A Lie bracket for the momentum kernel

Hadleigh Frost^{*}, Carlos R. Mafra^{α'} and Lionel Mason^{*}

, The Mathematical Institute, University of Oxford Andrew Wiles Building, ROQ, Woodstock Rd, Oxford OX2 6GG, United Kingdom

^{α'} Mathematical Sciences and STAG Research Centre, University of Southampton, Highfield, Southampton, SO17 1BJ, United Kingdom

We develop new mathematical tools for the study of the double copy and colour-kinematics duality for tree-level scattering amplitudes using the properties of Lie polynomials. We show that the S-map that was defined to simplify super-Yang-Mills multiparticle superfields is in fact a new Lie bracket on the dual space of Lie polynomials. We introduce *Lie polynomial currents* based on Berends-Giele recursion for biadjoint scalar tree amplitudes that take values in Lie polynomials. Field theory amplitudes are obtained from the Lie polynomial amplitudes by numerators characterized as homomorphisms from the free Lie algebra to kinematic data. Examples are presented for the biadjoint scalar, Yang-Mills theory and the nonlinear sigma model. That these theories satisfy the Bern-Carrasco-Johansson amplitude relations follows from the identities we prove for the Lie polynomial amplitudes and the existence of BCJ numerators.

A KLT map from Lie polynomials to their dual is obtained by nesting the S-map Lie bracket; the matrix elements of this map yield a recently proposed 'generalized KLT matrix', and this reduces to the usual KLT matrix when its entries are restricted to a basis. Using this, we give an algebraic proof for the cancellation of double poles in the KLT formula for gravity amplitudes. We finish with some remarks on numerators and colour-kinematics duality from this perspective.

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 $^{^{\}star}\,\mathrm{email:}\ \mathrm{frost@maths.ox.ac.uk}$

 $^{^{\}alpha'}$ email: c.r.mafra@soton.ac.uk

^{*}email: lmason@maths.ox.ac.uk

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1. Introduction

This paper develops Lie polynomials [1] and the combinatorics of words [2] as basic tools for the study of tree-level scattering amplitudes in QFT and string theory. We give streamlined self-contained proofs of the basic results that underpin coloured amplitudes and the double copy at tree-level using simply the elementary properties of Lie polynomials. We will see that cleanest description is in terms of the Berends-Giele currents of biadjoint scalar theory, with values in Lie polynomials.

The free Lie algebra, \mathscr{L} , is the space of linear combinations of 'Lie monomials', which are nested complete formal commutators of 'letters'; our letters will be taken to be the natural numbers, $1, 2, 3, \ldots, \mathscr{L}$ is a subspace of the space of linear combinations of 'words' formed from the natural numbers, with all letters distinct. There is a natural map from Lie monomials $\Gamma \in \mathscr{L}$ to the colour structures that appear in gauge theories, for any choice of gauge Lie algebra, and for any (single trace) gauge theory Lagrangian. There is also a correspondence between Lie monomials $\Gamma \in \mathscr{L}$, thought of as complete commutators of a word, and trivalent trees with a given root.

The double copy starts by expressing Yang-Mills tree amplitudes in the form [3]

$$A = \sum_{\Gamma} \frac{N_{\Gamma} c_{\Gamma}}{s_{\Gamma}} \,. \tag{1.1}$$

Here Γ denotes trivalent graphs, c_{Γ} denotes the corresponding colour factor¹, and s_{Γ} denotes the product of denominator propagator factors associated to the graph. The numerators N_{Γ} are functions of momenta and multilinear in the gluon polarization data. These are said to be 'BCJ numerators' if they satisfy colour kinematics duality: if $\Gamma + \Gamma' + \Gamma'' = 0$, then $N_{\Gamma} + N_{\Gamma'} + N_{\Gamma''} = 0$. In other words, the N_{Γ} are 'BCJ numerators' if $\Gamma \mapsto N_{\Gamma}$ is a homomorphism from \mathscr{L} to the kinematic data. Such numerators exist for Yang-Mills, and the key example of the double copy is that replacing c_{Γ} in (1.1) by another copy of N_{Γ} yields gravity amplitudes [4]. BCJ numerators are known for many coloured theories and can be used to obtain the tree amplitudes of any theory known to participate in the double copy. This includes gauge and gravity theories and their relatives, such as brane theories, with and without supersymmetry, see [5] for an up-to-date review of progress and references to the literature. The most basic example is to replace N_{Γ} in (1.1) by c_{Γ} : this

¹ formed from the graph by introducing the Lie algebra's structure constants at each vertex, Kronecker-deltas along each internal propagator and the external colours at the leaves.

gives the amplitudes of the biadjoint scalar theory. This theory forms the backbone of the double copy.

Lie polynomials are ubiquitous in the auxiliary structures that are used to study amplitudes, and with hindsight can be seen in the multiparticle vertex operators in conventional string theory [6], in the geometry of the space of Mandelstam variables [7], and in the CHY formulae and ambitwistor strings [8,9] via the structure of the moduli space of n-points on the Riemann sphere [10,11]. However, our aim here is to prove basic results directly using only the Lie polynomial structure.

The following is a detailed summary of results.

1.1. Berends-Giele recursion and planar binary trees

In §2 we review the properties of the vector space of Lie polynomials, \mathscr{L} . Important for the applications in this paper is the dual vector space, \mathscr{L}^* . Elements of \mathscr{L}^* can be expressed as words P modulo proper shuffles, i.e. the sum $R \sqcup S$ over ordered permutations with $R, S \neq \emptyset$.

In §3 we introduce perturbative \mathscr{L} valued fields for biadjoint scalar theory and use them to define corresponding Lie-polynomial Berends-Giele currents.² The Lie-polynomial currents b(P) satisfy a recursion [13]

$$b(P) = \frac{1}{s_P} \sum_{XY=P} [b(X), b(Y)], \qquad (1.2)$$

where s_P is the Mandelstam denoting the square of the off-shell momentum of the particles in the set $\{P\}$ and the commutator is that in \mathscr{L} . This defines a map $b: \mathscr{L}^* \to \mathscr{L}_S$ where \mathscr{L}^* encodes the colour ordering in the form of a words P up to proper shuffles, and \mathscr{L}_S is the space of Lie polynomials with coefficients in Mandelstam variables.

The currents b(P) give rise to *Lie polynomial amplitudes* obtained by removing the off-shell external propagator to give single colour ordered partial amplitudes m(Pn) valued in Lie polynomials:

$$m(Pn) := \lim_{s_P \to 0} s_P b(P) \in \mathscr{L}.$$
(1.3)

The pairing of (1.3) with an ordering gives the double colour ordered partial amplitudes of the biadjoint theory m(Pn, Qn) := (Q, m(Pn)) [14].

² The more familiar Yang-Mills case [12] is treated similarly in appendix A where the analogous objects are \mathscr{L} -valued Berends Giele currents.

We will interpret BCJ numerators N_{Γ} as homomorphisms from the free Lie algebra to appropriate functions of their kinematic data, as in [10]. The existence of such homomorphisms is not in principle guaranteed from this construction, but we will explicitly write down examples for NLSM and SYM theories in §7. All identities such as the Kleiss-Kuijf (KK) relations and the Bern Carrasco Johansson (BCJ) relations that are obeyed by b are inherited by tree-level scattering amplitudes obtained from the homomorphism.

1.2. BCJ amplitude relations and a Lie bracket

It was argued in [6,15] that BCJ amplitude relations could be expressed using the S-map defined in [6]. We will show that the S-map corresponds to a Lie bracket $\{,\}$ in the dual space of Lie polynomials and that the BCJ amplitude relations [3] follow from the identity

$$b(\{P,Q\}) = [b(P), b(Q)]$$
(1.4)

which generalizes the off-shell BCJ relations of [16]. Thus b maps the $\{,\}$ -bracket to the standard Lie bracket. Since b(P) is invertible as a map $\mathscr{L}^* \to \mathscr{L}$, this shows that $\{,\}$ is the pullback of [,] from \mathscr{L}_s to \mathscr{L}_s^* using b(P); in particular $\{,\}$ is a Lie bracket on \mathscr{L}^* .

For theories obtained from a homomorphism acting on the Lie polynomial amplitude (1.3), the BCJ relation for amplitudes follow from $m(\{P,Q\},n) = 0$ in the limit as $s_{PQ} \to 0$ as $b(\{P,Q\})$ no longer has a pole in $1/s_{PQ}$ due to (1.4).

