

The cluster adjacency for R-invariants was proved in [25] through a procedure in which one starts from the initial cluster of $\mathrm{Gr}(4, 6)$ and arrives at a cluster containing the poles of $R_{1\,i\,i+1\,j+1}$ through a sequence of (partial) cyclic rotations.

This observation, in particular the simple proof of the cluster adjacency of R-invariants, motivates the question of how far this property extends. In [42], it was conjectured that all (rational) Yangian invariants satisfy such cluster adjacency properties. It is also natural to ask whether this is a mathematical property of Yangian invariants or whether it is an extra physical constraint that BCFW terms are expected to satisfy.

Rational Yangian invariants. The natural question of whether the manifestation of cluster adjacency in BCFW terms extends to more general Yangian invariants was asked in [25]. The authors of [42] conjectured that the question has indeed an affirmative answer for rational Yangian invariants, providing a lot evidence with the use of Sklyanin brackets.

R-invariants and NMHV final entries. Finally, the fourth statement of cluster adjacency concerns NMHV loop amplitudes, which are sums of iterated integrals whose coefficients are R-invariants. Schematically they have the form

$$\mathcal{A}_{n,1}^{(L)} = \sum_{\alpha, i_1,\ldots,i_{2L}} R_\alpha c_{1,\ldots,2L} \phi_{i_1} \otimes \cdots \otimes \phi_{i_{2L}},$$

[1] We will denote tree-level N^kMHV n-point amplitudes by $\mathcal{A}_{n,k}$.

where the index α enumerates all relevant R-invariants, L is the loop order, and the indices i_k enumerate letters, the rational ones of which are $\mathcal{A}$-coordinates of the $\mathrm{Gr}(4, n)$ cluster algebra.

The observation which holds for all known such amplitudes is that the final entries of the symbols of the polylogarithms multiplying the R-invariants are cluster adjacent to all of the poles of the R-invariant that multiplies them.

It is also worth remembering that in general one needs to write out the amplitude with a redundant set of R-invariants that satisfy linear 6-term identities in order to make manifest this cluster adjacency property.

2.2. Leading singularities from the amplituhedron

We review here the concept of leading singularities. In particular, we show how leading singularities for $\mathcal{N} = 4$ SYM can be computed more geometrically via a Grassmannian approach and via the loop amplituhedron.

Leading singularities. The concept of leading singularities was originally introduced within the *Analytic Bootstrap Programme* in the 1960's [30]. At the beginning of this century, with the advent of novel on-shell techniques such as *generalised unitarity*, the concept of leading singularities was broadly employed and exploited in computation of scattering amplitudes, in particular in $\mathcal{N} = 4$ SYM [11].

Loop amplitudes in planar $\mathcal{N} = 4$ SYM are computed from *integrands*, which are rational functions of external kinematics and loop momenta, by integration over particular real-contours in the $4L$-dimensional loop momentum space. However, in general this contour is known not to preserve the symmetries of the theory and leads, for example, to IR-divergences. In this regard, it might seem natural to choose complex contours corresponding to computing residues of the integrand. Leading singularities are then the residues of the integrand computed around tori encircling the loci where a maximal set of internal propagators (e.g., four for one-loop) go on-shell.

Given a one-loop n-point scattering amplitude $\mathcal{A}(1, \ldots, n)$ and a partition $\mathcal{C}$ of $\{1, \ldots, n\}$ into 4 disjoint subsets $I_1, \ldots, I_4$, then the *leading singularity* of the amplitude is defined as

$$\int \prod_{a=1}^{4} d^4\eta_a d^4\ell_a \delta(\ell_a^2) \prod_{a=1}^{4} \mathcal{A}_a(\{\ell_a, \eta_a\}, I_a, \{-\ell_{a+1}, \eta_{a+1}\}),$$

where the index a is mod 4, the integral over ℓ is localised over the solutions of the delta function and the integral over the Grassmann coordinates[2] η_a amounts to

[2]See [4] for a good review on $\mathcal{N} = 4$ SYM and its conventions.

sum over all possible internal states flowing between the different sub-amplitudes $\{\mathcal{A}_1, \ldots, \mathcal{A}_4\}$. Since the four internal propagators are forced to vanish by the delta function, the internal particles can be taken on-shell. Therefore, leading singularities are in general simply the products of tree-amplitudes, summed over all the internal particles which can be exchanged, and integrated over the on-shell phase space of each.

Leading singularities from the Grassmannian. In [3], leading singularities were proposed as the complete set of IR-finite quantities that contains all the information needed to compute the S-matrix of $\mathcal{N} = 4$ SYM. Beautifully, both in momentum space and in momentum twistor space [44], all leading singularities of the theory, at any loop order, can be computed by a contour integral over the space of k-planes in n dimensions, called *Grassmannian* and denoted by $\mathrm{Gr}(k, n)$. Here k is the helicity sector of the amplitude. Remarkably, in [2], it was shown that only the "positive" part $\mathrm{Gr}_+(k, n)$ of this space, called the *positive Grassmannian* [41,46], is relevant for scattering amplitudes. Moreover, the integration contour providing leading singularities is performed on some of its *positroid cells*, in terms of which the positive Grassmannian has a beautiful stratification.

All positroid cells are in bijection with various nice combinatorial objects, including equivalence classes of reduced plabic graphs, also known as *on-shell diagrams* in the context of scattering amplitudes. A comprehensive summary about on-shell diagrams, their classification, evaluation, and relations was described in [2]. Formulae for one-loop leading singularities for $\mathcal{N} = 4$ SYM in momentum twistor variables were reported in [10] being used on-shell diagrams and will be used in an example in Section 2.2.1.

The loop amplituhedron. In 2013, the geometrisation of scattering amplitudes from polytopes à la Hodges [36] and from the positive Grassmannians came together in Arkani-Hamed and Trnka's work [8]. They introduced a novel mathematical object called the amplituhedron. Its canonical form gives all tree-level and the integrand of loop-level scattering amplitudes in planar $\mathcal{N} = 4$ SYM. Its boundaries geometrically encode all the singularities of the latter.

Let us fix a totally positive matrix $Z \in \mathrm{M}_+(n, k+4)$, i.e., all its maximal minors are positive. Let us consider $Y \in \mathrm{Gr}(k, k+4)$ and L lines $\mathcal{L}^{(l)} \in \mathrm{Gr}(2, 4+k)$, $l = 1, \ldots, L$, called *loop momenta*, in the four-dimensional complement of Y. Then the *loop amplituhedron* $\mathcal{A}_{n,k}^{(L)}$ is the set[3] of $(Y, \mathcal{L}^{(1)}, \ldots, \mathcal{L}^{(L)})$ such that

$$Y = C \cdot Z, \quad \mathcal{L}^{(l)} = D^{(l)} \cdot Z, \quad l = 1, \ldots, L, \tag{2.1}$$

[3]With abuse of notation, we will denote by $\mathcal{A}_{n,k}^{(L)}$ both the amplituhedron and the corresponding amplitude. It will be clear from the context which one we will be referring to.

where $C \in \mathrm{Gr}(k,n)$, $D^{(l)} \in \mathrm{Gr}(2,n)$ is in the four-dimensional complement of C and such that all the $(k+2s) \times n$ matrices

$$\begin{pmatrix} C \\ D^{(i_1)} \\ \vdots \\ D^{(i_s)} \end{pmatrix}, \quad 0 \le s \le L, \tag{2.2}$$

are *totally positive*, i.e., all they their maximal minors are positive.

An alternative definition of the loop amplituhedron based on *sign flips* and inequalities was introduced in [7] and conjectured to be equivalent to the definition given above. The canonical form of the loop amplituhedron $\mathcal{A}^{(L)}_{n,k}$ encodes the integrand of the L-loop N^{k}MHV n-point amplitude.

Let us now introduce some notation which will be useful in the following. Let us denote determinants of the $(4+k)\times(4+k)$ matrices obtained by stacking together Y and rows of Z specified by the indices i, j, l, s by

$$\langle Y i\ j\ l\ s\rangle := \varepsilon_{A_1 \dots A_k BCDE} Y_1^{A_1} \dots Y_k^{A_k} Z_i^B Z_j^C Z_l^D Z_s^E, \tag{2.3}$$

and analogously for brackets of the type $\langle Y \mathcal{L}^{(l)} i\ j\rangle$. As explained in [7], one can go from the space of bosonised momentum twistors, where $\mathcal{L}^{(l)}$ and Z_i live, to the space of physical momentum twistors[4] in $\mathbb{P}^3$ by projecting them through Y. Therefore, one can identify the brackets

$$\langle a\, b\, c\, d\rangle \equiv \langle Y a\, b\, c\, d\rangle,$$

where the left-hand side are brackets in momentum twistors and the right-hand side are brackets defined in (2.3). In the following, with abuse of notation, we will sometime denote both cases by $\langle a\, b\, c\, d\rangle$ and the meaning will be clear from the context.

Yangian invariants from the amplituhedron. For $L = 0$, i.e., tree-level, the definition of loop amplituhedron in (2.1) reproduces the definition of the *tree amplituhedron* [8]. This is the set of $Y \in \mathrm{Gr}(k, k+4)$ such that

$$Y = C \cdot Z, \tag{2.4}$$

where $C \in \mathrm{Gr}_+(k,n)$ and Z is the fixed totally positive $n \times (k+4)$ matrix defined above. The tree amplituhedron is therefore the image of the map $\widetilde{Z}$ induced by the fixed matrix Z from the positive Grassmannian $\mathrm{Gr}_+(k,n)$ to another Grassmannian $\mathrm{Gr}(k, k+4)$, i.e., $\widetilde{Z}\colon C \mapsto C \cdot Z = Y$. This map is not injective, since the dimension

[4] For conventions on momentum twistors, which we will denote by z_i, in a similar context, we refer the reader to, e.g., [42].

of the amplituhedron is $4k$, whereas the dimension of $\mathrm{Gr}_+(k,n)$ is $k(n-k)$, which is in general higher.

Let us consider positroid cells in $\mathrm{Gr}_+(k,n)$ which have the same dimension as the amplituhedron, i.e., $4k$, and have a full-dimensional image in the amplituhedron. This is equivalent to considering $4k$-dimensional cells which, within the physics community, are said to have "kinematic support", and were studied and classified in the context of the positive Grassmannians [2]. These cells are the same appearing as integration contours of the Grassmannian integral formulae in momentum twistors [44]. Given a $4k$-dimensional cell S in $\mathrm{Gr}_+(k,n)$ with kinematic support, if we perform such integral over S, we obtain a building block $\mathcal{Y}_S$ for leading singularities of $\mathcal{N}=4$ SYM (hence all tree-level amplitudes as well), which is referred to as[5] N^kMHV n-particle *Yangian invariant*. In this work, with a slight abuse of terminology, we will also refer to the image of S in the amplituhedron as *Yangian invariant*, and denote it by Y_S. It will be clear from the context which one we will be referring to.

For example, for NMHV amplitudes, Yangian invariants are called *R-invariants*, which can be compactly expressed as

$$R_{12345} = \frac{\delta^{0|4}(\langle 1234\rangle \chi_5 + \text{cyclic})}{\langle 1234\rangle\langle 2345\rangle\langle 1345\rangle\langle 1245\rangle\langle 1235\rangle},$$

where the brackets are in momentum twistors and are simply

$$\langle ijkl\rangle = \varepsilon_{ABCD} z_i^A z_j^B z_k^C z_l^D,$$

and χ_i are the Grassmann variables used to express amplitudes in $\mathcal{N}=4$ SYM in super-momentum twistors. Similarly, by R_I we will denote the analogous R-invariant with momentum twistor listed in I.

