Planar binary trees in scattering amplitudes

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These notes are a written version of my talk given at the CARMA workshop in June 2017, with some additional material. I presented a few concepts that have recently been used in the computation of tree-level scattering amplitudes (mostly using pure spinor methods but not restricted to it) in a context that could be of interest to the combinatorics community. In particular, I focused on the appearance of planar binary trees in scattering amplitudes and presented some curious identities obeyed by related objects, some of which are known to be true only via explicit examples.

1. Planar binary trees

The basic ingredients in the following discussions are the planar binary trees (pb trees). Recall that a planar tree is binary if every vertex is cubic (or trivalent), with one root and two leaves. It is customary to denote by PBT\(_n\) the set containing all planar binary trees with \(n\) leaves. Their sizes are given by the Catalan numbers; \(C_{n-1} = 1, 1, 2, 5, 14, 42, \ldots\) For example [1],

\[
PBT_1 = \{\} , \ PBT_2 = \{ \, \} , \ PBT_3 = \{ \, \, \, \} , \ PBT_4 = \{ \, \, \, \, \, \, \} .
\]

Let us now successively add more structure to planar binary trees. The motivation for doing this comes from the physics of scattering amplitudes but for the moment let us focus on their intrinsic combinatorial value.

In the subsequent discussions words are composed of permutations from the alphabet of natural numbers and will be written in upper case (e.g. \(A = 14532\)) while letters will be written in lower case (e.g. \(i = 3\)). The length of a word \(A\) is denoted \(|A|\). The generalized momenta \(k_A^m\) and the generalized Mandelstam variables \(s_P\) are defined as

\[
k_A^m = k_{a_1}^m + k_{a_2}^m + \cdots + k_{a_{|A|}}^m , \quad s_P \equiv \frac{1}{2} k_P \cdot k_P , \quad k_i \cdot k_j \equiv s_{ij} = s_{ji}, \quad (1.1)
\]

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where the momentum for a single letter squares to zero, $k_i \cdot k_i = 0$. For example $k_{12} \cdot k_3 = (k_1 \cdot k_3 + k_2 \cdot k_3) = s_{13} + s_{23}$ as well as $s_{123} = s_{12} + s_{13} + s_{23}$. In addition, every labelled object or function will be considered linear in words, for example $T_{123+321} \equiv T_{123} + T_{321}$.

This is also extended to cases such as

$$b\left(\frac{123}{s_{12}} + \frac{231}{s_{23}}\right) \equiv \frac{1}{s_{12}} b(123) + \frac{1}{s_{23}} b(231).$$  \hspace{1cm} (1.2)

1.1. Planar binary trees and Mandelstam variables

Let us associate to each pb tree a rational function of $s_{ij}$ following a recursive setup similar to that of Garsia [2]: to each word $P$ from the alphabet $X = \{1, 2, \ldots, n\}$ we let the pair $(P, T)$ represent the tree in which the letters of $P$ are successively assigned to the leaves of $T$ from left to right. Now let $T_1$ and $T_2$ be the left and right subtrees of $T$ and let $P_1$ and $P_2$ be their corresponding words such that $P = P_1 P_2$. The map from the tree $T$ to a function of $s_{ij}$ is defined by,

$$\phi(P, T) \equiv \frac{1}{s_P} \phi(P_1, T_1) \phi(P_2, T_2), \quad \phi(i, T) \equiv i \hspace{1cm} (1.3)$$

For example, the action of the map (1.3) on the two pb trees in PBT$_3$ is depicted in fig. 1.

Now let me illustrate a common theme in the discussions to follow. Suppose we are interested in the image of the map (1.3) not for an individual tree but for the sum over all pb trees in PBT$_n$. While it is straightforward to sum $\phi(P, T_j)$ over all pb trees in PBT$_n$, there is another way to get the answer: drop the tree specification $\phi(P, T) \equiv \phi(P)$ and evaluate the following recursion [3],

$$\phi(P) \equiv \frac{1}{s_P} \sum_{XY=P} \phi(X) \phi(Y), \quad \phi(i) \equiv i, \quad \phi(\emptyset) \equiv 0, \hspace{1cm} (1.4)$$

where $\sum_{XY=P}$ denotes the sum over all deconcatenations of the word $P$ into $X$ and $Y$. If we denote by $C_n$ the number of terms in the expansion of $\phi(12\ldots n+1)$, it is easy to see that (1.4) gives rise to the recurrence relation for the Catalan numbers, $C_0 = 1, C_{n+1} =$
\[ \sum_{i=0}^{n} C_i C_{n-i} \]. Therefore all the pb trees with \( n \) leaves can be generated by considering the deconcatenation of words of length \( n \). The first few expansions of (1.4) are given by

\[ \phi(1) = 1, \quad \phi(12) = \frac{1}{s_{12}}, \quad \phi(123) = \frac{1}{s_{12}s_{123}} + \frac{1}{s_{23}s_{123}}, \]

\[ \phi(1234) = \frac{1}{s_{1234}} \left( \frac{1}{s_{23}s_{123}} + \frac{1}{s_{34}s_{234}} + \frac{1}{s_{23}s_{234}} \right). \]

The definition (1.3) resembles the map \( \psi(T) \) defined by Chapoton in Proposition 3.2 of [4], but unfortunately they are not equivalent. In any case, as discussed in [4] the map \( \psi(T) \) gives rise to a mould [5], so one may ask similar questions here. As we will see below, one can modify the recursion (1.4) to obtain an alternate mould of planar binary trees.