1.3. The KLT inner product and its generalized matrix

The Kawai–Lewellen-Tye (KLT) matrix [17,18,19] is the inner product that is required to turn two sets of colour ordered Yang-Mills amplitudes into a gravity amplitude [20]. We show that its origins can be traced to the $\{,\}$ -bracket. The fact that $\{,\}$ forms a Lie bracket means that any Lie monomial Γ can be rebuilt out of $\{,\}$ in \mathscr{L}^* to form $\{\Gamma\} \in \mathscr{L}^*$. This gives our most abstract definition of the KLT kernel as the map $\mathscr{L} \to \mathscr{L}^*$ by $\Gamma \to \{\Gamma\}$; this determines the symmetric bilinear form on \mathscr{L} by the pairing $S(\Gamma_1, \Gamma_2) := (\{\Gamma_1\}, \Gamma_2)$. We show that the standard KLT matrix is most naturally understood as the components of this S in a special 'Lyndon' basis; the generalized KLT matrix of [13] is

$$S(P|Q) = (\ell\{P\}, \ell[Q]), \qquad (1.5)$$

where ℓ denotes the complete left bracketings:

$$\ell\{123...n\} := \{\ldots\{1,2\}...n\}, \quad \ell[123...n] := [\ldots[1,2]...n].$$
(1.6)

This generalized KLT matrix is symmetric and reduces to the standard KLT matrix in a Lyndon word basis of \mathscr{L}^* that singles out a special single particle.

Cachazo, He and Yuan [8] emphasize that biadjoint scalar amplitudes are in some sense the inverse to the KLT matrix, see [21]. Using the Berends-Giele amplitude formula for the biadjoint amplitudes of [14], this statement translates to the algebraic relation $\delta_{P,Q} = \sum_R S(P|R)_i b(iR|iQ)$. Using that the KLT matrix corresponds to a particular basis choice of a more fundamental KLT map, this identity will be proven in section 5.2.

1.4. Numerators and cobrackets

In §6 we show that the "contact term map" defined in [22] is the Lie co-bracket dual to the S-bracket; it gives rise to a *Lie co-algebra* structure on \mathscr{L}_{S}^{*} . As discussed in [22], the contact-term map encodes the BRST variations of local multiparticle superfield numerators satisfying generalized Jacobi identities [6] in the pure spinor formalism of the superstring [23]. These BRST variations play a central role in all recent developments in the explicit calculation of superstring amplitudes, from tree-level to 3-loops.

In §7 we discuss BCJ numerators from the perspectives of this paper. We discuss the distinctions in gauge freedoms between on-shell and Berends-Giele numerators; Berends-Giele off-shell extensions are not unique and depend on a choice of gauge and field redefinitions. Given such a choice, BCJ numerators are unique, but their locality will in general depend on the gauge choices etc.. We give a brief discussion of known numerators; the biadjoint scalar case is trivial being realized by the pairing (P, Γ) of a Lie polynomial with a word P. We give a conjecture for the non-linear sigma model (NLSM) that has now been proved elsewhere [24], and briefly describe how super-Yang-Mills (sYM), Z-theory and finally the open superstring including α' corrections fits into this framework. We end with a brief discussion of colour/kinematics duality within the framework of the Lie brackets discussed in the text.

2. Review of Lie polynomials, combinatorics on words and colour factors

Let W(A) be the vector space of linear combinations of words with non-repeated letters in the alphabet $A \subset \mathbb{N}^3$. The multilinear free Lie algebra $\mathscr{L}(A) \subset W(A)$ is the subspace

³ The definitions in this review section can be stated in the free associative algebra, in which the words may contain repetition of letters. However, in the context of scattering amplitudes we only use words that are permutations of a subset of \mathbb{N} with no repeated letters.

of W(A) linearly generated by the Lie monomials, Γ , that are defined to be complete bracketings of words with no repeated letters such as 123 - 132 - 231 + 321 = [1, [2, 3]]. We will also define $\mathcal{L}(A) \subset \mathscr{L}(A)$ to be the subspace of Lie polynomials of maximum length ($\mathscr{L}(A)$ has Lie polynomials of different lengths). In particular, we write $\mathcal{L}_{n-1} \equiv \mathcal{L}(1, 2, ..., n-1)$ to be the linear span of total bracketings of 1, ..., n-1.

The left- and right-bracketings are surjective maps from W onto \mathscr{L} given by

$$\ell[123\dots n] := [[[1,2],3],\dots,n], \qquad r[123\dots n] := [1, [2, [3,\dots, [n-1,n]\dots]]].$$
(2.1)

Clearly

$$\ell[Pi] = [\ell[P], i], \qquad r[iP] = [i, r[P]], \tag{2.2}$$

for a letter i and word P. This inductively implies Baker's identity [1]

$$\ell[P\ell[Q]] = [\ell[P], \ell[Q]].$$
(2.3)

Write |P| for the length of a word P. Then $\ell[P]$ and r[P] are related by $\ell[P] = -(-1)^{|P|}r[\overline{P}]$, where \overline{P} is the reverse of P.

2.1. The dual \mathcal{L}^* of \mathcal{L} , dual bases and their Kleiss-Kuijf relations

This section recalls the duality pairing between Lie polynomials and words defined up to shuffle products. This pairing is central to the results of the paper.

Define first the Kronecker inner product, for words $P, Q \in W$, by

$$(P,Q) := \begin{cases} 1 & \text{if } P = Q; \\ 0 & \text{otherwise.} \end{cases}$$
(2.4)

We will need the shuffle product on W, \sqcup , which is inductively defined by

$$(iP)\sqcup(jQ) := i(P\sqcup(jQ)) + j((iP)\sqcup Q), \tag{2.5}$$

for letters i, j, and words P, Q. The base case is $i \sqcup j = ij + ji$. The expression $P \sqcup Q$ is sometimes referred to as the sum over *ordered permutations* of P and Q, preserving the ordering of the letters of P and of Q. Ree's theorem characterizes \mathscr{L} in terms of the shuffle product. More precisely, $\Gamma \in W$ is a Lie polynomial iff [25]

$$(P \sqcup Q, \Gamma) = 0 \tag{2.6}$$

for all nonempty $P, Q \in W$.

If $Sh \subset W$ is the subspace spanned by all *proper shuffles*, $P \sqcup Q$ with P, Q nonempty, then Ree's theorem says that $\mathscr{L} = Sh^{\perp}$. Thus the dual vector space to \mathscr{L} is

$$\mathscr{L}^* = W/Sh. \tag{2.7}$$

We will write elements of \mathscr{L}^* as equivalence classes of the form P + Sh, for some $P \in W$. If two expressions, $P, Q \in W$ belong to the same equivalence class, write $P \sim Q$, i.e.

$$P \sim Q \quad \Leftrightarrow \quad P = Q + Sh \quad \Leftrightarrow \quad P = Q + \sum_{A, B \neq \emptyset} A \sqcup B.$$
 (2.8)

Dual bases of \mathscr{L} and \mathscr{L}^* can be obtained as follows. An element $P \in Lie^*$ can be represented by a particular expression $P \in W$ in many ways. Likewise, a Lie polynomial $\Gamma \in \mathscr{L}$ is not uniquely written as a sum of complete bracketings of words, because of the antisymmetry and Jacobi relations. It is therefore useful to find bases for \mathscr{L}^* and \mathscr{L} .

A word P is Lyndon if its first letter is also its smallest with respect to some fixed ordering of \mathbb{N} .⁴ The set of dual Lie elements, $P + Sh \in \mathscr{L}^*$, where P runs over all Lyndon words in W is a basis of \mathscr{L}^* [1]. Dually, the set of Lie monomials, $\ell[P]$, for all Lyndon words P is a basis of \mathscr{L} . These two bases are dual because, for two Lyndon words P and Q, the smallest letter must come first in both words. But, for any letter i,

$$(iP, \ell[iQ]) = (iP, iQ) = (P, Q),$$
 (2.9)

because the only term in the word expansion of $\ell[iQ]$ that has i at the beginning is iQ.

Restricting to \mathcal{L}_{n-1}^* this gives the basis of dual Lie elements 1Q + Sh, for all the (n-2)! permutations Q of 23...n-1. Their linear independence follows from the fact that they are dual to the set of Lie monomials $\ell[1P]$ in \mathcal{L} , for P a permutation of 23...n-1 by (2.9). Since 1Q spans \mathscr{L}^* , any $P + Sh \in \mathcal{L}^*$ must have the following basis expansion:

$$P + Sh = \sum_{Q} (P, \ell[1Q]) 1Q + Sh, \qquad (2.10)$$

where the sum is over all permutations, Q, of 23...n-1. The word expansions of $\ell[iP]$ and r[Pi] have the following explicit formulas

$$\ell[iP] = \sum_{P \in X \sqcup Y} (-1)^{|X|} \overline{X} iY, \qquad r[Pi] = \sum_{P \in X \sqcup Y} (-1)^{|Y|} X i \overline{Y}.$$
(2.11)

 $^{^4}$ P is assumed to have no repeated letters in our context. There is a more standard notion of Lyndon words for words that have repeated letters [2].