Among $4k$-dimensional cells with kinematic support corresponding to Yangian invariants, there are cells which are mapped injectively into the amplituhedron. The image of such cells in the amplituhedron are referred to as *generalised triangles* in [39, 40]. Generalised triangles are elements of triangulations of the amplituhedron. Cells corresponding to generalised triangles have *intersection number* one, see [2] for more details, and their corresponding Yangian invariants[6] are the building blocks for tree-level scattering amplitudes. Whereas, $4k$-dimensional cells with kinematic support, but with intersection number *higher* than one, are not mapped injectively into the amplituhedron: points in the image have a finite number (greater than one) of preimages in the cell. Yangian invariants associated with this type of cells do not enter

[5] In [29], it was indeed shown that the integral enjoys an infinite-dimensional symmetry, which is the Yangian of $\mathrm{psu}(2,2|2)$, and is simply called *the Yangian* in literature on scattering amplitudes. This symmetry is the hallmark of integrability of $\mathcal{N}=4$ SYM.

[6] Yangian invariants of this type were called *rational* in [42].

representations of scattering amplitudes at tree-level but are relevant for their leading singularities. These Yangian invariants can be written as a sum of terms which in general are algebraic (e.g., contain square roots), but the sum is still rational. See Section 3.2 for a relevant example.

Leading singularities from the amplituhedron. Let us now consider the boundaries of the loop amplituhedron and understand how they are related to leading singularities. It is known that the boundaries of the tree amplituhedron are on the vanishing locus of

$$\langle Y i_1\, i_1+1\, j_1\, j_1+1\rangle = 0, \quad \ldots, \quad \langle Y i_d\, i_d+1\, j_d\, j_d+1\rangle = 0 \tag{2.5}$$

for some $d > 0$ and all indices (considered cyclically) in $\{1, \ldots, n\}$. In order to make connection with leading singularities, we will not focus on this tree-level type of boundaries. Instead, we will consider boundaries where $(Y, \mathcal{L}^{(1)}, \ldots, \mathcal{L}^{(L)})$ satisfy *on-shell conditions*, which we define to be a subset of the following conditions:

$$\left\langle Y \mathcal{L}^{(l_a)} i_a, i_a+1\right\rangle = 0, \quad \left\langle Y \mathcal{L}^{(s_1)} \mathcal{L}^{(s_2)}\right\rangle = 0 \tag{2.6}$$

for $l_a, s_1, s_2 \in \{1, \ldots, \mathcal{L}\}$ and $i_a \in \{1, \ldots, n\}$, and Y does not lie on any of the tree-level type boundaries given by the equations in (2.5). Each set $\mathcal{C}$ of on-shell conditions has a certain number of solutions $\{\mathcal{L}_a^*\}_{\mathcal{C}}$, where we denoted by $\mathcal{L}_a^*$ the corresponding collection of L lines $(\mathcal{L}^{*(1)}, \ldots, \mathcal{L}^{*(L)})$. Following the terminology of [48], boundaries of the type (2.6) are called $\mathcal{L}$*-boundaries* and the connected components associated to each different solution of the same on-shell condition are called *branches*. If it exists, we denote by $\mathcal{B}[\mathcal{C}, \mathcal{L}^*]$ the boundaries of the loop amplituhedron, which are $\mathcal{L}$-boundaries determined by the set of on-shell conditions $\mathcal{C}$ and are in the branch corresponding to the solution $\mathcal{L}^*$. In [48], it was showed that, once we fix $\mathcal{C}$ and $\mathcal{L}^*$, there exists a minimum[7] k_{min} such that the loop amplituhedron $\mathcal{A}_{n,k}^{(L)}$ has the boundaries $\mathcal{B}[\mathcal{C}, \mathcal{L}^*]$ for all $k \geq k_{\text{min}}$.

Finally, we will focus on the $\mathcal{L}$-boundaries that are relevant for leading singularities, which correspond to *maximal cuts*. If $\mathcal{C}$ is a set of on-shell conditions, then $\mathcal{C}$ is a *maximal cut* if it is maximal by inclusion, i.e., we cannot add more on-shell conditions to $\mathcal{C}$ with Y not being on tree-level type boundaries of equation (2.5). In particular, an $\mathcal{L}$-boundary associated to a maximal cut has codimension $4L$ and the solutions in each branch have loop momenta localised in the points $\{\mathcal{L}^*\}$.

[7] Using *parity*, which is a symmetry of scattering amplitudes and of the amplituhedron, one can also establish an upper bound as $k \leq n - \bar{k}_{\text{min}} - 4$, where $\bar{k}_{\text{min}}$ is the minimal value of k for which the parity-conjugated branch appears.

For a maximal cut $\mathcal{C}$, boundaries $\mathcal{B}[\mathcal{C}, \mathcal{L}^*]$ of the loop amplituhedron correspond to leading singularities of the amplitude $\mathcal{A}_{n,k}^{(L)}$. In particular, as one can extract tree-level amplitudes $\mathcal{A}_{n,k}$ from the canonical form of the tree amplituhedron, one can extract the leading singularities $\text{LeS}[\mathcal{C}, \mathcal{L}^*]$ from the canonical form of the codimension-$4L$ boundaries $\mathcal{B}[\mathcal{C}, \mathcal{L}^*]$ of the loop amplituhedron.

It is known that all leading singularities of an amplitude $\mathcal{A}_{n,k}^{(L)}$ can be expressed as a sum of n-particle N^{k}MHV Yangian invariants, i.e., for a certain leading singularity LeS, there is a collection of $4k$-dimensional cells $\{S_a\}$ in $\text{Gr}_+(k, n)$ with kinematic support such that

$$\text{LeS} = \sum_a \mathcal{Y}_{S_a}. \tag{2.7}$$

This is just a rephrasing of the conjecture that the Grassmannian integral representation of scattering amplitudes provides leading singularities if integrated over proper contours, such as the one[8] provided by the above collection of cells $\{S_a\}$. The sum in (2.7) is the geometrical equivalent of "triangulating" the boundary of the loop amplituhedron, corresponding to the leading singularity, with the collection of Yangian invariants $\{\mathcal{Y}_{S_a}\}$. As different representations of a scattering amplitude $\mathcal{A}_{n,k}$ (tree-level or loop integrand) are just different ways to triangulate the amplituhedron (tree or loop), different representations of a leading singularity LeS as sum of Yangian invariants correspond to different triangulations of the corresponding boundary of the loop amplituhedron.

In Section 4, we will exploit the geometric definition of the loop amplituhedron to compute *all* Yangian invariants which can be part of a triangulation of a given boundary of the loop amplituhedron, i.e., all Yangian invariants which can be used to express a given leading singularity. Moreover, we will see how this connects to the Landau analysis in the next section.

2.2.1. Leading singularities at one-loop. In this section, we will provide an illustrative example on how to compute leading singularities from the Grassmannian for one-loop NMHV, following [10] (in particular, see Table 3). We will consider only some maximal cuts which will be relevant for our analysis. We will briefly comment on the N^{2}MHV case, and we will employ a different strategy based on the amplituhedron described in Section 3.

Given a cut $\mathcal{C} = \{I_1, \ldots, I_4\}$ for the loop amplitude $\mathcal{A}_{n,k}^{(1)}$, on-shell diagrams with tree sub-amplitudes $\mathcal{A}_{n_1,k_1}(I_1) \otimes \cdots \otimes \mathcal{A}_{n_4,k_4}(I_4)$, such that

$$\sum_{a=1}^{4} k_a = k - 2, \quad \sum_{a=1}^{4} n_a = n + 8, \tag{2.8}$$

[8] With suited orientation of each cell.

correspond to leading singularities of $\mathcal{A}_{n,k}^{(L=1)}$. Here we denoted sub-amplitudes by $\mathcal{A}_{n',k'}(I')$, where k', with $0 \leq k' \leq n-4$, is its $\mathrm{N}^{k'}$MHV helicity sector,[9] n' the number of legs, and I' denotes the indices the external particles contained.

Leading singularities for NMHV one-loop. Let us now list the types of leading singularities which can appear at NMHV at one-loop. By equation (2.8), we must have

$$k_1 + k_2 + k_3 + k_4 = 1 - 2 = -1.$$

Since we can have $k_a = -1$ only when one of the sub-amplitude is a 3-point amplitude, otherwise k_a are positive, then we must have at least a 3-point subamplitude to satisfy equation (2.8). Given a subamplitude $\mathcal{A}_{n',k'}(I')$, in the following we will omit the dependence of the sub-amplitudes on n' and we will use $\ldots$ for some or all indices in I'. They can be easily inferred from the context. All indices will be cyclically ordered $i < i+1 < j < j+1 < k < k+1$.

(1) The *two-mass easy box* $\mathcal{C}_{ij}^{E}$ is a maximal cut with the following on-shell conditions:

$$\langle \mathcal{L} i-1, i\rangle = \langle \mathcal{L} i, i+1\rangle = \langle \mathcal{L} j-1, j\rangle = \langle \mathcal{L} j, j+1\rangle = 0. \tag{2.9}$$

There are two possible on-shell diagrams contributing to this cut, whose leading singularities are

$$\mathrm{LeS}[\mathcal{A}_{-1}(i) \otimes \mathcal{A}_0(\ldots) \otimes \mathcal{A}_{-1}(j) \otimes \mathcal{A}_1(\ldots)] = \mathcal{A}_{\mathrm{NMHV}}(j, \ldots, i),$$
$$\mathrm{LeS}[\mathcal{A}_{-1}(i) \otimes \mathcal{A}_1(\ldots) \otimes \mathcal{A}_{-1}(j) \otimes \mathcal{A}_0(\ldots)] = \mathcal{A}_{\mathrm{NMHV}}(i, \ldots, j).$$

(2) The *two-mass hard box* $\mathcal{C}_{ij}^{H}$ is a maximal cut with the following on-shell conditions:

$$\begin{aligned}\langle \mathcal{L} i-1, i\rangle = \langle \mathcal{L} i, i+1\rangle = \langle \mathcal{L} i+1, i+2\rangle \\ = \langle \mathcal{L} j, j+1\rangle = 0.\end{aligned} \tag{2.10}$$

There are two possible on-shell diagrams contributing to this cut, whose leading singularities are

$$\mathrm{LeS}[\mathcal{A}_{-1}(i) \otimes \mathcal{A}_0(i+1) \otimes \mathcal{A}_0(\ldots, j) \otimes \mathcal{A}_0(\ldots)] = R_{i,i+1,i+2,j,j+1},$$
$$\mathrm{LeS}[\mathcal{A}_0(i) \otimes \mathcal{A}_{-1}(i+1) \otimes \mathcal{A}_0(\ldots, j) \otimes \mathcal{A}_0(\ldots)] = R_{i-1,i,i+1,j,j+1}.$$

[9] For $n = 3$, we also admit $k' = -1$, which corresponds to $\overline{\mathrm{MHV}}$, i.e., a *white* vertex. Moreover, note that $\mathcal{A}_0(\ldots) = 1$, since we are in the momentum twistor space.