1.2. An alternate mould of planar binary trees

A variation of the recursion (1.4) gives rise to an alternate mould of planar binary trees. Define \( \phi(P|Q) \) in terms of two words \( P \) and \( Q \) recursively as [3],

\[ \phi(P|Q) = \frac{1}{s_{P|Y=A}} \sum_{X=A} \left( \phi(X|A) \phi(Y|B) - (X \leftrightarrow Y) \right), \quad \phi(i|j) = \delta_{ij}, \quad \phi(\emptyset|B) = \phi(A|\emptyset) \equiv 0 \]

(1.6)

where \( \delta_{ij} = 1 \) if \( i = j \) and 0 otherwise. Note that \( \phi(P|Q) = \phi(Q|P) \). The first instances at multiplicity two are given by \( \phi(12|12) = 1/s_{12} = \phi(21|21) \) and \( \phi(12|21) = -1/s_{12} \), while at multiplicity three we have,

\[ \phi(123|123) = \frac{1}{s_{123}} \left( \frac{1}{s_{12}} + \frac{1}{s_{23}} \right), \quad \phi(123|132) = -\frac{1}{s_{23}s_{123}}, \quad \phi(123|213) = -\frac{1}{s_{12}s_{123}}, \]

\[ \phi(123|321) = \frac{1}{s_{123}} \left( \frac{1}{s_{12}} + \frac{1}{s_{23}} \right), \quad \phi(123|231) = -\frac{1}{s_{23}s_{123}}, \quad \phi(123|312) = -\frac{1}{s_{12}s_{123}}. \]

It follows from the antisymmetric deconcatenation in (1.6) that \( \phi(P|Q) \) satisfies the defining symmetry of an alternate mould [5],

\[ \phi(P|A \sqcup B) = \phi(A \sqcup B|Q) = 0, \quad \forall A, B \neq \emptyset, \]

(1.7)

where the shuffle product is defined by

\[ \emptyset \sqcup A = A \sqcup \emptyset = A, \quad A \sqcup B \equiv a_1(a_2 \ldots a_n \sqcup B) + b_1(b_2 \ldots b_m \sqcup A). \]

(1.8)

The identity (1.7) can be proved by induction [6] using the linearity of \( \phi(P|Q) \).

For the physics motivation: the construction of the map \( \phi(P|Q) \) in [3] followed the pioneering work of [7] where a similar map of planar binary trees was proposed and used to obtain the tree-level scattering amplitudes of a theory of bi-adjoint scalars.

\[ 1 \] In [4] the pb trees are mapped to variables \( 1/u_i \) defined by the intervals between sequential leaves, while the Mandelstam variables \( s_P \) may contain arbitrary leaves (such as \( s_{13} \)).
1.3. Planar binary trees and nested bracketings

It is well known that each pb tree can be mapped to a Lie polynomial in the Free Lie Algebra of the alphabet labelling its leaves [2,8]. For example, the trees in fig. 1 are mapped to the words $[[1,2],3] = 123 - 213 - 312 + 321$ and $[1,[2,3]] = 123 - 132 - 231 + 321$. So let us modify the map (1.3) of individual pb trees to also include bracketed words,

$$b(P, T) \equiv \frac{1}{s_P} \left[ b(P_1, T_1), b(P_2, T_2) \right], \quad b(i, T) \equiv i.$$  \hfill (1.9)

The setting is the same as in (1.3): the tree $T$ is decomposed in terms of its left $T_1$ and right $T_2$ subtrees with $P_1$ and $P_2$ denoting the subwords labelling their leaves. For example, the two pb trees from fig. 1 are now mapped to the expressions seen in fig. 2.

The map (1.9) can be extended to a sum over all pb trees in $\text{PBT}_n$ by deconcatenation: we drop the tree specification $b(P, T) \rightarrow b(P)$ and evaluate the following recursion:

$$b(P) = \frac{1}{s_P} \sum_{X, Y = P} \left[ b(X), b(Y) \right].$$  \hfill (1.10)

Just like (1.4), the deconcatenations generate all trees in $\text{PBT}_n$; but this time they are dressed with bracketed words and Mandelstam variables. For example,

$$b(1) = 1, \quad b(12) = \frac{[1,2]}{s_{12}}, \quad b(123) = \frac{[[1,2],3]}{s_{12}s_{123}} + \frac{[1,[2,3]]}{s_{23}s_{123}},$$  \hfill (1.11)

and see fig. 3 for the expression of $b(1234)$. The same mechanism used in proof of (1.7) can be used to prove that the recursion (1.10) satisfies,

$$b(A \sqcup B) = 0 \quad \forall A, B \neq \emptyset.$$  \hfill (1.12)

Therefore the additional bracketing structure in the numerators does not spoil the alternal mould symmetry of the pb trees from (1.6).
2. Berends–Giele currents

Apart from dressing pb trees with Mandelstam variables and Lie polynomials, even more structure can be added to them. In doing so, we obtain objects with direct relevance to the computation of tree-level amplitudes with the pure spinor formalism. They led to compact expressions for the amplitudes of both the open superstring and its field-theory limit [9,10].

2.1. Multiparticle unintegrated vertices

Let us briefly recall the existence of multiparticle unintegrated vertices $V_P$; a generalization of the vertex $V_i$ that plays a fundamental role in the pure spinor formalism [11]. They are defined recursively in a manner described in [12] but let us focus only on their high-level properties and leave aside the particularities of their assembly.