These can be proved by verifying that they satisfy (2.2). Substituting P = XiY into the explicit formula, (2.11), for the expansion of $\ell[iP]$, (2.10) implies that,

$$XiY \sim (-1)^{|X|} i(\overline{X} \sqcup Y), \qquad (2.12)$$

where XiY is a permutation of 12...n - 1, and *i* is some letter in 1, 2, ..., n - 1.⁵ Setting *Y* to be empty in (2.12) gives for any word *P* the special case $P \sim -(-1)^{|P|}\overline{P}$.

As explained in [15], (2.12) corresponds to the *Kleiss-Kuijf* (*KK*) relations among color-ordered amplitudes [29,30]

$$\mathcal{A}(X1Y,n) = (-1)^{|X|} \mathcal{A}(1(\overline{X} \sqcup Y),n)$$
(2.14)

expressed now as a general statement about \mathscr{L}^* under the numerator homomorphism from the Lie polynomial amplitude (1.3). Indeed we will see that the KK relations follow for any theory whose connected Feynman diagrams give rise to colour factors of the form (2.20).

We will also use basis expansions in \mathcal{L}_{n-1} . If $\Gamma \in \mathcal{L}_{n-1}$, then it has a basis expansion:

$$\Gamma = \sum_{Q} (1Q, \Gamma) \,\ell[1Q] \,, \tag{2.15}$$

where the sum is over all permutations, Q, of 23...n - 1. For example, this gives

$$[[1,2],[3,4]] = \ell[1234] - \ell[1243], \qquad (2.16)$$

which can also be verified directly using the Jacobi identity.

Finally, we will need to use the *adjoints* of ℓ and r, which we write as ℓ^* and r^* :

$$(\ell^*(P), Q) = (P, \ell(Q)), \qquad (r^*(P), Q) = (P, r(Q)).$$
 (2.17)

It follows from (2.2) that the adjoints can be computed recursively as

$$\ell^*(123...n) = \ell^*(123...n-1)n - \ell^*(23...n)1, \qquad \ell^*(i) := i, \qquad (2.18)$$
$$r^*(123...n) = 1r^*(23...n) - nr^*(123...n-1), \qquad r^*(i) := i,$$

Likewise, the explicit formulas (2.11) are equivalent to the following formulas [31]

$$\ell^*(A) = \sum_{A=XiY} (-1)^{|X|} i(\overline{X} \sqcup Y), \qquad r^*(A) = \sum_{A=XiY} (-1)^{|Y|} (X \sqcup \overline{Y}) i.$$
(2.19)

Note that ℓ^* and r^* are well-defined on \mathscr{L}^* as $\ell^*(P \sqcup Q) = 0 = r^*(P \sqcup Q)$ for nonempty P, Q. This follows from $(\ell^*(P \sqcup Q), R) = (P \sqcup Q, \ell[R])$ which vanishes due to (2.6).

$$BiA - (-1)^{|B|}i(A \sqcup \overline{B}) = -\sum_{\substack{XY=B\\X \neq \emptyset}} (-1)^{|X|} \overline{X} \sqcup (YiA).$$
(2.13)

This is stated in [26] and proven in [27] (see also equation (41) in [28]).

⁵ Another way to find (2.12) is to prove the following identity at the level of words:



Fig. 1 The product of propagators $\frac{1}{s_{\Gamma}}$ and the planar binary tree associated to the Lie monomial [[1,2],[3,4]] according to the definition (2.24).

2.2. Binary trees and colour structures

For any Lie monomial $\Gamma \in \mathcal{L}_{n-1}$, there is a rooted binary tree T_{Γ} [32]. The inductive definition is as follows. $T_{[1,2]}$ is the tree with two leaves, 1 and 2, connected by one vertex to the root. If $\Gamma = [\Gamma', \Gamma'']$, then T_{Γ} is the tree formed by connecting (or 'grafting') the roots of $T_{\Gamma'}$ and $T_{\Gamma''}$ to make a new vertex. Every pair of brackets in Γ corresponds to a vertex in T_{Γ} . An example is shown in fig. 1 for $\Gamma = [[1, 2], [3, 4]]$.

Fix *n* elements of a Lie algebra: $t_i^a \in \mathfrak{g}$, for i = 1, ..., n - 1. For any choice of the t_i , there is a map $\mathbf{t} : \mathcal{L}_{n-1} \to \mathfrak{g}$. For a Lie monomial $\Gamma \in \mathcal{L}_{n-1}$, $\mathbf{t}(\Gamma)$ is obtained by writing Γ as a nested bracketing of 1, ..., n - 1, and replacing every commutator bracket by the Lie bracket of \mathfrak{g} . If tr is the invariant inner product on \mathfrak{g} , then for every Lie monomial $\Gamma \in \mathcal{L}_{n-1}$, the associated *colour factor* is

$$c_{\Gamma} = \operatorname{tr}(\mathbf{t}(\Gamma)t_n). \tag{2.20}$$

The replacement $\Gamma \mapsto c_{\Gamma}$ defines a homomorphism out of \mathcal{L}_{n-1} ; in particular $c_{-\Gamma} = -c_{\Gamma}$. If T_{Γ} is treated as a cubic Feynman diagram in a gauge theory with Lie group \mathfrak{g} , then (up to a sign) c_{Γ} is the colour factor of that diagram.⁶

2.3. Mandelstam variables.

Massless scattering amplitudes are functions of external momenta, k_i^{μ} , i = 1, ..., n, with $k_i \cdot k_i = 0$. The Mandelstam variable s_{ij} is

$$s_{ij} := k_i \cdot k_j. \tag{2.21}$$

⁶ The caveat about signs is because a cubic tree Feynman diagram in gauge theory is not just a tree: the orientations at each vertex are important, and so the Feynman diagrams are sometimes drawn as quark graphs.

For every subset $I \subset \mathbb{N}$ with at least two elements, write

$$s_I := \sum_{\{i,j\} \subset I} s_{ij}, \qquad k_I^{\mu} := \sum_{i \in I} k_i^{\mu}, \tag{2.22}$$

so that $k_I \cdot k_J = \sum_{i \in I, j \in J} s_{ij}$.

Consider the Laurent ring with the variables s_I , for all subsets I (with at least two elements). Then let S be the subring of this Laurent ring defined by the relation, (2.22). For example, $1/(s_{12} + s_{23})$ is not a function in S. Whereas $1/(s_{12} + s_{23} + s_{13})$ is a function in S, because

$$\frac{1}{s_{12} + s_{23} + s_{13}} = \frac{1}{s_{123}}.$$
(2.23)

The functions in \mathcal{S} are the kind that arise in scattering amplitudes.

Fix a Lie monomial $\Gamma \in \mathcal{L}_{n-1}$. When written as a nested bracket expression, each pair of brackets in Γ defines a subset of $\{1, ..., n-1\}$. If I is a subset that appears like this, write $I \in \Gamma$, and define

$$s_{\Gamma} := \prod_{I \in \Gamma} s_I. \tag{2.24}$$

For example, $s_{[[1,2],[3,4]]} = s_{12}s_{34}s_{1234}$, as in fig. 1.

The inverse, $\frac{1}{s_{\Gamma}}$, is the *product of propagators* of the tree graph, T_{Γ} , associated to Γ , including a propagator for the root of T_{Γ} .

3. Berends-Giele recursion and Lie polynomials

Berends-Giele (BG) recursion [12] computes currents $J(P)^{\mu}$, labelled by permutations P, that can be used to find the on-shell gauge theory tree amplitudes. In [14] Berends-Giele recursion is applied to biadjoint scalar theory. This led to double colour-ordered currents b(P|Q) labelled by two permutations P and Q.⁷ The BG recursion from [14] satisfied by b(P|Q) induces a BG-like recursion for a parent object that was denoted b(P) in [13]. In this approach to Berends-Giele, b(P) is a Lie polynomial with coefficients in the Mandelstam variables. These b(P), and the associated partial *Lie polynomial amplitudes*, are the basic subject of the subsequent sections.

In the following we re-derive the results of [14] and the appendix of [26] using fields with values in Lie polynomials. Yang-Mills fields are similarly treated in appendix A.

⁷ In [14] these were denoted $\phi(P|Q)$.