(3) The *three-mass box* $\mathcal{C}_{ijk}$ is a maximal cut with the following on-shell conditions:

$$\langle \mathcal{L} i-1, i\rangle = \langle \mathcal{L} i, i+1\rangle = \langle \mathcal{L} j, j+1\rangle = \langle \mathcal{L} k, k+1\rangle = 0. \quad (2.11)$$

There is only one on-shell diagrams contributing to this cut, whose leading singularity is

$$\mathrm{LeS}[\mathcal{A}_{-1}(i) \otimes \mathcal{A}_0(\ldots, j) \otimes \mathcal{A}_0(\ldots, k) \otimes \mathcal{A}_0(\ldots)] = R_{i,j,j+1,k,k+1}.$$

Leading singularities for N^{2}MHV one-loop. For N^{2}MHV at one-loop, we have all cuts of the type appearing at NMHV, and in addition the *four-mass box cut* appears from 8 points. This is associated to leading singularities which contains non-rational Yangian invariants, and, by Landau analysis, to algebraic singularities of the loop amplitude. We leave these cases for explorations in future works.

N^{2}MHV leading singularities are in general expressed as

$$R_I \cdot R_J, \quad R_I \cdot \mathcal{A}_{\mathrm{NMHV}}(J), \quad \varphi R_I \cdot R_J, \quad (2.12)$$

where I, J are lists of twistors (in general, expressed as intersection of lines or planes defined from z_i), R_I are R-invariants with twistors in the list I, and φ is an extra function, not relevant for our purposes. Nevertheless, as discussed in (2.7) all of them are just combinations of N^{2}MHV Yangian invariants. For the purpose of the paper, we are not interested in representations of leading singularities like (2.12), but we will focus on their underline geometry. In particular, we are interested on the full list $\{\mathcal{Y}_a\}$ of Yangian invariants which can be used to express a given leading singularity. In Section 4, we will explain a way to obtain such list directly from the geometry of the loop amplituhedron.

2.3. Landau singularities from the amplituhedron

We will briefly review how the Landau analysis can be used to infer singularities of the *integral*, from the poles of the *integrand*. First, we will review the original definition in terms of Feynman diagrams and then following [48] we will review the role amplituhedron plays in this analysis.

Landau singularities. The concept of Landau singularities was originally introduced in 1959, when Landau stated a set of equations, called *Landau equations*, whose solutions parametrises the locus in the space of kinematic data, where a given Feynman integral has branch points [38].

Given a Feynman integral I contributing to an L loop scattering amplitude in D spacetime dimensions, we can always bring it to the following form by using Feynman parametrisation:

$$I = c \int \prod_{a=1}^{L} d^D \ell_a \int_{\Delta_{\nu-1}} \frac{\mathcal{N}(\{\ell_a\}, \{p_r\})}{\mathcal{D}^\nu(\alpha; \{q_i\})}, \quad \mathcal{D} = \sum_{i=1}^{\nu} \alpha_i (q_i^2 - m_i^2), \tag{2.13}$$

where c is just constant which does not enter our analysis, the integration is performed over the simplex $\Delta_{\nu-1}$, i.e., $\alpha_1 + \cdots + \alpha_\nu = 1$ and $\alpha_i \geq 0$, q_i is the momentum flowing along the corresponding propagator i, $\{p_r\}$ are the momenta of external particles, and $\mathcal{N}$ is a function of the kinematic data. It is known that the physical amplitude from (2.13) is obtained by performing the integral over a particular contour defined by the $i\varepsilon$ prescription in the propagators. However, in order to understand the analytic continuation outside the physical sheet in the space of kinematic, one has to study arbitrary contours.

The Landau analysis establishes that the integral I in (2.13) *can* develop singularities when the following equations admit a solution

$$\sum_{i \in \text{loop}} \alpha_i q_i = 0 \quad \text{for all loops and } \alpha_i (q_i^2 - m_i^2) = 0 \ \forall i. \tag{2.14}$$

In order to capture the analytic structure of I away from the physical sheet, one allows solutions of the following equations with α_i and ℓ_a away from the physical contour as well. When some of the α_i are different than zero, the second case in equation (2.14) corresponds to putting some internal propagators on-shell, and these will be related to “cuts”. In the following, we will be interested only when solutions exist on codimension-one subspaces of the external kinematic space, i.e., when they are parametrised by the vanishing locus of a certain function of external kinematic.

We notice that the power of this method seems to be affected by two major inconveniences. Firstly, this analysis does not know about the numerator $\mathcal{N}$ in equation (2.13), which can change the structure of singularities of the denominator, or even cancel some of them. Secondly, even when the numerator does not affect the singularities, singularities of individual Feynman integrals might not survive the summation to remain singularities of the full amplitude. In summary, the Landau analysis, even if predicts all potential singularities of the amplitude, in general, it predicts many “spurious” singularities as well, which are not actual singularities of the amplitude.

In [17], it was suggested that one can circumvent these issues by directly appealing to the geometry of the amplituhedron.

Landau singularities form the loop amplituhedron. Given a Landau singularity corresponding to setting to zero a certain number of internal propagators, i.e., a *cut*, this is an actual singularity of the amplitude if the cut corresponds to a boundary of the loop amplituhedron.

In order to make the connection with the amplituhedron more explicitly, as shown in [48], one can re-write the Landau equation in momentum twistors. If a cut $\mathcal{C}$ is a collection of constraints of the type

$$f_j(\mathcal{L}, z) = 0, \tag{2.15}$$

where $\mathcal{L}$ collectively denotes the momentum twistors associated to loops $\mathcal{L}^{(1)}, \dots, \mathcal{L}^{(L)}$, and $\{z\}$ are momentum twistors encoding the kinematic data of external particles. Then the Landau equations for this set of on-shell constraints include the above equations together with a set of equations of the type

$$\sum_{j=1}^{d} \alpha_j \frac{\partial f_j(\mathcal{L}(\beta), z)}{\partial \beta_s} = 0, \quad s = 1, \dots, 4L,$$

where the β's are $4L$ coordinates used to parametrise $\mathcal{L}^{(1)}, \dots, \mathcal{L}^{(L)}$. This latter equations are often referred to as *Kirchhoff conditions*. We observe that the Landau equations are $d + 4L$ equations in $d + 4L - 1$ variables (since we can always rescale all the α's in the Kirchhoff equations). Therefore, one might expect that they do not admit solutions for general kinematics. For the purpose of this analysis, one is then interested in knowing what the codimension-one loci in kinematic space of z's are, for which Landau equations admit solutions (with α's not all zero). Let such loci be the vanishing set of the function

$$\mathrm{LaS}[\mathcal{C}, \mathcal{L}^*](z) = \prod_{t=1}^{N} a_t(z) = 0,$$

where $\mathcal{C}$ is the cut associated to the Landau equations (2.15), $\mathcal{L}^*$ is one branch of solutions of the on-shell conditions we are considering, and $a_t(z)$ are certain polynomials of Plücker coordinates of z (i.e., brackets in momentum twistors, see p. 307). In the following, we will refer to $\mathrm{LaS}[\mathcal{C}, \mathcal{L}^*]$ as the *Landau singularity* associated to the cut $\mathcal{C}$ in the branch $\mathcal{L}^*$. With a slight abuse of terminology, we will also refer to $a_1, \dots, a_N$ as corresponding Landau singularities.

Finally, a given Landau singularity $\mathrm{LaS}[\mathcal{C}, \mathcal{L}^*]$ is a true singularity of the amplitude $\mathcal{A}_{n,k}^{(L)}$ if the loop amplituhedron has a boundary of the type $\mathcal{B}[\mathcal{C}, \mathcal{L}^*]$, see [17].

In summary, on one hand, the Landau analysis can connect the geometry of boundaries of the amplituhedron to the location of singularities of integrated amplitudes. On the other, the amplituhedron can tell which are the true singularities of the integrand, and therefore select the true Landau singularities, among the spurious ones coming from summing over Feynman diagrams.

2.3.1. Landau singularities at one-loop. We report below the Landau singularities corresponding to some maximal cuts that will be relevant for our analysis. These can be found in [48, Table 1]. We also report the points where the loop momenta localise on different cuts. In particular, for a maximal cut $\mathcal{C}$, there are two solutions $\mathcal{L}_1^*$, $\mathcal{L}_2^*$ (parity conjugate to each other), each of which can be expressed in term of momentum twistors of external kinematic as

$$\mathcal{L}_a^* = D[\mathcal{C}, \mathcal{L}_a^*] \cdot z, \tag{2.16}$$

where $D[\mathcal{C}, \mathcal{L}_a^*]$ is a $2 \times n$ matrix depending on Plückers coordinates of z, where z is the $n \times 4$ matrix whose rows are the momentum twistors of the external kinematics z_i. In the following, only the non-zero columns of D will be displayed explicitly. Moreover, we consider cyclically ordered indices $i < i+1 < j < j+1 < k < k+1$.

(1) The *two-mass hard box cut* $\mathcal{C}_{ij}^E$ in equation (2.9) has in general two solutions:

$$\mathcal{L}_1^* = (ij), \quad \mathcal{L}_2^* = \bar{i} \cap \bar{j},$$

the first is valid for $0 \leq k \leq n-6$ and the second for $2 \leq k \leq n-4$. The corresponding matrices are[10]

$$D[\mathcal{C}_{ij}^E, \mathcal{L}_1^*] = \overset{\begin{matrix} i & \;\; j \end{matrix}}{\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}}, \quad D[\mathcal{C}_{ij}^E, \mathcal{L}_2^*] = \overset{\begin{matrix} i-1 & \qquad\qquad i & \qquad\qquad i+1 \end{matrix}}{\begin{pmatrix} \langle i\, \bar{j}\rangle & -\langle i-1, \bar{j}\rangle & 0 \\ 0 & -\langle i+1, \bar{j}\rangle & \langle i\, \bar{j}\rangle \end{pmatrix}}.$$

For this cut and both of the branches,[11] we have the following Landau singularities:

$$\mathrm{LaS}[\mathcal{C}_{ij}^E, \mathcal{L}_1^*](z) = \mathrm{LaS}[\mathcal{C}_{ij}^E, \mathcal{L}_2^*](z) = \langle i\, \bar{j}\rangle\langle \bar{i}\, j\rangle.$$

(2) The *two-mass easy box cut* $\mathcal{C}_{ij}^H$ in equation (2.10) has in general two solutions:

$$\mathcal{L}_1^* = \overline{i+1} \cap (ijj+1), \quad \mathcal{L}_2^* = \bar{i} \cap (i+1, jj+1).$$

They are both valid for $1 \leq k \leq n-5$. The corresponding matrices are

$$\begin{aligned} D[\mathcal{C}_{ij}^H, \mathcal{L}_1^*] &= \overset{\begin{matrix} i & \qquad\qquad i+1 & \qquad\qquad\qquad i+2 \end{matrix}}{\begin{pmatrix} 1 & 0 & 0 \\ 0 & -\langle i, i+2, j, j+1\rangle & \langle i, i+1, j, j+1\rangle \end{pmatrix}}, \\ D[\mathcal{C}_{ij}^H, \mathcal{L}_2^*] &= \overset{\begin{matrix} i-1 & \qquad\qquad\qquad i & \qquad\qquad i+1 \end{matrix}}{\begin{pmatrix} 0 & 0 & 1 \\ -\langle i, i+1, j, j+1\rangle & \langle i-1, i+1, j, j+1\rangle & 0 \end{pmatrix}}. \end{aligned} \tag{2.17}$$

[10] They are of course determined up to GL(2) (and up to adding rows of C, see Definition 2.1).

[11] In general, we can have different Landau singularities for different branches of the same cut. However, this does not happen at one loop [48].