The vertices $V_P$ can be characterized by the symmetry relations they satisfy: the generalized Jacobi identities as defined in [13] (also referred to as Lie symmetries in [12]),

$$V_{A\ell(B)} + V_{B\ell(A)} = 0, \quad A, B \neq \emptyset, \quad \forall C,$$

where $\ell(A)$ is the left-to-right bracketing defined recursively by

$$\ell(123\ldots n) \equiv \ell(123\ldots n-1)n - n\ell(123\ldots n-1), \quad \ell(i) \equiv i.$$

For example, $V_{1234C} + V_{2143C} + V_{3412C} + V_{4321C} = 0$, for any word $C$. In addition, the vertices $V_P$ are Grassmann-odd, $V_PV_Q = -V_QV_P$. Moreover, with the understanding that a word $P$ inside $V_\_\_$ stands for $\ell(P)$ and using the notation $V_{\ell(123\ldots n)} \equiv V_{123\ldots n}$ it is always possible to rewrite arbitrary bracketings within $V_\_\_$ in terms of $V_P$ with unbracketed $P$, using Baker’s identity [13]. For example, $V_{[A,B]} = V_{A\ell(B)}$ implies that $V_{[1,[2,3,4]]} = V_{1234} - V_{1324} - V_{1423} + V_{1432}$. In particular, one can always fix the first letter of $V_P$ using

$$V_{A\ell(B)} = -V_{\ell(A)B}, \quad A \neq \emptyset.$$

Therefore the number of independent $V_P$ at multiplicity $n$ is $(n-1)!$, in agreement with the dimension of multilinear Lie polynomials$^2$ as stated in section 5.6.2 of [13].

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$^2$ A Lie polynomial is called multilinear when its words are restricted to be permutations.
2.2. Planar binary trees and nested bracketings of $V_P$

The discussions above can be understood in the context of Free Lie Algebras. However, in the setting of scattering amplitudes with pure spinor methods, the bracketed words in the definition (1.10) are replaced by vertices $V_\ldots$ with corresponding bracket structure. For example, the word expansions in (1.11) become Berends–Giele currents \cite{12}

$$M_1 = V_1, \quad M_{12} = \frac{V_{[1,2]}}{s_{12}}, \quad M_{123} = \frac{V_{[[1,2],3]}}{s_{12}s_{123}} + \frac{V_{[1,[2,3]]}}{s_{23}s_{123}}. \tag{2.4}$$

Obviously, the alternal mould property continues to hold and we get

$$M_{A\sqcup B} = 0, \quad M_{AiB} = (-1)^{|A|}M_{i(A\sqcup B)}, \quad \forall A, B \neq \emptyset, \tag{2.5}$$

where the second identity (henceforth called Schocker’s identity) was proven in \cite{14} and implies that $M_P$ for words of length $n$ admits a $(n-1)!$ dimensional basis.

Alternatively, the Berends–Giele currents $M_P$ can be defined via a product of $\phi(A|B)$ and unbracketed superfields $V_B$ \cite{3}:

$$M_A = \sum_B \frac{1}{|B|} \phi(A|B)V_B = \sum_C \phi(A|iC)V_{iC}. \tag{2.6}$$

The alternal mould symmetry of $\phi(A|B)$ identifies the sum over $B$ as that of a Lie polynomial \cite{15}. This means that the sum over the $|B|!$ permutations are reduced to a sum over $(|B|-1)!$ cyclic permutations of the form $B = iC$, cancelling the overall factor $1/|B|$. Assuming the equivalence between the definitions (1.10) and (2.6) allows to infer a different representation for $\phi(P|Q)$ as compared to (1.6),

$$\phi(P|Q) = \langle P, b(Q) \rangle, \tag{2.7}$$

where $\langle A, B \rangle = \delta_{A,B}$ is the scalar product of words and $\delta_{A,B} = 1$ if $A=B$ and 0 otherwise. For example, the expansion in (1.11) together with $\langle 213, [[1,2],3] \rangle = -1$ and $\langle 213, [1,[2,3]] \rangle = 0$ implies

$$\phi(213|123) = \langle 213, b(123) \rangle = -\frac{1}{s_{12}s_{123}}. \tag{2.8}$$

After defining

$$\Phi(A|B), \equiv \phi(iA|iB) \tag{2.9}$$
the definition (2.6) can be rewritten in the form of the so-called \( BG \)-map:

\[
M_{iA} = \sum_B \Phi(A|B)_i V_{iB} .
\]  

(2.10)

The first few examples of (2.9) are \( \Phi(2|2)_1 = \frac{1}{s_{12}} \) and

\[
\begin{align*}
\Phi(23|23)_1 &= \frac{1}{s_{12}s_{13}} + \frac{1}{s_{23}s_{12}}, & \Phi(23|32)_1 &= -\frac{1}{s_{23}s_{12}}, \\
\Phi(32|32)_1 &= \frac{1}{s_{13}s_{12}} + \frac{1}{s_{23}s_{12}}, & \Phi(32|23)_1 &= -\frac{1}{s_{23}s_{12}},
\end{align*}
\]

(2.11)

The above definition motivates the following question: Can we obtain a relation analogous to (2.10) where \( V_{iA} \) is written in terms of \( M_{iB} \)? In other words, can we invert \( \Phi(A|B)_i \)?

2.3. The KLT matrix as the inverse of the BG map

We have seen that the alternate mould \( \phi(A|B) \) can be used to map the superfields \( V_B \) (with unbracketed words) into the Berends–Giele currents \( M_A \); we are now going to consider its inverse map. We will encounter a fascinating object called the KLT matrix \( S(A|B)_i \) whose origins date back to the 80s when a relation between amplitudes of closed and open strings was found [16]. The precise relation of [16] was subsequently formulated in terms of a KLT matrix in the field-theory limit in [17] and later given its full string-theory version in [18], with a slight reformulation in [19]. In the following we will utilize a recent recursive definition given in [20].