3.1. Berends-Giele recursion for biadjoint scalar theories

Biadjoint scalars are scalar fields that take values in the tensor product of two Lie algebras $\Phi \in \mathfrak{g} \otimes \tilde{\mathfrak{g}}$. Let these have structure constants f^{abc} and $\tilde{f}^{\tilde{a}\tilde{b}\tilde{c}}$ and invariant inner products for which we take an orthonormal basis. Then the Lagrangian is

$$\mathcal{L}_{BS} = \frac{1}{2} \nabla_{\mu} \Phi_{a\tilde{a}} \nabla^{\mu} \Phi^{a\tilde{a}} + \frac{1}{3!} f_{abc} \tilde{f}_{\tilde{a}\tilde{b}\tilde{c}} \Phi^{a\tilde{a}} \Phi^{b\tilde{b}} \Phi^{c\tilde{c}} , \qquad (3.1)$$

where $\mu = 1, \ldots, d$ is a space-time index and $a, b \ \tilde{a}, \tilde{b}$ are Lie algebra indices for $\mathfrak{g}, \mathfrak{g}$. The field equations are

$$\Box \Phi_{a\tilde{a}} = \frac{1}{2} f_{abc} \tilde{f}_{\tilde{a}\tilde{b}\tilde{c}} \Phi^{b\tilde{b}} \Phi^{c\tilde{c}} \,. \tag{3.2}$$

Consider the field $\Phi(x) \in \mathscr{L} \otimes \mathscr{L}$ rather than $\mathfrak{g} \otimes \tilde{\mathfrak{g}}$ now satisfying

$$\Box \Phi = \frac{1}{2} \llbracket \Phi, \Phi \rrbracket, \qquad (3.3)$$

where $[\![,]\!]$ is the symmetric operation:

$$\llbracket \Gamma_1 \otimes \tilde{\Gamma}_1, \Gamma_2 \otimes \tilde{\Gamma}_2 \rrbracket := [\Gamma_1, \Gamma_2] \otimes [\tilde{\Gamma}_1, \tilde{\Gamma}_2].$$
(3.4)

Inverting the wave operator in (3.2) gives the recursion

$$\Phi_n = \Phi_1 + \operatorname{proj}_{\mathscr{L}_{\leq n} \otimes \mathscr{L}_{\leq n}} \Box^{-1} \frac{1}{2} \llbracket \Phi_{n-1}, \Phi_{n-1} \rrbracket, \qquad (3.5)$$

for a perturbative solution in the form of fields $\Phi_n \in \mathscr{L}_{\leq n} \otimes \mathscr{L}_{\leq n}$, where $\mathscr{L}_{\leq n}$ is the subspace spanned by Lie monomials Γ with length $|\Gamma| \leq n$. The iteration is seeded by the following homogeneous solution to $\Box \Phi_1 = 0$:

$$\Phi_1 = \sum_{j \in \mathbb{N}} e^{ik_j \cdot x} \, j \otimes j \, \in \mathscr{L} \otimes \mathscr{L} \,. \tag{3.6}$$

By our definition of \mathscr{L} , the letters appearing in monomials in Φ_n are distinct.⁸ The coefficient of a word P in Φ_n has x dependence $e^{ik_P \cdot x}$. The inverse wave operator, \Box^{-1} , acts on such a term to give $1/k_P^2 = 1/s_P$. By construction, Φ_n is symmetric in its two factors:

$$\Phi_n = \sum_j \phi_j \Gamma_j \otimes \Gamma_j , \qquad (3.7)$$

for some coefficients ϕ_j , and Lie monomials Γ_j . It follows that, for a word P, pairing with the left or right factor of Φ_n gives $(P, \Phi_n)_L = (P, \Phi_n)_R$. So write

$$\Phi(P) := (P, \Phi)_L = (P, \Phi)_R.$$
(3.8)

Define now the Berends-Giele currents to be

$$b(P) = e^{-ik_P \cdot x} \Phi(P) \quad \in \quad \mathscr{L}_s := \mathscr{L} \otimes \mathcal{S} \,, \tag{3.9}$$

i.e., Lie polynomials multiplied by rational functions of the Mandelstams, where the factor of $e^{-ik_P \cdot x}$ removes the x dependence.

 $^{^{8}}$ In the perturbiner approach this is enforced by introducing nilpotents into each seed solution.

Proposition [13]. The Berends-Giele currents satisfy

$$b(P) = \frac{1}{s_P} \sum_{XY=P} [b(X), b(Y)], \qquad b(i) = i, \qquad (3.10)$$

where the sum is over all deconcatenations, P = XY, of P.

Proof. This follows by pairing (3.5) with P and using the identity

$$(P, [\Gamma_{j_1}, \Gamma_{j_2}]) \otimes [\Gamma_{j_1}, \Gamma_{j_2}] = \sum_{XY=P} [(X, \Gamma_{j_1})\Gamma_{j_1}, (Y, \Gamma_{j_2})\Gamma_{j_2}] + [(X, \Gamma_{j_2})\Gamma_{j_2}, (Y, \Gamma_{j_1})\Gamma_{j_1}].$$
(3.11)

which together with the symmetry of Φ gives

$$\frac{1}{2} \llbracket \Phi, \Phi \rrbracket(P) = \sum_{XY=P} [\Phi(X), \Phi(Y)].$$
(3.12)

which gives (3.10).

For example, the recursion (3.10) gives

$$b(12) = \frac{[1,2]}{s_{12}},$$

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

$$b(1234) = \frac{[[[1,2],3],4]}{s_{12}s_{123}s_{1234}} + \frac{[[1,[2,3]],4]}{s_{123}s_{1234}s_{23}} + \frac{[[1,2],[3,4]]}{s_{12}s_{1234}s_{34}} + \frac{[1,[[2,3],4]]}{s_{1234}s_{23}s_{234}} + \frac{[1,[2,[3,4]]]}{s_{1234}s_{23}s_{234}}.$$
(3.13)

Since $\Phi \in \mathscr{L} \otimes \mathscr{L}$, Ree's theorem implies that

$$b(R \sqcup S) = 0, \qquad (3.14)$$

for nonempty R, S. Thus $b: P \mapsto b(P)$ defines a map

$$b: \mathscr{L}_s^* \to \mathscr{L}_s. \tag{3.15}$$

To obtain an *n*-particle amplitude from a Berends-Giele current, remove the last propagator by multiplying by $s_{12...n-1}$, and imposing momentum conservation this becomes k_n^2 which we then set to zero. Thus we define the \mathscr{L} -valued "amplitude" by

$$m(P,n) = \lim_{s_P \to 0} s_P \, b(P) \in \mathscr{L}_{\mathcal{S}},\tag{3.16}$$

for permutations P of 12...n – 1 (although (3.14) in fact gives $P \in \mathcal{L}_{n-1}^*$.)



Fig. 2 The Catalan expansion b(1234) from (3.10). Viewed as cubic graphs and removing the overall propagator $1/s_{1234}$, they correspond to the expansion of a color-ordered five-point tree amplitude A(12345) [3]. Note the leg 5 does not enter in the Lie elements in the numerators and that the root is unlabeled. By labelling the root and assigning leg 5 to the Catalan expansion of b(5) one recovers the free Lie algebra correspondence (3.22) for the case n = 5.

3.2. The tree diagram expansion of b(P)

The Feynman diagrams of biadjoint scalar theory are trivalent trees. Berends-Giele recursion generates the Feynman graphs with one off-shell leg decorated with an off-shell propagator, with the remaining legs on-shell. So b(P) can be written as a sum over binary trees as follows. Write

$$b := \sum_{\Gamma} \frac{\Gamma \otimes \Gamma}{s_{\Gamma}} \quad \in \quad \mathscr{L} \otimes \mathscr{L}, \tag{3.17}$$

where the sum is over all Lie monomials (up to sign), and where s_{Γ} is the product of variables s_I defined in (2.24). Then pairing b with a word P gives

$$b(P) = \sum_{\Gamma} \frac{(P, \Gamma)\Gamma}{s_{\Gamma}},$$
(3.18)

which is a sum over all planar rooted trees with respect to the ordering P.

The following Lemma shows that (3.18) is indeed the solution to the Berends-Giele recursion discussed in §3.1.

Lemma. The formula in (3.18) satisfies (3.10).

Proof. For any Lie monomial Γ there are Γ_1 and Γ_2 so that $\Gamma = [\Gamma_1, \Gamma_2]$, and these monomials are unique up to sign. So, for a fixed Lie monomial Γ ,

$$\frac{(P,\Gamma)\Gamma}{s_{\Gamma}} = \frac{(X,\Gamma_1)(Y,\Gamma_2)[\Gamma_1,\Gamma_2]}{s_P s_{\Gamma_1} s_{\Gamma_2}} - \frac{(Y,\Gamma_1)(X,\Gamma_2)[\Gamma_1,\Gamma_2]}{s_P s_{\Gamma_1} s_{\Gamma_2}},$$
(3.19)

where P = XY and $|X| = |\Gamma_1|$, $|Y| = |\Gamma_2|$. Summing over all Lie monomials (up to sign), Γ_1 and Γ_2 , that have length strictly smaller than |P| gives (3.10). \Box Regarding b as a map from $\mathscr{L}^*_{\mathcal{S}}$ to $\mathscr{L}_{\mathcal{S}}$ it follows from (3.17) that b is self-adjoint:

$$b(P|Q) := (P, b(Q)) = (b(P), Q) = b(Q|P), \qquad (3.20)$$

for any $P, Q \in \mathscr{L}^*_{\mathcal{S}}$. Since b(P) is a Lie polynomial it can be expanded in a basis as

$$b(P) = \sum_{R} b(P|iR)\ell[iR], \qquad (3.21)$$

where i is some letter in P and we used (2.15).