For this cut, we have the following Landau singularities:

$$\mathrm{LaS}\big[\mathcal{C}_{ij}^{H},\mathcal{L}_1^*\big](z)=\mathrm{LaS}\big[\mathcal{C}_{ij}^{H},\mathcal{L}_2^*\big](z)=\langle i,i+1,j,j+1\rangle. \tag{2.18}$$

(3) The *three-mass easy box* $\mathcal{C}_{ijk}$ in equation (2.11) has in general 2 solutions:

$$\mathcal{L}_1^*=(ijj+1)\cap(ikk+1),\quad \mathcal{L}_2^*=(\bar{i}\cap(jj+1),\bar{i}\cap(kk+1)).$$

The first is valid for $1\le k\le n-6$ and the second for $2\le k\le n-5$. The corresponding matrices are

$$D[\mathcal{C}_{ijk},\mathcal{L}_1^*]=\begin{pmatrix} \overset{i}{1} & \overset{i+1}{0} & \overset{j}{0}\\ 0 & \langle i,j,k,k+1\rangle & -\langle i,j+1,k,k+1\rangle\end{pmatrix},$$

$$D[\mathcal{C}_{ijk},\mathcal{L}_2^*]=\begin{pmatrix} \overset{j}{-\langle\bar{i},j+1\rangle} & \overset{j+1}{\langle\bar{i},j\rangle} & \overset{k}{0} & \overset{k+1}{0}\\ 0 & 0 & -\langle\bar{i},k+1\rangle & \langle\bar{i},k\rangle\end{pmatrix}.$$

For this cut, we have the following Landau singularities:

$$\mathrm{LaS}[\mathcal{C}_{ijk},\mathcal{L}_1^*](z)=\mathrm{LaS}[\mathcal{C}_{ijk},\mathcal{L}_2^*](z)=\langle i(i-1,i+1)(j,j+1)(k,k+1)\rangle.$$

Our notation for twistor brackets throughout the paper follows closely the literature, e.g., [48].

3. Cluster adjacency in Yangian invariants

We start unpacking cluster phenomena in the context of singularities of scattering amplitudes in $\mathcal{N}=4$ SYM. In this section, we focus on tree-level singularities, i.e., on poles of Yangian invariants (see Section 2.2).

In [25], it was conjectured that, given a Yangian invariant $\mathcal{Y}$ appearing in a BCFW representation of the tree-level amplitude $\mathcal{A}_{n,k}$, then *all* its poles are *cluster adjacent*, i.e., they are given by some collection of $\mathcal{A}$-coordinates of the $\mathrm{Gr}(4,n)$ cluster algebra that can be found together in a common cluster. In [42], the conjecture was generalised for all *rational* Yangian invariants of $\mathcal{N}=4$ SYM, where rationality in this context means intersection number one in the terminology of [2,9].

In particular, in [25] cluster adjacency between Yangian invariants was checked up to 8-point N^{2}MHV by looking at Yangian invariants appearing into a specific representation of the amplitude. This is not an exhaustive check since, starting from 8-point N^{2}MHV, one in general finds Yangian invariants which are not related by cyclic symmetry to any of the Yangian invariants appearing in a fixed representation. Whereas in [42], *pair-wise* cluster adjacency between poles of Yangian invariants was checked for all $k \leq 2$ and many $k = 3$ Yangian invariants, by employing Sklyanin Poisson brackets.

In this section, we prove that all (rational) N^2MHV Yangian invariants with are cluster adjacent by explicit calculation of the relevant clusters. Moreover, we provide explicitly the list of their actual poles in terms of polynomial in Plückers of momentum twistors which are $\mathcal{A}$-coordinates of the $\mathrm{Gr}(4,n)$ cluster algebra in the files `yik2n_.m`.

Poles of Yangian invariants from the amplituhedron. All Yangian invariants for $k = 2$ were fully classified in [2]. However, the advantage of presenting Yangian invariants written as products of R-invariants (with, in some cases, auxiliary multiplicative rational functions) is shadowed by a drawback. In this way, the actual poles of the Yangian invariant are not always exposed: their numerator might indeed cancel some poles in the denominator. Moreover, the relation between these poles and $\mathcal{A}$-cluster coordinates of $\mathrm{Gr}(4,n)$ is not manifest either.

We will now explain how to improve on both aspects using a geometric approach from the amplituhedron, which automatically detects only actual poles of a Yangian invariant. Moreover, given an $\mathcal{A}$-cluster coordinate, it can easily tell whether it is a pole of a given Yangian invariant, without computing its full expression.

We recall from Section 2.2 that, given a $4k$-dimensional cell S of $\mathrm{Gr}_+(k,n)$ with kinematic support, the Yangian invariant Y_S is its full-dimensional image in the amplituhedron and $\mathcal{Y}_S$ is the corresponding function of (super-)momentum twistors obtained from the Grassmannian integral formula. Then there is a bijection between (actual) poles of $\mathcal{Y}_S$ and codimension-one boundaries of Y_S. Geometrically, these boundaries are simply described as the image of some of the boundaries of the cell S into the amplituhedron. In details, let $\partial S^{(i)}$ be one $(4k-1)$-dimensional cell in the boundary of the cell S that has a full-dimensional image[12] (i.e., $4k-1$) into the amplituhedron. Then the image of $\partial S^{(i)}$ is a boundary of Y_S. Moreover, being of codimension one, this boundary in the amplituhedron lies on an hyper-surface determined by the vanishing locus of a function

$$P(\langle Y Z_{i_1}\, Z_{i_2}\, Z_{i_3}\, Z_{i_4}\rangle) = 0,$$

which depends on the brackets defined in equation (2.3). By projecting to momentum twistor space, the corresponding pole of $\mathcal{Y}_S$ will be at

$$P(\langle z_{i_1} z_{i_2} z_{i_3} z_{i_4}\rangle) = 0.$$

[12] Even if a cell S has kinematic support, in general, it has some boundaries whose dimension might be dropped when mapping into the amplituhedron. One has to disregard such boundaries, as they do not contribute to the codimension-one boundary of Y_S.

Vice-versa, if we start with a polynomial[13] $P(\langle z_{i_1} z_{i_2} z_{i_3} z_{i_4}\rangle)$ in Plückers, e.g., an $\mathcal{A}$-cluster coordinate, then we can claim it is a pole of a given Yangian invariant $\mathcal{Y}_S$ if

$$P(\langle Y Z_{i_1}\, Z_{i_2}\, Z_{i_3}\, Z_{i_4}\rangle)\big|_{Y=C\cdot Z} = 0, \quad \forall C \in \partial S^{(i)},$$

where we parametrised Y as in definition (2.4), i.e., $Y = C \cdot Z$, with C any representative of a point in $\partial S^{(i)}$. In this way, we can detect (actual) poles of every Yangian invariant purely from the geometry of the amplituhedron. In order to handle positroid cells in the Grassmannian, we used the MATHEMATICA package `positroids.m` [9].

3.1. Cluster adjacency in all (rational) N^{2}MHV Yangian invariants

In this section, we report all poles of each N^{2}MHV Yangian invariant explicitly expressed as $\mathcal{A}$-cluster coordinates and explore their cluster properties.

$n = 6$. There is only one Yangian invariant and all its poles correspond to frozen variables $\{\langle i, i+1, i+2, i+3\rangle\}_{i\in[6]}$. Therefore, this Yangian invariant satisfies cluster adjacency trivially.

In the following, we will write $\langle i\rangle := \langle i, i+1, i+2, i+3\rangle$, which will be frozen variables in the Gr$(4,n)$cluster algebra. Note that the definition of $\langle i\rangle$ is depends on n. Nevertheless, we suppress this information to avoid notational clutter.

$n = 7$. There are only 3 Yangian invariants $\{\mathcal{Y}_a\}_{a\in[3]}$, up to cyclic symmetry. Only the Yangian invariants number 2, 3 are of the new type which appear at $n = 7$, whereas $\mathcal{Y}_1$ is just a relabelling of the type $n = 6$. We list here the poles of each of them in terms of polynomial of brackets of momentum twistors:

$$\begin{aligned}
\partial\mathcal{Y}_1 &= \{\langle 2\bar{6}\rangle, \langle 2367\rangle, \langle \bar{3}7\rangle, \langle 2\rangle, \langle 3\rangle, \langle 4\rangle\},\\
\partial\mathcal{Y}_2 &= \{\langle 1\bar{4}\rangle, \langle 5(67)(12)(34)\rangle, \langle 3(45)(67)(12)\rangle, \langle 1\rangle, \langle \bar{4}7\rangle, \langle 2\rangle, \langle 3\rangle, \langle 4\rangle\},\\
\partial\mathcal{Y}_3 &= \{\langle 3471\rangle, \langle 7(12)(34)(56)\rangle, \langle \bar{2}7\rangle, \langle 3467\rangle, \langle 1\rangle, \langle \bar{4}7\rangle, \langle 3\rangle, \langle \bar{3}7\rangle, \langle 4\rangle\}.
\end{aligned}$$

As expected, all the poles are cluster variables of Gr$(4,7)$ and we checked they are cluster adjacent.

$n = 8$. There are 24 Yangian invariants up to cyclic symmetry; 4 of them are of $n = 6$ type, 14 are of $n = 7$ type. There are only 6 new types which appear for $n = 8$. We provide a full list of these Yangian invariants in an ancillary file, `yik2n8.m`, and the labels we use to denote them below refer to this list.

[13]We assume the polynomials are irreducible in the Plücker variables.

In this case, we observe explicitly that writing $k = 2$ Yangian invariants in terms of products of R-invariants might obscure the actual poles. Let us consider the Yangian invariant $\mathcal{Y}_{11}$, which can be written as

$$\mathcal{Y}_{11} = R_{12345} R_{678,(123)\cap(45),5}. \tag{3.1}$$

If we write the poles explicitly, we can see that some factorise

$$\langle(123) \cap (45)567\rangle = \langle 1235\rangle\langle 4567\rangle,$$

where $\langle 1235\rangle$ is also a pole of R_{12345} and will therefore seem to appear as a double pole in (3.1). Since we appeal purely to the geometry of the amplituhedron, we will only see the actual poles of the Yangian invariants, and in this case $\langle 1235\rangle$ is not an actual pole. In the following, we will write Yangian invariants which show this phenomenon explicitly, otherwise, we will write their poles as unions of 10 poles of 2 R-invariants:

$$\partial\mathcal{Y}_{12} = \partial R_{123,(45)\cap\bar{7},8} \cup \partial R_{45678}, \tag{3.2}$$

$$\partial\mathcal{Y}_{15} = \partial R_{81234} \cup \partial R_{45678}, \tag{3.3}$$

$$\partial\mathcal{Y}_{16} = \partial R_{1234,\bar{5}\cap(78)} \cup \partial R_{45678}, \tag{3.4}$$

$$\partial\mathcal{Y}_{11} = \{\langle 1\bar{4}\rangle, \langle 1245\rangle, \langle 123(45)\cap\bar{7}\rangle, \langle 1\rangle, \langle 4578\rangle, \langle 2\rangle, \langle\bar{5}8\rangle, \langle 4\rangle, \langle 5\rangle\}, \tag{3.5}$$

$$\begin{aligned}\partial\mathcal{Y}_{13} = \{&\langle 6(13)(45)(78)\rangle, \langle 6(12)(45)(78)\rangle, \langle 123, \bar{5}\cap(78)\rangle, \langle 4\bar{7}\rangle,\\ &\langle 123(45)\cap\bar{7}\rangle, \langle\bar{5}8\rangle, \langle 6(23)(45)(78), \langle 4\rangle, \langle 5\rangle\},\end{aligned} \tag{3.6}$$

$$\begin{aligned}\partial\mathcal{Y}_{24} = \{&\langle 1(34)(56)(78)\rangle, \langle 7\rangle, \langle 6(12)(34)(78)\rangle, \langle 3(12)(56)(78)\rangle, \langle 1\rangle,\\ &\langle 8(12)(34)(56)\rangle, \langle 5(12)(34)(78)\rangle, \langle 3\rangle, \langle 2(34)(56)(78)\rangle,\\ &\langle 7(12)(34)(56)\rangle, \langle 5\rangle, \langle 4(12)(56)(78)\rangle\}.\end{aligned} \tag{3.7}$$

All of these Yangian invariants, including those of four-mass box type, have poles that are polynomial in momentum twistor brackets. These polynomials are all cluster variables of $\mathrm{Gr}(4, 8)$.