More precisely, let \( S(A|B)_i \) for words \( A, B \) and letter \( i \) denote a symmetric matrix that vanishes if \( A \) is not a permutation of \( B \) and otherwise given by

\[
S(P,j|Q,j,R)_i \equiv (k_iQ \cdot k_j)S(P|Q,R)_i, \quad S(\emptyset|\emptyset)_i \equiv 1, \quad |Q| + |R| = |P| .
\]  

(2.12)

For an example application of the recursion (2.12) consider the following sequence:

\[
S(243|432)_1 = (k_1 \cdot k_3)S(24|42)_1, \quad S(24|42)_1 = (k_1 \cdot k_4)S(2|2)_1 \quad \text{and} \quad S(2|2)_1 = (k_1 \cdot k_2).
\]

Therefore \( S(243|432)_1 = (k_1 \cdot k_3)(k_1 \cdot k_4)(k_1 \cdot k_2) \). As an additional example, the entries of the symmetric \( 2! \times 2! \) matrix composed of permutations from \( A,B=23 \) with \( i=1 \) are:

\[
S(23|23)_1 = s_{12}(s_{13} + s_{23}), \quad S(23|32)_1 = s_{12}s_{13}, \quad S(32|32)_1 = s_{13}(s_{12} + s_{23}).
\]  

(2.13)

As one can easily check from the examples above, we have \( S(2|2)_1 \Phi(2|2)_1 = 1 \) as well as

\[
\begin{align*}
S(23|23)_1 \Phi(23|23)_1 + S(23|32)_1 \Phi(32|23)_1 &= 1 \quad (2.14) \\
S(23|23)_1 \Phi(23|32)_1 + S(23|32)_1 \Phi(32|32)_1 &= 0 .
\end{align*}
\]

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Following the arguments of [7] in the context of scattering amplitudes and its reformulation in terms of \( \phi(A|B) \) from [3], there is a strong expectation that this must be true in general:

\[
\sum_C S(A|C)_i \Phi(C|B)_i = \delta_{A,B} .
\] (2.15)

The sum over \( \sum_C \) instructs to sum over all words \( C \) but the condition that \( S(A|C)_i \) is zero if \( C \) is not a permutation of \( A \) leads to a finite sum. In the subsequent discussions we will obtain a more general relation that reduces to (2.15) in a particular case, leading to an alternative avenue to prove it.

### 2.3.1. KLT matrix and labelled trees

If \( s_{ij} \) is depicted as the edge between the vertices labelled \( i \) and \( j \), the entries of the KLT matrix \( S(A|B)_i \) for words \( A, B \) of length \( n \) generate all rooted labelled trees with \( n + 1 \) vertices and \( n \) edges, whose total number is \((n + 1)^n - 1\) [21].

To see this, note that the recursion (2.12) removes the letter \( j \) to generate an edge \( k_R \cdot k_j \) at each iteration for a total of \( n \) edges; in particular, \((k_i \cdot k_j)^2\) is never generated. In addition, we see from (2.12) that there is always a path from any given vertex to the vertex \( i \). Therefore the recursion (2.12) gives rise to rooted labelled trees. Conversely, if a given tree with \( n \) vertices appears in \( S(A|B)_i \), then a new tree obtained by appending an edge \( s_{j(n+1)} \) where \( j = 1, \ldots, n \) is necessarily contained in \( S(A(n+1)|B(n+1))_i = k_iB \cdot k_{n+1} S(A|B)_i \).

Relabelling the vertices if necessary, the new vertex \( n+1 \) can always be chosen to appear in a single edge of the new tree where the argument above applies, finishing the proof.

For example, the tree representation of \( S(234|423)_1 = s_{12}s_{13}s_{14} + s_{14}s_{12}s_{23} \) is:

\[
S(234|423)_1 = 2 \quad 3 \quad 4 \quad + \quad 4 \quad 1 \quad 2 \quad 3
\]

For another application, note that a symmetric \( 3! \times 3! \) matrix naively contains 21 elements. By the above proof there are only \( 4^2 = 16 \) cubic monomials of \( s_{jk} \) in the permutations of \( S(234|234)_1 \), so there must be five relations among them. An explicit search yields:

\[
S(432|234)_1 = S(342|243)_1, \quad S(423|324)_1 = S(342|243)_1 ,
\]

\[
S(432|342)_1 = S(423|342)_1 - S(342|243)_1 + S(432|324)_1 ,
\]

\[
S(432|243)_1 = S(342|243)_1 - S(423|234)_1 + S(423|243)_1 ,
\]

\[
S(432|243)_1 = S(324|243)_1 - S(324|234)_1 + S(342|243)_1 .
\]
By the same token, any other choice of the fixed letter \( i \) can be expanded in terms of a basis where \( i = 1 \).

It is amusing to note that \((n+1)^{n-1}\) is also the number of ways to factorize the cycle \((12\ldots(n+1))\) as a product of transpositions [22]. For example, the factorizations of the cycle \((123)\) corresponding to the three labelled trees with three vertices are \((123) = (12)(23) = (13)(12) = (23)(13)\) (see e.g. exercise 5.47 of [21]).

2.4. An extended KLT matrix

Given the conjectural relation (2.15) and the definition (2.6) it is not difficult to see that the KLT matrix inverts (2.6) leading to [19],

\[
V_{iA} = \sum_B S(A|B)_{i} M_{iB}. \tag{2.17}
\]

Unlike the definition (2.6) where \( \phi(\cdot|\cdot) \) can be used for arbitrary permutations of both words (thereby manifesting the alternal mould symmetry of \( M_A \)) the relation (2.17) fixes the first letter in the left-hand side to be \( i \). This is unsatisfactory since we know from (2.1) that \( V_P \) satisfies generalized Jacobi identities when all permutations of \( P \) are considered but (2.17) manifestly defines only a cyclic orbit of \( P \equiv iA \). Although nothing prevents using different choices of \( i \) on demand, a more general definition akin to (2.6) is desirable.

The lack of manifest Lie symmetry in (2.17) is due to the definition of \( S(A|B)_i \), which obviously singles out \( i \). Therefore the quest is to find a general definition for the KLT matrix without this restriction. Luckily, this can be done with the following arguments.

One can explicitly verify in examples that when \( S(P|Q)_i \) is considered as a function of permutations of the extended words \( iP,iQ \) it satisfies the following constraint:

\[
S(AjB|RjS)_i = S(\ell(iA)B|\ell(iR)S)_{j}. \tag{2.18}
\]

For example, \( S(314|314)_2 = S(234|234)_1 - 2S(234|324)_1 + S(324|324)_1 \).