The usual biadjoint scalar partial tree amplitude is [14]

$$m(Pn, Qn)) =: \lim_{s_P \to 0} s_P b(P|Q) = (Q, m(Pn)).$$
 (3.22)

We will see in §7 how b(P) can be dressed with BCJ numerators to give BG currents and hence amplitudes for certain coloured theories.

4. A Lie bracket for tree-level scattering amplitude relations

This section introduces a Lie bracket on $\mathscr{L}^*_{\mathcal{S}}$, and uses it to prove the fundamental BCJ relation. Following [13], this Lie bracket is then used to define a generalized KLT matrix in §5 and to prove the identities conjectured in [13].

4.1. The S-bracket

The *S*-map was introduced in [6,15] to express the BCJ relations for super-Yang-Mills amplitudes from its action on Berends-Giele currents M_P from [33]. It was abstracted to a map acting on words in [13] and the off-shell BCJ relations for b(P) was conjectured, but no general proof was given. Here we will see that the S-map defines a Lie bracket on \mathscr{L}^* and this will lead to a proof of the fundamental BCJ relations.

Definition (S bracket). Define a multilinear pairing $\{,\}: \mathcal{L}^* \otimes \mathcal{L}^* \to \mathcal{L}^*$ by [13]

$$\{P,Q\} := r^*(P) \star \ell^*(Q), \tag{4.1}$$

where r^* and ℓ^* are defined in (2.18) and

$$Ai \star jB := s_{ij} AijB \tag{4.2}$$

for words A, B and letters i, j. Equivalently, for $P, Q \in \mathscr{L}^*$, equation (2.19) gives [6]

$$\{P,Q\} = \sum_{\substack{XiY=P\\RjS=Q}} s_{ij} \left(X \sqcup \alpha(Y)\right) ij(\alpha(R) \sqcup S).$$

$$(4.3)$$

Alternatively, a recursive definition is given by

$$\{iAj, B\} = i\{Aj, B\} - j\{iA, B\},$$

$$\{B, iAj\} = \{B, iA\}j - \{B, Aj\}i,$$

$$\{i, j\} = s_{ij} ij$$
(4.4)

as can be verified from the explicit form of the adjoint maps ℓ^* and r^* in (2.19). For example,

$$\{1, 2\} = s_{12}12, \qquad (4.5)$$

$$\{1, 23\} = s_{12}123 - s_{13}132, \qquad (12, 3) = s_{23}123 - s_{13}213, \qquad (1, 234\} = s_{12}1234 - s_{13}1324 - s_{13}1342 + s_{14}1432, \qquad (123, 4) = s_{34}1234 - s_{24}1324 - s_{24}3124 + s_{14}3214, \qquad (12, 34) = s_{23}1234 - s_{24}1243 - s_{13}2134 + s_{14}2143.$$

Given that the adjoints r^* and ℓ^* annihilate proper shuffles, the definition (4.1) manifestly satisfies $\{A \sqcup B, C\} = 0$.

The S bracket is antisymmetric in \mathscr{L}^* . Indeed, by (4.3),

$$\{Q,P\} = \sum_{\substack{XiY=P\\RjS=Q}} s_{ij} \left(R \sqcup \alpha(S)\right) ji(\alpha(X) \sqcup Y) \sim -(-1)^{Q+P} \overline{\{P,Q\}},\tag{4.6}$$

because, in \mathscr{L}^* , X is shuffle equivalent to $-(-1)^X \overline{X}$. Using (2.8) this means that,

$$\{P,Q\} \sim -\{Q,P\}.$$
 (4.7)

In fact, we show in §5.1 that the S bracket is a Lie bracket on $\mathscr{L}^*_{\mathcal{S}}$, and so it also satisfies the Jacobi identity.

4.2. The BCJ amplitude relations

This section proves the main property of the S bracket which amounts to a generalization of the well-known off-shell fundamental BCJ relation [16]. Following [6], we call the relations implied by the S bracket BCJ amplitude relations. The on-shell identities follow directly from the off-shell relations, as is explained at the end of this section.

Proposition. For $P, Q \in \mathscr{L}^*$, the S-bracket satisfies

$$b(\{P,Q\}) = [b(P), b(Q)], \qquad (4.8)$$

i.e., b maps the S bracket to the Lie bracket.

The proposition is proved in appendix B. It is interesting to observe that the property (4.8) mimics the identity obeyed by the Poisson bracket $\{,\}$ of Hamiltonian vector fields $X_f: X_{\{f,g\}} = [X_f, X_g]$ for functions f and g.

Corollary (Fundamental off-shell BCJ relations [16]). Taking P = i, a single letter, we obtain

$$b(\{i,Q\}) := \sum_{Q=XjY} s_{ij} b(ij\alpha(X) \sqcup Y) = [i, b(Q)],$$
(4.9)

where $\alpha(X) = (-1)^{|X|} \overline{X}$.

The expression in (4.9) can also be written as

$$\{i, Q\} \sim \sum_{Q=XY} k_i \cdot k_Y X i Y \tag{4.10}$$

To see this, use (2.10) to write the RHS (4.10) in the basis of words beginning with the letter i,

$$\sum_{Q=XY} (k_i \cdot k_Y) X i Y \sim \sum_{Q=XY} (k_i \cdot k_Y) i(\alpha(X) \sqcup Y)$$
(4.11)

Further manipulations give

$$RHS = \sum_{Q=XjY} (k_i \cdot k_{jY}) \, ij(\alpha(X) \sqcup Y) - (k_i \cdot k_Y) \, ij(\alpha(X) \sqcup Y), \qquad (4.12)$$
$$= \sum_{Q=XjY} s_{ij} \, ij(\alpha(X) \sqcup Y),$$

where we use the property (2.5) of the shuffle product.

Corollary (BCJ relations). The tree-level partial amplitudes (3.16) satisfy

$$m(\{P,Q\},n) = 0, \qquad (4.13)$$

where P and Q are words that partition 1, 2, ..., n-1 into two parts.

Proof. By the definition (3.16),

$$m(\{P,Q\},n) = \lim_{s_{PQ}\to 0} s_{PQ}b(\{P,Q\}) = \lim_{s_{PQ}\to 0} s_{PQ}[b(P),b(Q)] = 0.$$
(4.14)

The last term vanishes because neither b(P) nor b(Q) has a $1/s_{PQ}$ pole.

The original fundamental BCJ relations are [34,35]

$$m(\{i, Q\}n) = \sum_{Q=RS} (k_i \cdot k_S)m(RiSn) = 0, \qquad (4.15)$$

which follows from (4.10). For example, by (4.5), [3]

$$0 = m(\{1, 23\}4) = s_{12}m(1234) - s_{13}m(1324),$$

$$0 = m(\{1, 234\}, 5) = s_{12}m(12345) - s_{13}m(13245) - s_{13}m(13425) + s_{14}m(14325).$$
(4.16)

But, as observed in [6,15], (4.13) also implies other BCJ relations, such as

$$0 = m(\{12, 34\}, 5) = s_{23}m(1234, 5) - s_{13}m(2134, 5) - s_{24}m(1243, 5) + s_{14}m(2143, 5), \quad (4.17)$$

while similar formulas using the shuffle product appear in [36,37,38]. The BCJ relations for Yang–Mills theory were first proven from the field-theory limit of string theory in [36] and [37]. By now these relations have been proven for a variety of theories at tree-level. See the recent review [5] and references therein.

5. The KLT map

This section introduces a canonical KLT map $S : \mathscr{L}_S \to \mathscr{L}_S^*$. S is the inverse of b, and this implies that the S-bracket is a Lie bracket. When S is written out in terms of a pair of bases for \mathscr{L} and \mathscr{L}^* , the matrix elements of S are the generalized KLT matrix S(P|Q)proposed in [13]. We prove the properties conjectured in [13] as well as additional ones.

5.1. The KLT map

Let Γ be a Lie monomial, and write it as a nested bracketing. Let $\{\Gamma\} \in \mathscr{L}^*$ be obtained by replacing every commutator [,] in the bracketed expression of Γ with a $\{, \}$. This is well defined because the S-bracket is antisymmetric. By nested applications of (4.8), it follows from the proposition in the previous section that for any Lie monomial Γ ,

$$\Gamma = b(\{\Gamma\}). \tag{5.1}$$

For example,

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

$$= s_{12}s_{34}(s_{23}b(1234) - s_{24}b(1243) - s_{13}b(2134) + s_{14}b(2143)).$$
(5.2)

where we used $\{\{1,2\},\{3,4\}\} = s_{12}s_{34}\{12,34\}$, the example (4.5) and the relations among Mandelstam invariants.