We verified that cluster variables corresponding to all the poles of these Yangian invariants are cluster adjacent with a single exception. Namely, the Yangian invariant $\mathcal{Y}_{24}$, which corresponds to the four-mass box, contains non-cluster adjacent poles. We will comment on this in Section 3.2.

The $\mathrm{Gr}(4, n)$ cluster algebras are infinite for $n \geq 8$ but recent understanding [6,26, 35] suggest natural truncations of these in terms of *positive tropical Grassmannians* or their generalisations. For $n = 8$ there have been three such constructions, by considering all tropicalised Plücker coordinates, only a parity-invariant subset thereof, or the parity completion of the set of Plücker coordinates. These, as polytopes, have 274, 260 and 548 vertices, respectively.

One may also wonder if and which of the proposed truncations of the infinite cluster algebras via tropical fans do accommodate the adjacencies we found for 8-point N^{2}MHV Yangian invariants. We find that all Yangian invariants, except $\mathcal{Y}_{24}$, are also cluster adjacent in the more restrictive sense of tropical fans. In particular, the corresponding g-vectors of their unfrozen poles always form a cone of the tropical fan with 274 vertices, obtained by tropicalising the maximal parity-invariant subset of the Plücker coordinates.

$n = 9$. There are 108 Yangian invariants up to cyclic symmetry; 10 of them are of $n = 6$ type, 56 are of $n = 7$ type, and 38 are of $n = 8$ type. There are only 4 new types which appear for $n = 9$. We report below the boundaries in terms of brackets of momentum twistors for these 4 types:

$$\partial\mathcal{Y}_{45} = \partial R_{12349} \cup \partial R_{56789}, \tag{3.8a}$$

$$\partial\mathcal{Y}_{46} = \partial R_{1234,(567)\cap(89)} \cup \partial R_{56789}, \tag{3.8b}$$

$$\partial\mathcal{Y}_{48} = \partial R_{1234,(56)\cap(789)} \cup \partial R_{56789}, \tag{3.8c}$$

$$\begin{aligned}\partial\mathcal{Y}_{101} = \{&\langle 5\,6\,\bar{2} \cap \bar{8}\rangle, \langle 4\,6\,\bar{2} \cap \bar{8}\rangle, \langle 4\,5\,\bar{2} \cap \bar{8}\rangle,\\ &\langle 2\,3\,\bar{5} \cap \bar{8}\rangle, \langle 1\,3\,\bar{5} \cap \bar{8}\rangle, \langle 1\,2\,\bar{5} \cap \bar{8}\rangle,\\ &\langle 8\,9\,\bar{2} \cap \bar{5}\rangle, \langle 7\,9\,\bar{2} \cap \bar{5}\rangle, \langle 7\,8\,\bar{2} \cap \bar{5}\rangle\},\end{aligned} \tag{3.8d}$$

where the labels refer to the list in the ancillary file `yik2n9.m`, where we give a full list of these Yangian invariants (up to cyclic rotations). All 108 of these objects are cluster adjacent in Gr(4, 9), except the two, which are of the $n = 8$ four-mass box type.

We also present the cluster that contains the poles of a Yangian invariant which is particularly interesting, namely $\mathcal{Y}_{101}$ in (3.8d). Informally, it is called the *spurion*, since it does not contain any physical pole. Therefore, it cannot appear in any of the BCFW representations of the amplitude $\mathcal{A}_{9,2}$. Nevertheless, from the perspective of the amplituhedron, it is a generalised triangle and can be part of a triangulation, giving a representation of $\mathcal{A}_{9,2}$ not obtainable with standard BCFW.

This cluster has the quiver diagram displayed in Figure 1, where we abbreviated the relevant $\mathcal{A}$-coordinates as

$$\begin{aligned} a_1 &= \langle 5\,6\,\bar{2} \cap \bar{8}\rangle, & a_2 &= \langle 4\,6\,\bar{2} \cap \bar{8}\rangle, & a_3 &= \langle 4\,5\,\bar{2} \cap \bar{8}\rangle,\\ a_4 &= \langle 2\,3\,\bar{5} \cap \bar{8}\rangle, & a_5 &= \langle 1\,3\,\bar{5} \cap \bar{8}\rangle, & a_6 &= \langle 1\,2\,\bar{5} \cap \bar{8}\rangle,\\ a_7 &= \langle 8\,9\,\bar{2} \cap \bar{5}\rangle, & a_8 &= \langle 7\,9\,\bar{2} \cap \bar{5}\rangle, & a_9 &= \langle 7\,8\,\bar{2} \cap \bar{5}\rangle, \end{aligned}$$

while the remaining irrelevant ones are

$$s_1 = \langle 1456\rangle, \quad s_2 = \langle 1237\rangle, \quad s_3 = \langle 4789\rangle.$$

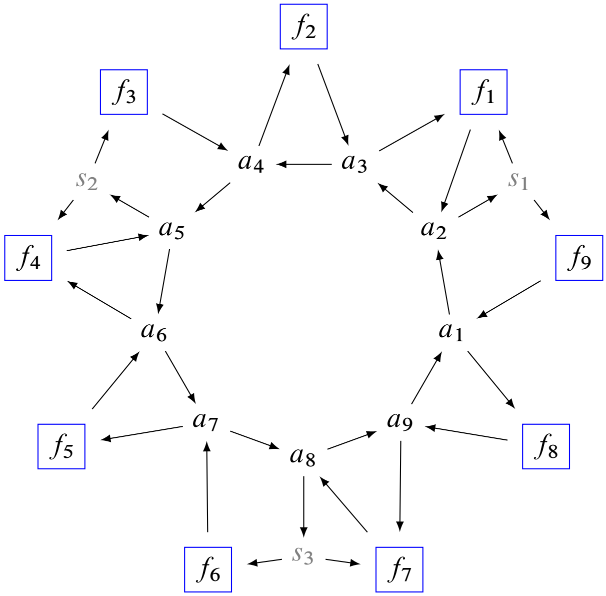

Figure 1. Quiver diagram for a Gr(4, 9) showing cluster adjacency of the poles of $\mathcal{Y}_{101}$ for $n = 9$.

These three irrelevant $\mathcal{A}$ coordinates can be freely mutated and therefore one may say that this Yangian invariant corresponds to a cube in the cluster polytope. Note also the $\mathbb{Z}_3$ symmetry of the spurion is reflected in this cluster.

$n = 10$. There are 395 Yangian invariants up to cyclic symmetry; 22 of them are of $n = 6$ type, 168 are of $n = 7$ type, 174 are of $n = 8$ type, 30 are of $n = 9$ type and only 1 is of $n = 10$. As observed in [2], there are no new types of Yangian invariants beyond $n = 10$. This comes immediately from the fact that Yangian invariants correspond to $4k$-dimensional cells in $\text{Gr}_+(k, n)$, whose number of types is bounded for fixed k. The only new type of Yangian invariant for $n = 10$ is very simple:

$$\partial\mathcal{Y}_1 = \partial R_{12345} \cup \partial R_{6789,10}.$$

In Figure 2, we represent a cluster in Gr(4, 10) cluster algebra which contains all poles of $\mathcal{Y}_1$. We observe that all poles of R_{12345} are in the left-most position, whereas all the poles of $R_{6789,10}$ are in the right-most position.

With this, we proved cluster adjacency for *all* N^2MHV Yangian invariants corresponding to generalised triangles. Moreover, we observe that Yangian invariants of the four-mass box type, which are not generalised triangles, do not satisfy cluster adjacency. The corresponding cluster algebras are infinite, and one may wonder how one can check this conclusively. We comment on this in the next section.

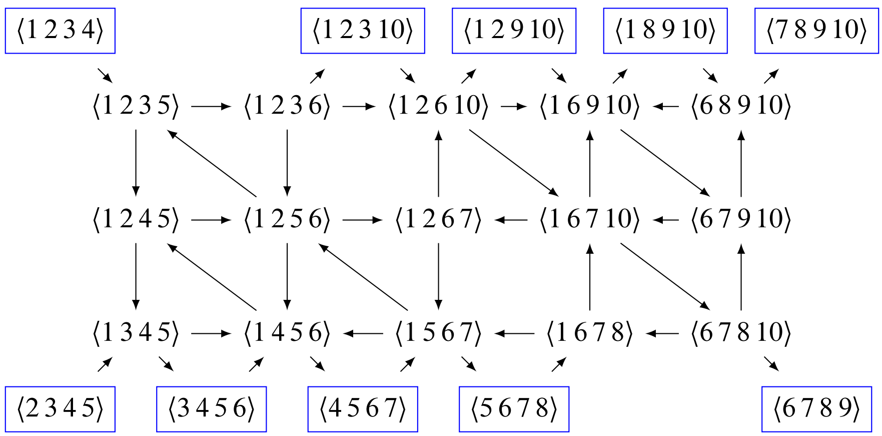

Figure 2. The cluster in Gr(4, 10) demonstrating the adjacency of the Yangian invariant $\mathcal{Y}_1$ for $n = 10$.

3.2. Four-mass box Yangian invariants

The $n = 8$ Yangian invariant $\mathcal{Y}_{24}$ corresponds to a four-mass box cut. These types of Yangian invariants fall in the category of Yangian invariants with intersection number higher than one, see Section 2.2 and they have always been excluded in cluster adjacency analysis, e.g., in [42].

In particular, for the case of $\mathcal{Y}_{24}$, points in the amplituhedron have 2 pre-images in the associated cell S_{24} in $\mathrm{Gr}_+(k, n)$. From an algebraic perspective, this corresponds to the fact that $\mathcal{Y}_{24}$ can be expressed as the sum of two contributions:

$$\mathcal{Y}_{24} = \mathcal{Y}_{24}^{(1)} + \mathcal{Y}_{24}^{(2)},$$

each of which contains square-roots, however the sum is of course rational. Moreover, the boundaries of $\mathcal{Y}_{24}$ will only correspond to the actual poles of the sum in equation (3.2). We reported these poles in equation (3.7) and checked that they are *not* cluster adjacent.[14] The infinite nature of the Gr(4, 8) cluster algebra might make it difficult to perform exhaustive checks, especially when the poles may not be mutation pairs.[15] Nevertheless, we explain below how one proves that this Yangian invariant is not cluster adjacent.

[14]Invariant $\mathcal{Y}_{24}$, as other Yangian invariants with intersection number higher than one, can be rewritten as a sum of other rational Yangian invariants, each of which we showed to satisfy cluster adjacency.