The identities (2.3) and (2.18) suggest the existence of a more general KLT matrix \( S(A|B) \) with no fixed letter \( i \) that reduces to (2.12) when the first letters of \( A,B \) coincide

\[
S(iP|iQ) \equiv S(P|Q)_i. \tag{2.19}
\]

To see this, note that if this extended matrix \( S(A|B) \) satisfies Lie symmetries in both row and columns, namely (note \(|A| = |B|\)),

\[
S(\ell(A)|B) = S(A|\ell(B)) = |A|S(A|B), \tag{2.20}
\]
then the identity (2.18) is explained, according to (2.3), as a “change of basis” of multilinear Lie polynomials whose first letter is fixed to be $i$ or $j$. This observation can be exploited to define an extended KLT matrix $S(A|B)$ as a multilinear Lie polynomial in both (arbitrary) words $A$ and $B$ as follows: Without loss of generality we write $A = PiQ$ and $B = RiS$ and move the letter $i$ to the front via (2.3) to obtain,

$$S(P, i, Q|R, i, S) \equiv (-1)^{\delta_{|P|,|Q|}}(-1)^{\delta_{|R|,|S|}} S(\ell(P)Q|\ell(R)S)_i,$$  \hspace{1cm} (2.21)

where the sign factors account for the possibility of either $P$ or $Q$ being the empty word of length zero\(^3\). One can now check that (2.21) and (2.19) imply the identity (2.18):

$$S(AjB|RjS)_i \equiv S(iAjB|iRjS)_i \equiv S(\ell(iA)B|\ell(iR)S)_j \equiv S(\ell(iA)B|\ell(R)S)_j.$$  \hspace{1cm} (2.22)

For example, the entries of the extended KLT matrix for sample permutations of $A, B=123$ are given by

$$S(213|213) = S(123|123) = S(23|23)_1,$$

$$S(213|231) = S(123|123) - S(123|132) = S(23|23)_1 - S(23|32)_1,$$

which are reduced to the cases that can be computed by (2.12). Note that any common letter $i$ between $A$ and $B$ can be chosen in (2.21) because (2.18) guarantees their equality. For example, $S(213|321)$ with $i=1$ leads to $S(213|321) = S(23|32)_1 - S(23|23)_1 = -s_{12}s_{23}$ whereas $i=2$ gives $S(213|321) = -S(13|31)_2 = -s_{12}s_{23}$.

2.4.1. Extended KLT matrix as an inverse to the BG map

Using the general matrix $S(A|B)$ given in (2.21) the definition (2.17) can be promoted to

$$V_A = \sum_B \frac{1}{|B|} S(A|B)M_B.$$  \hspace{1cm} (2.24)

Given (2.20), the definition (2.24) manifests the Lie symmetries of $V_A$ and accomplishes the task initiated in the last subsection. But now the compatibility between (2.17) and (2.6) suggests a relation between $S(A|B)$ and $\phi(A|B)$. Experimentally one finds,

$$\sum_B S(A|B)\phi(B|C) = \langle \ell(A), \rho(C) \rangle,$$  \hspace{1cm} (2.25)

\(^3\) The sign in $PiQ = -i\ell(P)Q$ is negative only if $P \neq \emptyset$ as there is nothing to do in case $P = \emptyset$. We set $\ell(\emptyset) \equiv 0$ and write $PiQ = -(1)^{|P|}\cdot i\ell(P)Q$ to extend its validity also when $P = \emptyset$.\n
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where \( \ell(A) \) is defined in (2.2) while \( \rho(C) \) is given by [13]

\[
\rho(123\ldots n) \equiv 1\rho(23\ldots n) - n\rho(123\ldots n-1), \quad \rho(i) \equiv i,
\]

and \( \langle P,Q \rangle = \delta_{P,Q} \) denotes the scalar product of words. From the fact that \( \rho \) and \( \tilde{\ell} \) are adjoint maps w.r.t the scalar product together with \( \tilde{\ell}\ell(A) = |A|\ell(A) \) and \( \tilde{\rho}\rho(C) = |C|\rho(C) \) [13], it follows that the RHS of (2.25) can be written as \( |C|\langle A,\rho(C) \rangle = |A|\langle \ell(A),C \rangle \) and that it is not positive definite.

We can now demonstrate that (2.25) implies the conjectural relation (2.15).

Proposition 1. If \( \sum_C \phi(A|C)S(C|B) = \langle \rho(A) , \ell(B) \rangle \) then (2.15) is true,

\[
\sum_R \Phi(P|R)_i S(R|Q)_i = \delta_{P,Q}.
\]

Proof: The shuffle symmetry of \( \phi(A|C) \) makes the sum over all \( C \) reduce to a cyclic subset of permutations with an overall factor \( |C|=|B| \). Setting \( C \equiv iC' \), we get

\[
\langle \rho(A) , \ell(B) \rangle = \sum_C \phi(A|C)S(C|B) = \sum_{C'} |B|\phi(A|iC')S(iC'|B).
\]

Since \( \rho \) is the adjoint of the right-to-left bracketing map \( r \) and \( r(P)=|P|P \) if \( P \) is a Lie polynomial (which \( \ell(B) \) certainly is) [13]; \( \langle \rho(A) , \ell(B) \rangle = |B|\langle A,\ell(B) \rangle \). Therefore we get \( \sum_{C'} \phi(A|iC')S(iC'|B) = \langle A,\ell(B) \rangle \). Choosing \( A \equiv iA' \) and \( B \equiv iB' \) leads to

\[
\sum_{C'} \Phi(A'|C')_i S(C'|B')_i = \langle iA',\ell(iB') \rangle = \delta_{A',B'},
\]

where we used (2.9) and (2.19). To prove the last equality, note that the identity \( \ell(aP) = \sum_{X_iY_i=P}(-1)^{|X|} \bar{X}aY \) [23] implies \( \ell(iB') = iB' + \sum RiS \) with \( R \neq \emptyset \) and therefore \( \langle iA',\ell(iB') \rangle = \delta_{A',B'} \). Renaming \( A'=P,B'=Q \) and \( C'=R \) finishes the proof \( \square \).