Define the KLT map $S: \mathscr{L}_{\mathcal{S}} \to \mathscr{L}_{\mathcal{S}}^*$ by

$$S: \Gamma \mapsto \{\Gamma\},\tag{5.3}$$

for Lie monomials Γ . As written, it is not obvious that S is well defined. The reason (5.3) is well defined is that it turns out that S-bracket is Lie. This is shown in the proof of the following main proposition:

Proposition. The maps $b : \mathscr{L}^* \to \mathscr{L}$ and $S : \mathscr{L} \to \mathscr{L}^*$ are inverses. In particular, b is invertible.

Proof. Choose an ordering of A, which defines dual Lyndon bases of $\mathscr{L}^*(A)$ and $\mathscr{L}(A)$, as in §2.1. Then define a map, S':

$$S': \ell(a) \mapsto \{\ell(a)\},\tag{5.4}$$

for monomials $\ell(a)$ in the given basis of $\mathscr{L}(A)$. We show that (i) S' and b are inverse, and (ii) that the S' in (5.4) is the map, S, in (5.3). This proves that (5.3) is well-defined.

By (5.1),

$$b(S'(\Gamma)) = \sum_{P \in Basis} (\Gamma, P)b(\{\ell(P)\}) = \sum_{P \in Basis} (\Gamma, P)\ell(P) = \Gamma.$$
 (5.5)

Conversely,

$$S'(b(P)) = \sum_{Q \in Basis} (b(P), Q) \{\ell(Q)\}.$$
(5.6)

Expanding $\{\ell(Q)\} \in \mathscr{L}^*$ in the given basis gives (by (2.10)),

$$\{\ell(Q)\} = \sum_{R \in Basis} (\{\ell(Q)\}, \ell(R))R.$$
(5.7)

But notice that

$$(\{\Gamma\}, \Gamma') = (\{\Gamma\}, b(\{\Gamma'\})) = (b(\{\Gamma\}), \{\Gamma'\}) = (\Gamma, \{\Gamma'\}),$$
(5.8)

by the self-adjointness of b. Combining (5.7) and (5.8) gives that

$$S'(b(P)) = \sum_{Q,R \in Basis} b(P,Q)(\ell\{Q\},\ell(R))R = \sum_{R \in Basis} (P,\ell(R))R = P.$$
(5.9)

So b is invertible, with inverse S'. But $b({\Gamma}) = \Gamma$, by (5.1). So $S'(\Gamma) = {\Gamma}$.

Notice that the self-adjointness of b implies (as in (5.8)) that the KLT map, S, is self adjoint:

$$(S(\Gamma), \Gamma') = (\Gamma, S(\Gamma')).$$
(5.10)

Corollary. The S-bracket is Lie.

Proof. Given that S and b are inverse, (4.8) shows that $\{ , \}$ is the pull back of [,] from \mathscr{L} to \mathscr{L}^* by b^{-1} . i.e. $\{ , \}$ is skew and satisfies the Jacobi relation. \Box

5.2. The generalized and standard KLT matrix

This section finds explicit formulas for the KLT map, S, in terms of the matrix elements of S. In the next section, it is shown how these reduce to the standard formula for the KLT matrix elements.

If P_i, Γ_i is a pair of dual bases for \mathscr{L}^* and \mathscr{L} , then

$$S: \Gamma \mapsto \sum_{i,j} (P_i, \Gamma)(\{\Gamma_i\}, \Gamma'_j) P'_j.$$
(5.11)

In other words, the matrix elements of S are

$$S(\Gamma_1, \Gamma_2) = (\{\Gamma_1\}, \Gamma_2), \tag{5.12}$$

for two Lie monomials Γ_1, Γ_2 .

For the rest of this section, we again take pairs of dual Lyndon bases: $P \in \mathscr{L}^*$ for every Lyndon word P, and $\ell[P] \in \mathscr{L}$ for every Lyndon word P. In these bases, the matrix elements, (5.12), are labelled by Lyndon words. So define the *generalized KLT matrix* (introduced in [13])⁹ to be these matrix elements:

$$S^{\ell}(P|Q) := (\ell\{P\}, \ell[Q]).$$
(5.13)

In this formula, we introduce the notation $\ell\{P\}$ for $\{\ell[P]\}^{10}$ This is given explicitly by:

$$\ell\{12...n\} := \{...\{1,2\},...,n\}.$$
(5.14)

For example,

$$\ell\{12\} = s_{12}12, \tag{5.15}$$

$$\ell\{123\} = s_{12}s_{23}123 - s_{12}s_{13}213, \tag{5.14}$$

$$\ell\{1234\} = +s_{12}s_{23}s_{34}1234 - s_{12}s_{23}s_{24}1324 - s_{12}s_{13}s_{34}2134 + s_{12}s_{13}s_{14}2314 - s_{12}s_{13}s_{24}3124 - s_{12}s_{23}s_{24}3124 + s_{12}s_{13}s_{14}3214 + s_{12}s_{14}s_{23}3214.$$

Some example entries of the generalized KLT matrix are

$$S^{\ell}(12|12) = s_{12}, \qquad S^{\ell}(123|123) = s_{12}(s_{13} + s_{23}), \qquad S^{\ell}(132|123) = s_{12}s_{13}, \\S^{\ell}(12|21) = -s_{12}, \qquad S^{\ell}(312|123) = -s_{12}s_{13}. \qquad S^{\ell}(321|123) = s_{12}s_{23}.$$
(5.16)

The generalized KLT matrix is the matrix of coefficients that arises in the basis expansion of $\ell\{P\}$:

$$\ell\{P\} \sim \sum_{Q \in Basis} (\ell\{P\}, \ell[Q])Q = \sum_{Q \in Basis} S^{\ell}(P|Q)Q,$$
(5.17)

as in (5.7). As pointed out in [13], the generalized KLT matrix $S^{\ell}(P|Q)$ can be defined for any two words P, Q, instead of restricting P, Q to a set of Lyndon words.

⁹ Alternative formulas for the generalized KLT matrix arise by choosing any pair of dual bases. E.g. one can define $S^r(P,Q) := (r\{P\}, r(Q))$, but as $P,Q \in \mathscr{L}$, by Lemma 1.7 of [1], $r\{P\} = -\ell\{\alpha(P)\}$ and $r(P) = -\ell(\alpha(P))$ so $S^r(P|Q) = S^\ell(\overline{P}|\overline{Q})$. These alternative choices explain redefinitions w.r.t reversal of permutations $P \to \overline{P}$, see e.g. footnote 10 in [39].

¹⁰ In [13] the map ℓ{A} was denoted $\sigma(A)$.

It follows from (5.8) that the generalized KLT matrix is symmetric:

$$S^{\ell}(P|Q) = S^{\ell}(Q|P).$$
 (5.18)

Moreover, (5.5) implies that the generalized KLT matrix satisfies

$$\ell[P] = \sum_{Q \in Basis} S^{\ell}(P|Q) \, b(Q). \tag{5.19}$$

Or, equivalently,

$$(R, \ell[P]) = \sum_{Q \in Basis} S^{\ell}(P|Q) \, b(Q|R), \qquad (5.20)$$

and so, also:

$$b(P|Q) = \sum_{X,Y \in Basis} b(P|X) S^{\ell}(X|Y) b(Y|Q).$$
(5.21)

We now show that the standard KLT matrix arises from the restriction [13]

$$S(P|Q)_i := S^{\ell}(iP|iQ), \qquad (5.22)$$

for some fixed letter *i*, called the 'fixed leg'. An explicit formula for $S(P|Q)_i$ was given in [17,18]. This explicit formula can be recovered¹¹ from (5.22) using the following recursion, originally conjectured in [40].

Lemma. The standard KLT matrix (5.22) can be recursively computed using

$$S(Aj|BjC)_i = k_j \cdot k_{iB} S(A|BC)_i, \qquad (5.23)$$

where *i* is the fixed leg. The recursion is seeded by $S(\emptyset|\emptyset)_i := 1$.

Proof. By definition, $\ell{Aj} = {\ell{A}, j}$. Using the formula (4.10) for ${P, j}$,

$$\ell\{Aj\} = \sum_{X,Y} k_j \cdot k_X \, (XY, \ell\{A\}) X jY.$$
(5.24)

Since $S(Aj|BjC)_i = (\ell\{iAj\}, \ell(iBjC))$, it follows from (5.24) that

$$S(Aj|BjC)_i = \sum_{X,Y} k_j \cdot k_X(XY, \ell\{iA\})(XjY, \ell(iBjC)).$$
(5.25)

¹¹ An alternative explicit derivation using (5.22) is given in appendix C, where the steps are closer in spirit to the argument in [16].