[15]See Section 2.1 for the terminology.

We can easily find a cluster containing only two of the poles of this Yangian invariant, e.g.,

$$\langle 6(12)(34)(78)\rangle, \quad \langle 8(12)(34)(56)\rangle. \tag{3.9}$$

Then, by freezing these two nodes and mutating them in all other directions, we can start exploring the "face" corresponding to these and ask whether we are able to generate any of the other poles of this Yangian invariant. This turns out to be infinite. However, after a relatively small number of mutations, one finds that all mutations are exhausted apart from those corresponding to the 1-dimensional infinite sub-affine-A_2 sequences. Each mutation in these sequences produces Plücker polynomials of increasing degree, exhausting the possibility of generating any of the poles of equation (3.7). One might wonder[16] whether these mutations cover all possible clusters containing the two letters (3.9) we began with. The answer is positive thanks to [12, Theorem 6.2]. This indeed guarantees that for *any* skew-symmetrisable cluster algebra, the seeds whose clusters contain a given collection $\mathcal{A}$-coordinates form a connected subgraph of the exchange graph of the cluster algebra.

4. Patterns in leading and Landau singularities

In this section, we state the main conjecture of this work. We enhance the tree-level cluster adjacency of Yangian invariants explored in Section 3 to include information of loop-level singularities, i.e., Landau singularities. In particular, we provide evidence that all poles of a Yangian invariant in a given cut and the corresponding Landau singularity can be found together in a cluster.

Cluster adjacency seems to know about compatibility between different singularities or, equivalently, between boundaries. We have seen at tree-level how the collection of poles of a Yangian invariant (or, equivalently, of their boundaries) corresponds to cluster variables in a common cluster. One can naturally extend this compatibility, thinking of a Yangian invariant as being located "inside" a given leading singularity. Algebraically, this means that it can be used as an addend to express the leading singularity. Geometrically, this means literally that the Yangian is inside the codimension-$4L$ boundary of the loop amplituhedron which corresponds to the maximal cut giving the leading singularity, as explained in Section 2.2. By Landau analysis, we have seen how this boundary of the loop amplituhedron (equivalently, the leading singularity) is accessed by the *integrated* amplitude having a branch points in the corresponding Landau singularity. Vice-versa, given a Landau singularity which corresponds to branch points of the integrated amplitude, by "reverse" Landau analysis we can list

[16] We are grateful to Andrew McLeod for raising this question.

the maximal cuts of the integrand which are responsible for these singularities. The leading singularities of these maximal cuts will be then expressed in terms of Yangian invariants, which themselves have certain poles. Cluster algebras seem to tell us that we can find the Landau singularity *and* all the poles of a given Yangian as above in a common cluster.

Let us state our conjecture more explicitly. Given a maximal cut $\mathcal{C}$ of an L-loop n-point N^{k}MHV amplitude and a branch of its solutions $\mathcal{L}^*$, let LaS[$\mathcal{C}, \mathcal{L}^*$] be the corresponding Landau singularity and let LeS[$\mathcal{C}, \mathcal{L}^*$] be the corresponding leading singularity, as defined in Sections 2.2 and 2.3. Let us express them as

$$\mathrm{LaS}[\mathcal{C}, \mathcal{L}^*](z) = \prod_{t=1}^{N} a_t(z), \quad \mathrm{LeS}[\mathcal{C}, \mathcal{L}^*] = \sum_i \mathcal{Y}_i,$$

where $\{a_1(z), \dots, a_N(z)\}$ and the poles of the n-point N^{k}MHV Yangian invariants $\mathcal{Y}_i$ are $\mathcal{A}$-coordinates of the $\mathrm{Gr}(4, n)$ cluster algebra. Then we conjecture:

Conjecture 4.1. *$\{\mathcal{Y}_i, a_1, \dots, a_N\}$ are cluster adjacent, i.e., all the poles of $\mathcal{Y}_i$ and $a_1, \dots, a_N$ can be found in a common cluster of the* $\mathrm{Gr}(4, n)$ *cluster algebra.*

This refers to *any* Yangian invariant $\mathcal{Y}$ that can be used to represent the given leading singularity LeS.

We will refer to the cluster adjacency predicted by this conjecture as the *LL-cluster adjacency* (i.e., leading and Landau singularities cluster adjacency). In this paper, we checked for all amplitudes up to one-loop and 9-point (both NMHV and N^{2}MHV) ones that LL-cluster adjacency (4.1) holds true. We leave the checks for higher loops or points for future work.

Yangian invariants from the loop amplituhedron. For an L-loop n-point N^{k}MHV amplitude, let $\mathcal{C}$ be a maximal cut and $\mathcal{L}^*$ one branch of its solutions. Then we can directly use the definition of the loop amplituhedron to determine whether a given Yangian invariant $\mathcal{Y}$ can be used to express the corresponding leading singularity LeS[$\mathcal{C}, \mathcal{L}^*$]. In geometric terms, this means that the Yangian invariant $\mathcal{Y}$ is inside the codimension-$4L$ boundary $\mathcal{B}[\mathcal{C}, \mathcal{L}^*]$ of the loop amplituhedron $\mathcal{A}_{n,k}^{(L)}$.

As mentioned in equation (2.16), on the maximal cut $\mathcal{C}$ and on the branch of solutions $\mathcal{L}^*$, the loop momentum twistors are localised in terms of twistors of external kinematic,

$$\mathcal{L}^{(l)^*} = D^{(l)^*}\big(\langle z_{i_1} z_{i_2} z_{i_3} z_{i_4}\rangle\big) \cdot z, \quad l = 1, \dots, L, \tag{4.1}$$

where $D^{(l)^*}$ are $2 \times n$ matrices depending on Plückers coordinates of z, where z is the $n \times 4$ matrix whose rows are the momentum twistors of the external kinematics z_i.

On the amplituhedron side, on the boundary $\mathcal{B}[\mathcal{C},\mathcal{L}^*]$, the loop momentum twistors are localised as

$$\mathcal{L}^{(l)^*} = D^{(l)^*}\big(\langle Y Z_{i_1} Z_{i_2} Z_{i_3} Z_{i_4}\rangle\big) \cdot Z, \quad l = 1, \dots, L,$$

where $D^{(l)^*}$ are the same as in equation (4.1), however their dependence on brackets $\langle z_{i_1} z_{i_2} z_{i_3} z_{i_4}\rangle$ of momentum twistors has been uplifted in the amplituhedron into a dependence on $\langle Y Z_{i_1} Z_{i_2} Z_{i_3} Z_{i_4}\rangle$.

Let S be a $4k$-dimensional cell in $\mathrm{Gr}_+(k,n)$ with kinematic support. Then a Yangian invariant Y_S belongs to the boundary $\mathcal{B}[\mathcal{C},\mathcal{L}^*]$ if the positivity conditions in (2.2) are satisfied, i.e.,

$$\begin{pmatrix} C \\ D^{(i_1)^*}|_{Y=C\cdot Z} \\ \vdots \\ D^{(i_s)^*}|_{Y=C\cdot Z} \end{pmatrix}, \quad 0 \le s \le L, \tag{4.2}$$

are totally positive matrices for all representative matrices C in the cell S. In (4.2), $D^{(i_a)^*}|_{Y=C\cdot Z}$ denotes the matrix which depends on $\langle Y Z_{i_1} Z_{i_2} Z_{i_3} Z_{i_4}\rangle$, with Y in the image of the cell S, i.e., $Y = C \cdot Z$. As in previous sections, in order to handle positroid cells in the positive Grassmannian, we use the MATHEMATICA package `positroids.m`.

Using this procedure, by scanning over all $4k$-dimensional cells (with kinematic support) in $\mathrm{Gr}_+(k,n)$, we get a list $\{S_i\}_i$ such that $\{Y_{S_i}\}_i$ are all the Yangian invariants in the boundary $\mathcal{B}[\mathcal{C},\mathcal{L}^*]$. Finally, this means that we obtain the list of Yangian invariants $\{\mathcal{Y}_{S_i}\}_i$ which can appear as summands to represent the leading singularity $\mathrm{LeS}[\mathcal{C},\mathcal{L}^*]$.

4.1. LL-cluster adjacency for one-loop NMHV

Let us consider the case of one-loop n-point NMHV amplitudes and state the expected LL-cluster adjacencies by matching Yangian invariants in representations of a leading singularity with the corresponding Landau singularities associated to the same maximal cut. We note that our studies focus on the non-trivial cases when Landau singularities are not only products of frozen variables, which are the ones presented in Section 2.3. We will refer to Section 2.2 for the corresponding leading singularities.

The Landau singularity for the two easy-mass box cut $\mathcal{C}^E_{ij}$ is given by the product of the cluster variables $\langle i\,\bar{j}\rangle$ and $\langle \bar{i}\,j\rangle$. Whereas the leading singularities for the cut $\mathcal{C}^E_{ij}$ are $\mathcal{A}_{\mathrm{NMHV}}(i,\dots,j)$ and $\mathcal{A}_{\mathrm{NMHV}}(j,\dots,i)$, it is straightforward to see that the R-invariants which can appear in a representation of these leading singularities are just the ones of the type R_I, with I a 5-element subset of the set $\{j,\dots,i\}$ or of $\{i, \ldots, j\}$. The two-mass hard box cut $\mathcal{C}^H_{ij}$ has a Landau singularity which is just the cluster variable $\langle i, i+1, j, j+1\rangle$, whereas its leading singularities are $R_{i-1,i,i+1,j,j+1}$ and $R_{i,i+1,i+2,j,j+1}$. Since $\langle i, i+1, j, j+1\rangle$ is already a pole of both the latter two R-invariants, LL-cluster adjacency is trivially satisfied in this case. Finally, the three-mass box $\mathcal{C}_{ijk}$ has an associated Landau singularity which is $\langle i(i-1\, i+1)(jj+1)(kk+1)\rangle$ and the leading singularity is $R_{i,j,j+1,k,k+1}$.

In summary, the LL-cluster adjacency for all points one-loop NMHV relies on the following conjecture:

Conjecture 4.2. *In the* $\mathrm{Gr}(4,n)$ *cluster algebra, there are always clusters containing the following lists of* $\mathcal{A}$*-coordinates:*

$$\begin{aligned}&\big\{\partial R_I, \langle i\,\bar{j}\rangle, \langle \bar{i}\, j\rangle\big\}, \quad I \in \binom{\{j,\ldots,i\}}{5}, \binom{\{i,\ldots,j\}}{5},\\ &\big\{\partial R_{i,j,j+1,k,k+1}, \langle i(i-1\, i+1)(jj+1)(kk+1)\rangle\big\},\end{aligned} \tag{4.3}$$

where ∂R_J *denotes the list of all poles of the* R*-invariant* R_J*, and* $i < i+1 < j < j+1 < k < k+1$ *are cyclically ordered indices in* $\{1,\ldots,n\}$.

While we provide an *all-n proof* of the second type of adjacencies (4.3) in Section 4.1.4, in the following we report checks of the LL-cluster adjacencies up to 9 points, with corresponding cluster mutations, as explained in Appendix A.