In addition, the extended KLT matrix (2.21) satisfies

\[
S(A|b(C)) = \langle \ell(A),\rho(C) \rangle,
\]

where the \( b(C) \) map is defined in (1.10). This follows from plugging in \( \phi(B|C) = \langle B,b(C) \rangle \) into the relation (2.25) and using the definition of the scalar product \( \langle P,Q \rangle = \delta_{P,Q} \).
For example, on the one hand $\langle \ell(123), \rho(123) \rangle = 3$ while on the other hand the expansion (1.11) of $b(123)$ leads to

$$S(123|b(123)) = \frac{1}{s_{12}s_{123}} \left( S(123|123) - S(123|213) - S(123|312) + S(123|321) \right)$$

$$+ \frac{1}{s_{23}s_{123}} \left( S(123|123) - S(123|132) - S(123|231) + S(123|321) \right)$$

$$= \frac{1}{s_{12}s_{123}} \left( 3S(23|23) \right) + \frac{1}{s_{23}s_{123}} \left( 3S(23|23) - 3S(23|32) \right)$$

$$= 3,$$

where in the last step we used the expressions (2.13).

We have defined the extended KLT matrix by reducing its permutations to the standard KLT matrix via (2.19) where the recursive algorithm (2.12) can be applied. After introducing the so-called S-map defined in [12], we will obtain a direct formula to compute the entries of the extended KLT matrix without recoursing to its old definition (2.12).

2.5. The S-map and bracketed numerators of planar binary trees

It is easy to see from (1.10) that $[1, 2] = s_{12}b(12)$, but already at the next order

$$[[1, 2], 3] = s_{12}s_{23}b(123) - s_{12}s_{13}b(213),$$

$$[1, [2, 3]] = s_{12}s_{23}b(123) - s_{13}s_{23}b(132),$$

an interplay between the Jacobi identity and $s_{123} = s_{12} + s_{13} + s_{23}$ is needed to cancel all denominators. The identities in (2.32) motivate the search for a general procedure that generates the expansions on the right-hand side for any given numerator of an arbitrary pb tree. Surprisingly, an algorithm discovered in [12] (while in pursuit of other objectives) can be used to achieve precisely that.

The algorithm is based on the so-called S-map $\{A, B\}$ between words $A$ and $B$ defined as follows:

$$\{A, B\} \equiv (-1)^{|B|+1} \rho(A) \otimes^s \tilde{\rho}(B),$$

where $\rho(B)$ is defined in (2.26) and $\tilde{\rho}(B)$ denotes its reversal while $\otimes^s$ denotes a weighted concatenation product between words

$$Ai \otimes^s jB \equiv s_{ij}Ai jB.$$
The claim based on experimental data is that the map \( b(A) \) defined in (1.10) acting on a nested application of the S-map gives rise to a pb tree numerator with corresponding bracketed structure

\[
[[\ldots[i,j],k]\ldots] = b(\{\ldots\{i,j\},k\}\ldots). \tag{2.35}
\]

For example, the relations in (2.32) are obtained from

\[
[[1,2],3] = b(\{1,2\},3), \quad [1,[2,3]] = b(\{1,\{2,3\}\}), \tag{2.36}
\]

while \([[1,2],[3,4]] = b(\{\{1,2\},\{3,4\}\})\) implies

\[
[[1,2],[3,4]] = s_{12}s_{34}\left(s_{23}b(1234) - s_{24}b(1243) - s_{13}b(2134) + s_{14}b(2143)\right), \tag{2.37}
\]

which can be verified with some effort. The examples above suggest that it is convenient to define a nested left-to-right S-map by

\[
\sigma(123\ldots n) = \{\sigma(12\ldots n-1), n\}, \quad \sigma(i) = i, \tag{2.38}
\]

for example \( \sigma(123) = \{1,2\},3 = s_{12}(s_{23}123 - s_{13}213) \). Using (2.38) the conjectural relation (2.35) implies

\[
\ell(A) = b(\sigma(A)), \tag{2.39}
\]

which can be verified at high multiplicities. The S-map was originally defined in [12] in terms of Berends–Giele currents \( M_A \) using the notation \( M_{S[AB]} \equiv M_{\{AB\}} \) as follows

\[
M_{S[AB]} \equiv \sum_{i=1}^{\lvert A \rvert} \sum_{j=1}^{\lvert B \rvert} (-1)^{i+j+\lvert A \rvert-1} s_{ai} b_j M(a_1 a_2 \ldots a_{i-1} w a_i a | A| a_{i+1} \ldots a_{\lvert A \rvert}) a_i b_j (b_{j-1} \ldots b_{2i} b_{i+1} \ldots b_{\lvert B \rvert}) \tag{2.40}
\]

for \( A = a_1 a_2 \ldots a_{\lvert A \rvert} \) and \( B = b_1 b_2 \ldots b_{\lvert B \rvert} \). The equivalence between the definition (2.33) and (2.40) follows from the following general identity of words

\[
\rho(A) = \sum_{X_j Y = A} (-1)^{|Y|} (X_{\perp Y}) j, \tag{2.41}
\]

which can be proven by induction using the definitions (2.26) and (1.8).
Fig. 4 The graphical depiction of the grafting \( b(123) \lor b(45) \). The right-hand side can be expressed in terms of the S-map as \( b(\{123, 45\}) \).