Expanding ℓ{iA} in a basis, as in (5.17),

$$\ell\{iA\} = \sum_{P} S(A|P)_i \, iP. \tag{5.26}$$

So (5.25) becomes

$$S(Aj|BjC)_i = \sum_{X,Y,P} k_j \cdot k_X S(A|P)_i(XY,iP)(XjY,\ell(iBjC)).$$
(5.27)

The only contributions in the sum come from words, X = iX', that begin with the letter *i*. Expanding $\ell(iBjC)$, one sees that $(iX'jY, \ell(iBjC)) = \delta_{X',B}\delta_{Y,C}$. \Box

The identity, (5.20), together with the definition (5.22) is a purely algebraic proof that the standard KLT matrix is the inverse to the biadjoint scalar BG double current:

$$\sum_{R} S^{\ell}(P|R)_{i}b(iR|iQ) = \delta_{P,Q}.$$
(5.28)

This is in accord with the discussions of [8] and [14].

5.3. The momentum kernel and the KLT gravity formula

The (n-2)! version of the KLT relation, as given by [18,35], is

$$M_n = \lim_{s_{1P} \to 0} \sum_{P,Q \in S_{n-2}} \frac{1}{s_{1P}} A(1Pn) S(P|Q)_1 \tilde{A}(1Qn),$$
(5.29)

where $\tilde{A}(1Qn)$ is obtained from its left-moving counterpart by replacing the polarization vectors, e_i^{μ} , by some other set of polarization vectors, \tilde{e}_i^{μ} . It takes some effort to see directly that the limit on the RHS of (5.29) is well defined. The cancellation of the $1/s_{1P}$ pole on the RHS is easily understood in terms of the above discussion of $S(P|Q)_1$ in §5.1.

For example, starting from (5.28), we recover the well known fact that the KLT matrix (5.13) annihilates the on-shell biadjoint scalar amplitudes,

$$\sum_{Q} S^{\ell}(1P|1Q)m(1Q,n|R,n) = 0, \qquad (5.30)$$

where $m(1Q, n|R, n) = \lim_{s_{iP}\to 0} s_{iP}b(1Q|R)$. The expression vanishes because there is no $1/s_{iP}$ pole in (5.28). This is a remarkable identity, because the components $S(P,Q)_i$ do not have s_{iP} as a factor. On the other hand, b(iP, iQ) does have a $1/s_{iP}$. This cancellation is the key reason why (5.29) is well defined.

In the rest of this section, we explain how a Lie polynomial version of (5.29) follows immediately from the main result in §5.1. We have already shown, in (5.21), that the KLT matrix satisfies the following off-shell, (n-2)! KLT relation

$$b(P|Q) = \sum_{R,U} b(P|iR)S(R|U)_i b(iU|Q).$$
 (5.31)

To obtain a relation of the form (5.29), write

$$A(1P,n) := s_{1P}b(1P) = s_{1P} \sum_{R \in S_{n-2}} b(1P|1R)\ell[1R], \qquad (5.32)$$

for the Lie polynomial 'precursor' of a gauge theory amplitude. And write

$$M_n = \sum_{P,Q \in S_{n-2}} s_{1P} \,\ell[1P] b(1P|1Q) \ell[1Q] \tag{5.33}$$

for the precursor of a gravity amplitude. Notice that, by (3.21), (5.33) is equivalently written as

$$M_n = s_{12...n-1} \sum_{|\Gamma|=n-1} \frac{\Gamma \otimes \Gamma}{s_{\Gamma}}.$$
(5.34)

Then (5.31) implies the following KLT relation

$$M_n = \lim_{s_{1P}=0} \sum_{P,Q \in S_{n-2}} \frac{1}{s_{1P}} S(P|Q)_1 m(1Pn) \otimes m(1Qn).$$
(5.35)

All the double poles from the right-hand side of (5.29) are manifestly absent in its free Lie algebra version (5.35) due to the generalized KLT matrix property (5.31). The only poles in (5.31) are those that appear in b(1P|1Q).

Our results also make it clear why the existence of a 'BCJ form' for gravity is equivalent to the KLT relation. As an example, the four-point "gravity" amplitude has the following double copy expansion:

$$M_{4} = s_{123} \Big(b(123|123)\tilde{\ell}[123]\ell[123] + b(123|132)\tilde{\ell}[123]\ell[132]$$

$$+ b(132|123)\tilde{\ell}[132]\ell[123] + b(132|132)\tilde{\ell}[132]\ell[132] \Big)$$

$$= \frac{[[1,2],3] \otimes [[1,2],3]}{s_{12}} + \frac{[[1,3],2] \otimes [[1,3],2]}{s_{13}} + \frac{[1,[2,3]] \otimes [1,[2,3]]}{s_{23}},$$
(5.36)

where we used $\ell[123] - \ell[132] = [1, [2, 3]].$

The main property of the bracket the S-bracket is that

$$b(\{P,Q\}) = [b(P), b(Q)].$$
(5.37)

Since b and S are inverse, this is equivalent to

$$\{P,Q\} = S([b(P), b(Q)]).$$
(5.38)

The bracket $\{P, Q\}$ is polynomial in the Mandelstam variables, whereas S([b(P), b(Q)]) is naively a rational function of the Mandelstam variables. The cancellation of the poles in [b(P), b(Q)] by the KLT matrix is not at all obvious from its concrete formula.

As observed in $\S5.1$, (5.38) implies that the S-bracket is Lie, and so satisfies

$$\{1,2\} \sim -\{2,1\} \qquad \{\{1,2\},3\} + \{\{2,3\},1\} + \{\{3,1\},2\} \sim 0, \tag{5.39}$$

as identities in \mathscr{L}^*_S . It follows that the S-bracket satisfies generalized Jacobi identities [1]

$$\ell\{PiQ\} \sim -\ell\{i\ell[P]Q\} \tag{5.40}$$

which can be deduced from two applications of (2.3). This makes it clear that the definition of $S^{\ell}(P,Q)$, given in (5.13) also satisfies such generalized Jacobi identities in P and Q [13],

$$S(XiY|Q) = -S(i\ell[X]Y|Q).$$
(5.41)

Notice that this property of the generalized KLT matrix has no analog for the standard KLT matrix, $S(XiY|Q)_j$, because of the fixed leg j.¹²

Finally, another consequence of (5.38) is that

$$\sum_{XY=P} \{X, Y\} \sim s_P P.$$
(5.42)

This follows immediately from (3.10), by acting with the KLT map on both sides.

¹² The identity (5.41) motivated the introduction of the generalized KLT matrix in [13]. In the multiparticle pure spinor superfield framework, where V_P are local superfields satisfying generalized Jacobi identities and M_Q are Berends-Giele current superfields satisfying shuffle symmetries, we have the relation $V_{iA} = \sum_B S(A|B)_i M_B$ [39]. However, the fixed leg *i* prevents the Jacobi identities of V_{iA} being manifest.

6. The contact term map as a Lie co-bracket

A series of studies of string theory correlators and BCJ numerators led to the so-called contact term map [22] appearing in the action of the pure spinor BRST operator on local multiparticle superfields [6]. This section identifies the contact term map as the Lie cobracket dual to the S-bracket and proves its main properties as a result of this identification.

Definition (Contact term map). The contact term map, $C : \mathscr{L}_{S} \to \mathscr{L}_{S} \land \mathscr{L}_{S}$, is the dual of the S-bracket; i.e. for a Lie monomial, Γ ,

$$(P \otimes Q, C(\Gamma)) := (\{P, Q\}, \Gamma).$$

$$(6.1)$$

An explicit formula for $C(\Gamma)$ follows from (6.1) by choosing a basis, for example:

$$C(\Gamma) = \sum_{P,Q} (\{P,Q\},\Gamma) \ \ell[P] \otimes \ell[Q], \tag{6.2}$$

where the sum is over a Lyndon basis of $\mathscr{L}^*.^{13}$

Defining $P \wedge Q := P \otimes Q - Q \otimes P$, the first few examples of the map C are

$$C([1,2]) = (k_1 \cdot k_2)(1 \wedge 2),$$

$$C([1,[2,3]]) = (k_2 \cdot k_3) ([1,2] \wedge 3 + 2 \wedge [1,3]) + (k_1 \cdot k_{23}) (1 \wedge [2,3]).$$
(6.3)

C satisfies the dual Jacobi identity (A is the swap map, $X \otimes Y \mapsto Y \otimes X$.)

$$(C \otimes Id) \circ C - (Id \otimes C) \circ C - (Id \otimes A) \circ (C \otimes 1) \circ C = 0, \tag{6.4}$$

which is equivalent to the Jacobi identity for the S-bracket. Also, recall the main property,

$$b(\{P,Q\}) = [b(P), b(Q)].$$
(6.5)

This is equivalent to:

¹³ Other explicit formulas follow from choosing different pairs of dual basis. e.g. we could write a 'left-right' version of (6.2): $C(\Gamma) = \sum_{P,Q} (\{P,Q\},\Gamma) \ell[P] \otimes r[Q]$, which is related to (6.2) by $Q \sim (-1)^Q \overline{Q}$ and $\ell[Q] = (-1)^Q r[\overline{Q}]$.