4.1.1. LL-cluster adjacency for one-loop 7-point NMHV. Up to cyclic shifts, for $n = 1$ there are only 3 types of R-invariants:

$$(12),\ (13),\ (14), \quad (i_1,\ldots,i_{n-5}) := R_{[n]/\{i_1,\ldots,i_{n-5}\}}.$$

The adjacencies between Landau and leading singularities read:

$$\begin{aligned}(12) &\quad \text{is CA with } \langle 3\bar{7}\rangle, \langle \bar{3}7\rangle,\\ (13) &\quad \text{is CA with } \langle 2(13)(45)(67)\rangle.\end{aligned}$$

Both the adjacencies are manifested in the cluster polytope by the presence of a subpolytope made out of clusters that contain all active poles of the Yangian invariants and the Landau singularities. The R-invariant (12) has three active poles, and together with the Landau singularity, these correspond to four $\mathcal{A}$-coordinates. The remaining two degrees of freedom correspond to a pentagonal face of the cluster polytope, i.e., an A_2 subalgebra.

The pentagons that correspond to $\{(12), \langle 1367\rangle\}$ and $\{(12), \langle 2347\rangle\}$ share an edge, i.e., the subpolytope of two cluster that contain the poles of (12) as well as both the parity-conjugate Landau singularities. This will be a recurring feature for higher n:

R-invariant	Landau singularity	Mutation sequence	Subalgebra
(123)	$\langle 3\bar{8}\rangle\langle\bar{3}8\rangle$	(1,5,9,1,2,8,1,2,5,7,1,2,4,2,3,1,5,6)	D_5
	$\langle 4\bar{1}\rangle\langle 1\bar{4}\rangle$	(1,4,7,5,9,1,5,8,1,4,5)	D_4
(124)	$\langle 3\bar{8}\rangle\langle 8\bar{3}\rangle$	(2,6,5,8,9,4,5,4,7,3,1,2,4)	A_3
(125)	$\langle 3\bar{8}\rangle\langle 8\bar{3}\rangle$	(2,5,8,6,9,1,2,4,5,4,7,3,1,4)	$A_1 \times A_1$
(126)	$\langle 3\bar{8}\rangle\langle\bar{3}8\rangle$	(2,5,8,2,4,6,2,4,5,9,1,2,1,7,1,3)	$A_1 \times A_1$
(127)	$\langle 3\bar{8}\rangle\langle\bar{3}8\rangle$	(2,5,8,5,7,9,6,1,2,5,1,2,4,1,2,3)	A_3
	$\langle 8(71)(34)(56)\rangle$	(7,8,9,2,6,1,2,5,4,7,1,2)	D_4
(147)	$\langle 8(71)(23)(56)\rangle$	(2,3,6,7,8,9,2,5,4,7)	$A_1 \times A_1 \times A_1$

Table 1. Checks of the cluster adjacencies of $n = 8$ R-invariants and NMHV Landau singularities. The mutation sequences describe a cluster starting from the initial cluster. See Appendix A for labelling conventions. The subalgebras donate the residual freedom of mutations, which leave the collective set of poles invariant.

When the Landau analysis predicts the product of two parity-conjugate Plücker coordinates, there is a cluster that contains both of them as well as the Yangian invariant. We will omit the parity-conjugate singularity to keep notation short.

The R-invariant (13) has 4 active poles, and together with the Landau singularity $\langle 2(13)(45)(67)\rangle$, this adjacency corresponds to a line segment.

4.1.2. LL-cluster adjacency for one-loop 8-point NMHV. There are 7 cyclically inequivalent R-invariants in this case, and we find that all associated Landau singularities are cluster adjacent. In Table 1, we provide the checks for the cases that are not implied by the $n = 7$ case. We also omit the cases where the Landau singularity is a pole of the NMHV invariant.

For example, the cluster adjacency statements that

$$(123) \quad \text{is CA} \;\; \text{with } \langle 4\bar{8}\rangle, \langle\bar{4}8\rangle,$$
$$(124) \quad \text{is CA} \;\; \text{with } \langle 3(24)(56)(78)\rangle$$

follow from the adjacencies of (12) to $\langle 3\bar{7}\rangle$ and of (13) to $\langle 2(13)(45)(67)\rangle$. We also omit everywhere Landau singularities that are poles of the Yangian invariants, trivially satisfying the cluster adjacency based on that of Yangian invariants.

4.1.3. LL-cluster adjacency for one-loop 9-point NMHV. There are 14 R-invariants up to cyclic symmetry. The adjacencies we need to check along with their verifications are listed in Table 2. We note that the cluster adjacencies between Landau

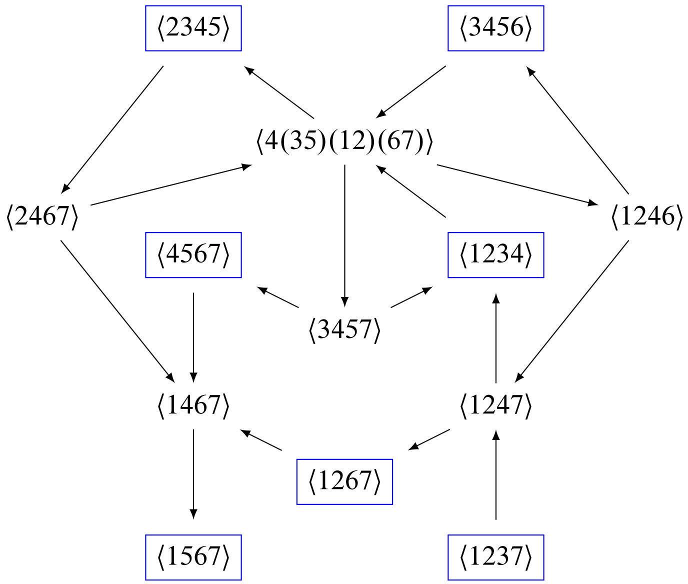

Figure 3. The quiver diagram of a $\mathrm{Gr}(4,7)$ cluster containing the poles of the R-invariant R_{12467} and the $\mathcal{A}$-coordinate $\langle 4(23)(12)(67)\rangle$. This cluster is enough to prove the LL-cluster adjacency for all one-loop NMHV amplitudes.

singularities and leading singularities at $n = 7$ and $n = 8$ are embedded in $n = 9$, as we should expect.

4.1.4. An all-n proof. It is straightforward to prove that the Landau singularities $\langle i\,(i-1 i+1)\,(j j+1)\,(k k+1)\rangle$ are cluster adjacent to the poles of the R-invariants $R_{i\,j\,j+1\,k\,k+1}$ in the strict sense, i.e., there exists a cluster that contains both this Landau singularity and all the poles of the said R-invariant in any $\mathrm{Gr}(4,n)$ cluster algebra, with n sufficiently large to accommodate the former. Without loss of generality, we can fix $j = 1$ and assume $k+1 < i-1$. All other cases are related to this case by cyclic symmetries.

We will show this by explicitly constructing such a cluster closely following [25], where the cluster adjacency of any R-invariant was proved based on partial rotations.

We first find a cluster that contains the poles of R_{12467} and $\langle 4(23)(12)(67)\rangle$ in the $\mathrm{Gr}(4,7)$ cluster algebra. This cluster can be obtained after a sequence of mutations, which we shall denote by Σ_0. The resulting cluster has the quiver diagram displayed in Figure 3.

The cluster we aim to find is just a relabelling of the cluster above, and this can be achieved through partial cyclic rotations. In particular, we need to find a sequence of rotations that maps the labels of $(1,2,3,4,5,6)$ to $(k, k+1, i-1, i, i+1, 1, 2)$.

R-invariant	**Landau singularity**	**Mutation sequence**	**Subalgebra**
(1234)	$\langle 1\bar{4}\rangle\langle 4\bar{1}\rangle$	(4,7,10)	E_7
(1235)	$\langle \bar{1}4\rangle\langle 1\bar{4}\rangle$	(2,1,4,4,10)	E_6
	$\langle 3\bar{9}\rangle\langle 9\bar{3}\rangle$	(2,1,4,4,10,11,12)	E_7
(1236)	$\langle 4\bar{1}\rangle\langle 1\bar{4}\rangle$	(3,6,9,10,11,12,1,2,1,3)	E_7
	$\langle 3\bar{9}\rangle\langle 9\bar{3}\rangle$	(3,6,9,10,11,12,1,6,1)	E_6
(1237)	$\langle 4\bar{1}\rangle\langle 1\bar{4}\rangle$	(7,1,2,1,3,6)	E_6
	$\langle 3\bar{9}\rangle\langle 9\bar{3}\rangle$	(7,1,3,1)	E_6
(1238)	$\langle 4\bar{1}\rangle\langle 1\bar{4}\rangle$	(1,2,3,5,10)	$\tilde{D}_5$
	$\langle 3\bar{9}\rangle\langle 9\bar{3}\rangle$	(1,2,3,5,11,7,10,12)	E_6
	$\langle 4\bar{9}\rangle\langle 9\bar{4}\rangle$	(1,2,3,5,7,10)	D_6
	$\langle 9(81)(45)(67)\rangle$	(1,2,3,5,6,5)	$\tilde{E}_6$
(1278)	$\langle 9\bar{6}\rangle\langle 6\bar{9}\rangle$	(5,1,2,4,7,8,5,10,2,5,2,7,8,10)	E_6
	$\langle 3\bar{9}\rangle\langle 9\bar{3}\rangle$	(5,1,2,4,7,8,5,10,2,8)	E_6
	$\langle 9(81)(34)(56)\rangle$	(5,1,2,4,7,8,5,10,2,5)	E_7
(1246)	$\langle 3\bar{9}\rangle\langle 9\bar{3}\rangle$	(2,5,7,8,1,3,6)	$A_2 \times A_2$
(1247)	$\langle 3\bar{9}\rangle\langle 9\bar{3}\rangle$	(3,4,6,8,9,1,5,1)	$A_3 \times A_2 \times A_1$
	$\langle 3(24)(56)(89)\rangle$	(3,4,6,8,9,1,6)	$D_6 \times A_1$
(1248)	$\langle 3\bar{9}\rangle\langle 9\bar{3}\rangle$	(2,6,7,4,5,8,9,12,2,5,2,6,7,9)	$D_6 \times A_1$
(1267)	$\langle 8\bar{5}\rangle\langle 5\bar{8}\rangle$	(2,5,6,1,3,1,2)	$A_4 \times A_1$
(1257)	$\langle 3\bar{9}\rangle\langle 9\bar{3}\rangle$	(3,6,7,8,9,1,6,1)	$A_3 \times A_2 \times A_2$
	$\langle 6(57)(89)(34)\rangle$	(1,4,5,3,6,3)	$A_5 \times A_1$
(1258)	$\langle 3\bar{9}\rangle\langle 9\bar{3}\rangle$	(3,4,5,6,1)	$A_3 \times A_1 \times A_1$
(1268)	$\langle 3\bar{9}\rangle\langle 9\bar{3}\rangle$	(2,5,8,7,10,1,3)	A_5

Table 2. Checks of the cluster adjacencies of $n = 9$ R-invariants and NMHV Landau singularities. The mutation sequences describe a cluster starting from the initial cluster. See Appendix A for labelling conventions. The subalgebras donate the residual freedom of mutations, which leave the collective set of poles invariant.

These rotations are

$$(1,2,3,4,5,6,7) \xrightarrow{-2|_{k+4}} (k+3,k+4,1,2,3,4,5) \xrightarrow{-3|_{i+1}} (k,k+1,i-1,i,i+1,1,2),$$

where $r|_m$ denotes r rotations in the Gr$(4,m)$ algebra. In [25], it was explained how to find a mutation sequence that realises such a transformation, and we denote this sequence by Σ_m^r. For negative r, it is understood that the mutation sequence is applied in reverse.