2.5.1. Grafting of trees and an algebra for \( b(A) \)

Recall that the grafting operation on pb trees \( T_1 \) and \( T_2 \) is denoted \( T_1 \lor T_2 \) and gives rise to a new pb tree where the roots of \( T_1 \) and \( T_2 \) are glued together [24,25]. For example, 

\[
\begin{array}{c}
1 \\
\downarrow \\
2 \\
\downarrow \\
3 \\
\downarrow \\
4 \\
\downarrow \\
5 \\
\end{array} \lor 
\begin{array}{c}
1 \\
\downarrow \\
2 \\
\downarrow \\
3 \\
\downarrow \\
4 \\
\downarrow \\
5 \\
\end{array} = 
\begin{array}{c}
1 \\
\downarrow \\
2 \\
\downarrow \\
3 \\
\downarrow \\
4 \\
\downarrow \\
5 \\
\end{array} \lor 
\begin{array}{c}
1 \\
\downarrow \\
2 \\
\downarrow \\
3 \\
\downarrow \\
4 \\
\downarrow \\
5 \\
\end{array} = 
\begin{array}{c}
1 \\
\downarrow \\
2 \\
\downarrow \\
3 \\
\downarrow \\
4 \\
\downarrow \\
5 \\
\end{array} \lor 
\begin{array}{c}
1 \\
\downarrow \\
2 \\
\downarrow \\
3 \\
\downarrow \\
4 \\
\downarrow \\
5 \\
\end{array}.
\]

Given that each pb tree corresponds to a Lie polynomial composed of bracketed words, the grafting of trees induces a map between Lie polynomials. For example, the above grafting implies \([[[1, 2], 3] \lor [4, 5]] = [[[1, 2], 3], [4, 5]]\). An interesting observation (confirmed by explicit examples) is that the S-map seems to capture the effect of grafting all the trees and associated Mandelstam variables in \( b(A) \lor b(B) \). More precisely, 

\[
b(A) \lor b(B) = b(\{A, B\}),
\]

(2.42)
giving rise to an algebraic structure of \( b(A) \) trees.

A non-trivial example of the above algebra is obtained by considering the grafting of \( b(123) \lor b(45) \). On the one hand we get (see fig. 4), 

\[
b(123) \lor b(45) = \frac{[[[1, 2], 3], [4, 5]]}{s_{12}s_{45}s_{123}} + \frac{[[[1, 2, 3], [4, 5]]}{s_{23}s_{45}s_{123}}.
\]

(2.43)

On the other hand, the S-map between the words \( A=123 \) and \( B=45 \) is given by 

\[
\{123, 45\} = s_{34}12345 - s_{35}12354 - s_{24}13245 + s_{25}13254 - s_{24}31245 + s_{25}31254 + s_{14}32145 - s_{15}32154.
\]

(2.44)

A long calculation using the \( b(A) \) map (1.10) together with the linearity condition (1.2) yields 

\[
b(\{123, 45\}) = \frac{[[[1, 2], 3], [4, 5]]}{s_{12}s_{45}s_{123}} + \frac{[[1, [2, 3]], [4, 5]]}{s_{23}s_{45}s_{123}}.
\]

(2.45)

Therefore we see from (2.43) and (2.45) that \( b(123) \lor b(45) = b(\{123, 45\}) \).
2.6. An alternative definition for the extended KLT matrix

The introduction of the S-map in the last subsection suggests that a direct definition for the extended KLT matrix which does not rely on the standard KLT matrix as in (2.21) may be possible. The reasoning is similar to the one that led us to the relation (2.7) and exploits the fact that $V_P$ can be obtained from two different ways. Consider the example of $V_{123}$. On the one hand it can be obtained from the definition (2.24),

$$V_{123} = \sum_B \frac{1}{3} S(123|B)M_B = S(123|123)M_{123} + S(123|132)M_{132}.$$  \hspace{1cm} (2.46)

On the other hand it follows from the S-map on the Berends–Giele currents

$$V_{123} = s_{12}s_{23}M_{123} - s_{12}s_{13}M_{213} = (s_{12}s_{23} + s_{12}s_{13})M_{123} + s_{12}s_{13}M_{132},$$  \hspace{1cm} (2.47)

by exploiting the relation of $[[1, 2], 3] \rightarrow V_{123}$ and $b(123) \rightarrow M_{123}$. In the last equality we used Schocker’s identity (2.5) to rewrite $M_B$ in a basis of $M_{1B'}$. Comparing (2.46) and (2.47) leads to the expressions for $S(123|123)$ and $S(123|132)$. Note that both definitions do not necessarily rely on any particular basis of $M_{iA'}$ and are valid in general. Thus the S-map gives rise to a recipe for unlocking the expressions of $S(A|B)$ for arbitrary permutations. In fact, the considerations to be given below lead to the following proposal,

$$S(P|Q) \equiv \langle \ell(P), \sigma(Q) \rangle.$$  \hspace{1cm} (2.48)

For example, from $\ell(123) = 123 - 213 - 312 + 321$ and $\sigma(123) = s_{12}s_{23}123 - s_{12}s_{13}213$ one immediately gets $S(123|123) = s_{12}(s_{13} + s_{23})$. Higher-multiplicity examples are similarly verified.