If we then apply the mutation sequence Σ_0 to the appropriately relabelled cluster, in other words, if we mutate the Gr$(4,n)$ initial cluster into the sequence

$$\Sigma_{i+1}^{-3}\Sigma_{k+4}^{-2}\Sigma_0,$$

we obtain a cluster which contains all the poles of the R-invariant $R_{1\,2\,k\,k+1\,i}$ as well as the letter $\langle i(i-1\,i+1)(12)(k\,k+1)\rangle$.

4.1.5. An amplitude in a manifestly LL-cluster adjacent form. In [25], it was argued that to make the adjacency of the final entries of symbols with the R-invariants of NMHV loop amplitudes, one has to expand the symbol of the amplitude over the full set of R-invariants, which satisfy linear six-term relations between them. This way of writing the amplitude is certainly not unique due to these identities, and cluster adjacency between the R-invariants and the final entries can be made manifest in a number of ways.

We can suggest our observation of the cluster adjacency of Landau singularities and R-invariants as a further constraint on the final entry condition. More precisely, we can rule out any final entry – R-invariant pairs that are not related to each other through LL-cluster adjacency.

It turns out that the one-loop NMHV amplitude can be uniquely fixed in a form in which it obeys the adjacency discussed above,

$$\begin{aligned}\mathcal{A}_{1,7}^{\text{BDS-like},(1)} = &-(13)[a_{11}\otimes a_{62}+a_{13}\otimes a_{62}]\\ &+(14)[-a_{11}\otimes a_{11}+a_{11}\otimes a_{14}+a_{14}\otimes a_{11}-a_{14}\otimes a_{14}]\\ &+(12)[a_{11}\otimes a_{15}-a_{11}\otimes a_{22}-a_{11}\otimes a_{31}+a_{12}\otimes a_{15}\\ &\qquad -a_{12}\otimes a_{22}-a_{12}\otimes a_{31}-2a_{15}\otimes a_{15}\\ &\qquad +a_{15}\otimes a_{22}+a_{15}\otimes a_{31}]+\text{cyclic},\end{aligned}$$

where the notation a_{ij} for the symbol letters follows the literature on 7-point amplitudes.

It would be interesting to show that any one-loop NMHV amplitude can be written in such a way. Then one may speculate whether this leads to a final entry condition for a given MHV degree and loop order.

4.2. LL-cluster adjacency for one-loop N^2MHV

We now use results from Section 3, in particular the lists of poles of (rational) N^2MHV Yangian invariants expressed as cluster coordinates, to test LL-cluster adjacency at one-loop for N^2MHV amplitudes. Moreover, for a given cut, we use positivity as in equation (4.2) to get the full list of N^2MHV Yangian invariants which appear in a representation of the corresponding leading singularity. For example, if we consider the two-mass hard box cut $\mathcal{C}^H_{15}$ and the branch as in equation (2.17), then for 8 points, we find a list of six N^2MHV Yangian invariants, whereas for $n = 9$ and the same cut and branch, we find that there are 21. Each of these N^2MHV Yangian invariants has poles which can be found in the same cluster together with the Landau singularity of the corresponding cut in equation (2.18), i.e., $\langle 1256\rangle$.

$n = 7$. This case is related to the $n = 7$ NMHV case discussed above through parity conjugation. Up to cyclic shifts, for $n = 7$ there are only 3 types of Yangian invariants $\mathcal{Y}_{1,2,3}$, which are parity conjugates of (12), (13) and (14), respectively. Their poles have been explicitly presented in Section 3.1.

For these Yangian invariants, we only have the following associated Landau singularity that is not implied by a case worked out earlier in the paper:

Yangian invariant	**Landau singularity**	**Mutation sequence**	**Subalgebra**
$\mathcal{Y}_1$	$\langle 3\bar{6}\rangle, \langle 6\bar{3}\rangle$	(3)	A_1
$\mathcal{Y}_2$	$\langle 4(12)(35)(67)\rangle$	(6,5,4,1,2)	A_1

where, as before, the mutation sequences describe a cluster proving the cluster adjacency.

$n = 8$. There are 24 Yangian invariants up to cyclic symmetry. We see that for some of the Landau singularity – Yangian invariant pairs, cluster adjacency is implied either by checks for $n = 6$ and $n = 7$ or by the cluster adjacency of the Yangian invariant itself when the Landau singularity is a pole of the former. The remaining cases are listed in the table below together with the clusters that contain of all said singularities:

Yangian invariant	**Landau singularity**	**Mutation sequence**	**Subalgebra**
$\mathcal{Y}_1$	$\langle 1378\rangle$	(2,5,8,6,9,1,2,4,5,1,4,7)	$A_3 \times A_2$
$\mathcal{Y}_{10}$	$\langle 8(71)(23)(56)\rangle$	(7,8,9,3,6,2,5,7,1,4)	$A_3 \times A_1$
$\mathcal{Y}_{14}$	$\langle 7(68)(23)(45)\rangle$	(1,5,9,3,5,6,1,2,3,4,5,4,8,7)	$A_1 \times A_1$
$\mathcal{Y}_{18}$	$\langle 8(71)(23)(45)\rangle$	(7,8,9,4,5,6,3,1,2,7,8,1,4,7)	$A_1 \times A_1$

We have also checked the cluster adjacency properties for Landau singularities and Yangian invariants of N^{2}MHV $n = 9$ one-loop amplitudes. These considerations are too lengthy to present here and we refer to the ancillary file `LLCAk2n9.m`.

5. Conclusions and outlook

Cluster phenomena have become increasingly relevant in understanding singularities of scattering amplitudes. The remarkable observation that building blocks of scattering amplitudes in planar $\mathcal{N} = 4$ SYM satisfy a property called *cluster adjacency*, provided both paths to understand their deep mathematical structures and tools to perform computations which otherwise would be beyond reach. At tree-level, scattering amplitudes are rational functions whose singularity structure is encoded in the location of its poles. They can be expressed as sums of Yangian invariants, which have their own singularities, some of which are “spurious” as they do not appear in the final amplitude. Nevertheless, collections of all poles of each Yangian invariant which can appear in a representation of tree-level scattering amplitudes seem themselves to be part of a beautiful mathematical story.

In this paper, we argued for an enhancement of the phenomenon of cluster adjacency of Yangian invariants to include singularities of loop amplitudes in $\mathcal{N} = 4$ SYM. In particular, via an amplituhedron-based approach, we observed a new manifestation of cluster adjacency for leading and Landau singularities, which we called “LL-cluster adjacency” for brevity. Given a maximal cut of a loop amplitude, the corresponding Landau singularities are found in the same cluster as the poles of each Yangian invariant which can appear in a representation of the leading singularity related to the cut. Moreover, we checked LL-cluster adjacencies for all one-loop amplitudes, both NMHV and N^{2}MHV, up to 9 points. Interestingly, one-loop NMHV 7-point amplitude are uniquely fixed by LL-cluster adjacencies, once these are interpreted as a final-entry conditions. On the way, we proved that all N^{2}MHV Yangian invariants corresponding to generalised triangles are cluster adjacent, confirming the conjectures of [25,42]. We also show that, for Yangian invariants of the four-mass box type, the poles of the rational sum of their algebraic terms violate cluster adjacency.

Studies of cluster adjacency of Yangian invariants [39, 42] motivate the question of whether this phenomenon should be regarded as a built-in mathematical feature of Yangian invariants that is by their definition, or whether it is a physical constraint. While cluster adjacency may be a mathematical fact for rational Yangian invariants, the inclusion of Landau singularities is certainly a new, “physical” information, just like extended-Steinmann conditions on symbol letters. Our observation calls for a geometric understanding that unifies all the related incarnations of cluster adjacency and makes manifest how the more physical ones are implied by the mathematical ones and vice versa.

At each loop L and helicity sector k, LL-cluster adjacencies provide a natural set of pairings between Yangian invariants and symbol letters of the corresponding Landau singularities. This set is in general much smaller than the full set of adjacencies obtained from $\mathrm{Gr}(4,n)$ cluster algebras, which is loop- and helicity-agnostic. It would be interesting to see if LL-cluster adjacencies could be interpreted as *refined* set one can use to contain amplitudes at fixed loop order and MHV degree, instead of relying on the full cluster algebra. We provided an example of how this principle can be interpreted as a final-entry condition and fix the $n = 7$ one-loop amplitude. Such a principle would be even more restrictive than the recently proposed truncations of infinite cluster algebras [6, 26, 35], but without further examples with higher multiplicity and loop order, it is merely a wishful speculation.

On this regard, extending our analysis to non-rational Yangian invariants and Landau singularities corresponding to algebraic letters could be natural direction to pursue. There have been many promising results on how to understand algebraic letters in a cluster algebra fashion with the help of tropical positive Grassmannians [6, 26, 35]. However, a full understanding of $\mathrm{Gr}(4,n)$ infinite cluster algebras is still missing, e.g., notions of "adjacencies" involving algebraic letters have still to be defined.

Our work is in the direction of making steps towards answering the long-standing question of how the cluster structure of integrands in $\mathcal{N} = 4$ SYM is related to the cluster structure of the integrated amplitudes. The manifestation of the physical information carried by LL-cluster adjacencies which relates leading singularities with Landau singularities shows further evidence that cluster phenomena know about the mathematical structure encoding (the singularities of) loop amplitudes.

A. Initial clusters and the encoding of mutations

To prove the cluster adjacency properties we claim the hold, we present clusters containing these poles as the results of a sequence of mutations starting from the initial cluster.

We enumerate the active nodes of the initial cluster, starting from $\langle 1235\rangle$ going downwards and continuing in the second column starting with $\langle 1236\rangle$, numbered 4. In Figure 4, we remind the reader the initial cluster for $\mathrm{Gr}(4,n)$ and describe this way of labelling the nodes. Clearly, the mutation sequence that relates two clusters is not unique.

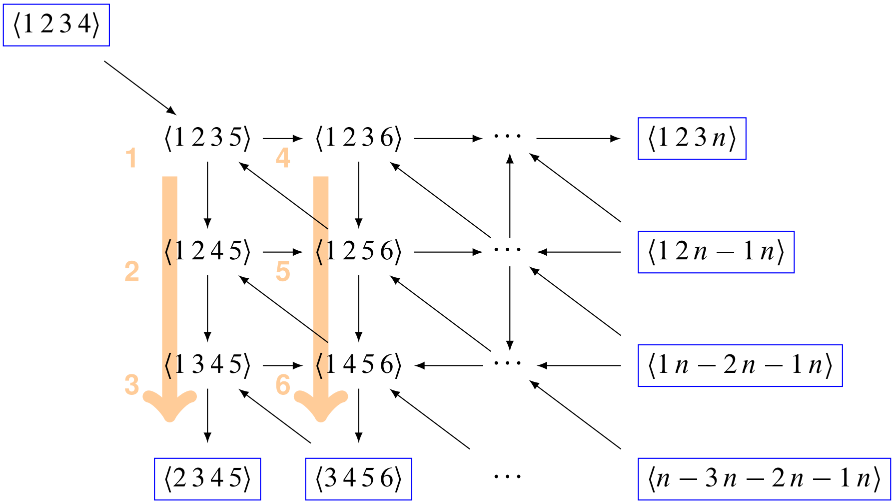

Figure 4. Initial cluster for $\mathrm{Gr}(4,n)$ and a numbering of its nodes to encode mutation sequences.

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