After the experimental observation that $\sigma(AjD) = -k_A \cdot k_j j\sigma(AD) + \ldots$ where the omitted terms do not contain the letter $j$ at the last position \footnote{The definition of (2.38) implies that the last letter in $\sigma(A)$ is always the last letter of $A$.} one can see that (2.48) reduces to the recursion (2.12) for $S(Aj|CjD)_i$,

$$S(Aj|CjD)_i = \langle \ell(iA)_j, \sigma(iCD) \rangle = -k_{iC} \cdot k_j \langle \ell(iA)_j - j\ell(iA), j\sigma(iCD) + \ldots \rangle$$

$$= k_{iC} \cdot k_j \langle \ell(iA), \sigma(iCD) \rangle = k_{iC} \cdot k_j S(A|CD)_i, \quad D \neq \emptyset.$$  \hspace{1cm} (2.49)

In addition, it is straightforward to see using (2.48) and (2.7) the proof of (2.25) reduces to showing that $\langle \ell(A), \sigma(b(C)) - \rho(C) \rangle = 0$, which has been verified to high multiplicity.
A few words about the proposal (2.48) are in order. In the left-hand side of (2.47), one can interpret \( V_A \) as an “ordinary” word \( A \) but \( M_A \) in the right-hand side does not admit such an interpretation as they satisfy the shuffle symmetries (2.5). This means that one cannot read off the coefficients \( S(A|B) \) from the standard scalar product of words in a similar fashion as in (2.7); a different prescription is needed. The simplest trial is as follows: If \( S_P \) satisfies shuffle symmetries as \( S_{A\mu B} = 0 \) then we define \( \langle A, S_P \rangle_s \) between an ordinary word \( A \equiv iB \) and \( S_P \equiv S_{C_1D} \) as

\[
\langle A, S_P \rangle_s = \langle iB, S_{C_1D} \rangle_s \equiv \langle iB, (-1)^{|C|}i(\tilde{C}_{\square D}) \rangle = (-1)^{|C|}\langle B, \tilde{C}_{\square D} \rangle, \tag{2.50}
\]

in terms of the standard scalar product. Using the above definition and the identity \( \ell(iB) = \sum_{X\sqcup Y = B}(-1)^{|X|}\tilde{X}iY \) [23] one can show that

\[
\langle A, S_P \rangle_s = \langle \ell(A), P \rangle. \tag{2.51}
\]

Now define the shuffle-extension \( \sigma_s(A) \) of \( \sigma(A) \) by mapping the words in the right-hand side of (2.38) to shuffle-satisfying objects according to \( P \to S_P \). For example, \( \sigma(12) = s_{12}12 \) while \( \sigma_s(12) = s_{12}S_{12} \). Similarly \( \sigma(123) = s_{12}s_{23}123 - s_{13}s_{23}213 \) while \( \sigma_s(123) = s_{12}s_{23}S_{123} - s_{13}s_{23}S_{213} \). Using the definitions above and the intuition gained from the example (2.47) suggests that \( S(P|Q) \) can be extracted using the shuffle-aware scalar product (2.50) as \( S(P|Q) \equiv \langle P, \sigma_s(Q) \rangle_s \), which is experimentally checked to be correct. The identity (2.51) then leads to (2.48) in terms of the standard scalar product.

2.7. Deconcatenation of Berends–Giele currents

In the pure spinor formalism there is a nilpotent Grassmann-odd BRST operator \( Q^2 = 0 \) [11]. It was argued in [12] that a very interesting pattern arises in the computation of \( QV_P \):

\[
QV_1 = 0, \quad QV_{12} = (k_1 \cdot k_2)V_1V_2 \\
QV_{123} = (k_1 \cdot k_2)[V_1V_{23} + V_{13}V_2] + (k_{12} \cdot k_3)V_{12}V_3 \\
QV_{1234} = (k_1 \cdot k_2)[V_1V_{234} + V_{13}V_{24} + V_{14}V_{23} + V_{134}V_2] \\
+ (k_{12} \cdot k_3)[V_{12}V_{34} + V_{124}V_3] + (k_{123} \cdot k_4)V_{123}V_4.
\]

A non-trivial consistency check of the above identities consists in checking that the right-hand side preserves the symmetries (2.1) of the left-hand side (we use that \( V_P \) is
Grassmann-odd). It turns out that these identities admit the following generalization, as suggested from the equations of motion of the superfields defined recursively in \[12\] \((k_0 \equiv 0)\)

\[
QV_P = \sum_{\substack{P = X\cdot j \\ Y = R \sqcup S}} (k_X \cdot k_j) V_X R_j S,
\]

(2.53)

where \(Y = R \sqcup S\) represents the deshuffle of \(Y\) into the words \(R\) and \(S\). An algorithmic procedure to obtain the pairs \((R, S)\) in the sum in (2.53) follows from the map \(\delta_2(Y)\) \[13\],

\[
\delta_2(Y) = \sum_{R, S} \langle Y, R \sqcup S \rangle R \otimes S.
\]

(2.54)

For example \(\delta_2(123) = \emptyset \otimes 123 + 1 \otimes 23 + 2 \otimes 13 + 12 \otimes 3 + 3 \otimes 12 + 13 \otimes 2 + 23 \otimes 1 + 123 \otimes \emptyset\).

It turns out that the identity (2.53) gives rise to a beautiful deconcatenation formula for \(QM_P\) using the definition (2.6). For example, note that the \(1/s_{12}\) factor in the definition of \(M_{12}\) cancels the numerator from \(QV_{12} = s_{12} V_1 V_2\) so that \(QM_{12} = M_1 M_2\). Similarly and rather surprisingly one finds the precise cancellations of numerators and denominators to get \(QM_{123} = M_1 M_{23} + M_{12} M_3\). It has been experimentally checked to high multiplicities that the following fascinating identity holds true \((M_0 \equiv 0)\)

\[
QM_P = \sum_{P = XY} M_X M_Y.
\]

(2.55)

It would be desirable to prove (2.55) using the combinatorial definitions (2.6) and (2.53).

The above Berends–Giele currents have been constructed in pursuit of a general formula for the \(n\)-point scattering amplitude of super-Yang–Mills at tree-level using BRST cohomology methods \[10\]. The formula reads

\[
A(123\ldots n) = E_{123\ldots n-1} M_n, \quad E_P \equiv \sum_{P = XY} M_X M_Y,
\]

(2.56)

and has been shown in \[26\] to be the supersymmetric generalization of the standard Berends–Giele recursion given in \[27\].

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