Lemma. C satisfies [22]

$$C(b(P)) = \sum_{P=XY} b(X) \wedge b(Y).$$
(6.6)

Proof. (6.5) implies that

$$(P \otimes Q, C(b(R))) = ([b(P), b(Q)], R).$$
(6.7)

The RHS can be expanded by deconcatenation (as in the derivation of (3.10)):

$$RHS = \sum_{R=XY} (b(P), X)(b(Q), Y) - (X \leftrightarrow Y).$$
(6.8)

But b is self-adjoint, and so

$$(P \otimes Q, C(b(R))) = \sum_{R=XY} (P, b(X))(Q, b(Y)) - (X \leftrightarrow Y), \tag{6.9}$$

and this is equivalent to (6.6). (6.6) can also be checked using the formula, (6.2). \Box

The rest of this section derives a recursive formula for C. First define the standard extension of the adjoint representation of \mathscr{L} to $\mathscr{L} \otimes \mathscr{L}$:

$$[P, X \otimes Y] := [P, X] \otimes Y + X \otimes [P, Y],$$
$$[X \otimes Y, Q] := [X, Q] \otimes Y + X \otimes [Y, Q].$$

This makes $\mathscr{L}\otimes\mathscr{L}$ into an adjoint representation of \mathscr{L} .

Lemma (Recursion). For $\Gamma_1, \Gamma_2 \in \mathscr{L}$, the action of C on $[\Gamma_1, \Gamma_2]$ is given by

$$C([\Gamma_1, \Gamma_2]) := k_1 \cdot k_2 \, \Gamma_1 \wedge \Gamma_2 + [C(\Gamma_1), \Gamma_2] + [\Gamma_1, C(\Gamma_2)], \tag{6.11}$$

where k_1 and k_2 are the momenta associated to Γ_1 and Γ_2 . With C(i) := 0, (6.11) can be taken as a definition of C, as in [22].

Proof. This is a consequence of the identity, (B.5), used in the proof of the defining property of the S bracket, (6.5). We again use deconcatenation (as in (6.7), above) to write

$$(\{P,Q\},[\Gamma_1,\Gamma_2]) = (\delta\{P,Q\},\Gamma_1\otimes\Gamma_2) - (1\leftrightarrow 2).$$
(6.12)

Then (B.5) gives

$$(P \otimes Q, C([\Gamma_1, \Gamma_2])) = k_P \cdot k_Q(P, \Gamma_1)(Q, \Gamma_2)$$

$$+ \sum_{P = XY} (X, \Gamma_1)(\{Y, Q\}, \Gamma_2) - \sum_{Q = XY} (\{P, X\}, \Gamma_1)(Y, \Gamma_2) - (1 \leftrightarrow 2).$$
(6.13)

But $({Y,Q}, \Gamma_2) = (Y \otimes Q, C(\Gamma_2))$ and $({P,X}, \Gamma_1) = (P \otimes X, C(\Gamma_1))$, and so (6.13) is equivalent to (6.11). \Box

The recursive relation, (6.11), can be solved to find an explicit formula for $C(\Gamma)$. To see this, write

$$D(\Gamma) := k_1 \cdot k_2 \,\Gamma_1 \wedge \Gamma_2, \tag{6.14}$$

for Lie monomials $\Gamma = [\Gamma_1, \Gamma_2]$. Nesting (6.11) leads to a sum over the edges in the tree T_{Γ} . For $I \in \Gamma$ an edge in the tree T_{Γ} , let Γ_I be the associated Lie monomial. For example, if $\Gamma = [[1, 2], [3, 4]]$, then $\Gamma_{12} = [1, 2]$. Then the solution to the recursion, (6.11), is

$$C(\Gamma) = \sum_{I \in \Gamma} \Gamma / \Gamma_I [D(\Gamma_I)], \qquad (6.15)$$

where $\Gamma/\Gamma_I[D(\Gamma_I)]$ denotes the replacement, in Γ , of Γ_I by $D(\Gamma_I)$.

For example, if $\Gamma = [[1, 2], [3, 4]]$, then $C(\Gamma)$ is

$$C(\Gamma) = D(\Gamma) + \Gamma / \Gamma_{12}[D(\Gamma_{12})] + \Gamma / \Gamma_{34}[D(\Gamma_{34})], \qquad (6.16)$$

where

$$\Gamma/\Gamma_{34}[D(\Gamma_{34})] = s_{34}[[1,2], 3 \otimes 4] = s_{34}\left([[1,2],3] \otimes 4 + 3 \otimes [[1,2],4]\right), \tag{6.17}$$

and

$$D(\Gamma) = k_{12} \cdot k_{34} [1, 2] \wedge [3, 4].$$
(6.18)

6.1.1. The contact-term map and equations of motion

The contact term map plays a role in the equations of motion of the V_{Γ} [6,26,22]. Associated to the V_{Γ} are SYM Berends-Giele currents, $M_P = V(b(P))$, where $V(\Gamma) := V_{\Gamma}$. For example,

$$M_1 = V_1, \quad M_{12} = \frac{V_{[1,2]}}{s_{12}}, \quad M_{123} = \frac{V_{[1,2],3]}}{s_{12}s_{123}} + \frac{V_{[1,[2,3]]}}{s_{23}s_{123}}.$$
 (6.19)

The equation of motion of M_P under the action of the pure spinor BRST charge Q is given by [26]

$$QM_P = \sum_{XY=P} M_X M_Y \,. \tag{6.20}$$

Whereas the equation of motion for the local superfields V_{Γ} can be written as

$$QV_{\Gamma} = \frac{1}{2} (V \otimes V, C(\Gamma)) = \frac{1}{2} \sum_{P,Q} V_{\ell(P)} V_{\ell(Q)} (P \otimes Q, C(\Gamma)),$$
(6.21)

where the sum is over a basis. For example,

$$QV_{[1,2]} = (k_1 \cdot k_2)V_1V_2,$$

$$QV_{[1,2],3]} = (k_1 \cdot k_2)(V_{[1,3]}V_2 + V_1V_{[2,3]}) + (k_{12} \cdot k_3)V_{[1,2]}V_3,$$

$$QV_{[1,[2,3]]} = (k_2 \cdot k_3)(V_{[1,2]}V_3 + V_2V_{[1,3]}) + (k_1 \cdot k_{23})V_1V_{[2,3]},$$
(6.22)

and it can be checked that these imply (6.20) for P = 123. In fact, given (6.6), equation (6.21) implies equation (6.20), as explained in [22]. This was previously only known from explicit calculations at low multiplicities.

7. BCJ numerators

In the previous sections we used Berends-Giele currents to recast and prove relations for our Lie polynomial version of biadjoint scalar theory. When dressed with BCJ numerators these results apply directly to other coloured theories. In this section, we first argue that any coloured theory that admits the Berends-Giele framework can be understood in this way. There are clear distinctions between the behaviour of numerators for on-shell amplitudes, versus those for the partially off-shell Berends-Giele currents; for a given Berends-Giele description we will see that numerators are unique, but the Berends-Giele description itself has a gauge freedom as exploited in [26]. We then discuss explicit examples of numerators $N_{\Gamma}^{\text{theory}}$ for different theories.

7.1. BCJ numerators for coloured theories

Many gauge theories have perturbation expansions that can be expanded in colour factors of the form (2.20); this is the case for any gauge theory whose Lagrangian is second order and single trace in the Lie algebra, with interaction terms formed out of total Lie bracketings. For such a theory, there is an iteration for \mathscr{L} -valued fields, analogous to the one for biadjoint scalar in §3 and for Yang-Mills in appendix A. For a particular gauge choice, this iteration generates colour ordered Berends-Giele currents, $B^{\text{theory}}(P)$, with the partial amplitudes of the theory given by $\mathcal{A}^{\text{theory}}(Pn) = \lim_{s_P \to 0} s_P B^{\text{theory}}(P) \cdot \epsilon_n$, where ϵ_n is the polarization of the *n*th particle. These partial amplitudes trivially satisfy shuffle relations [41] as a consequence of the BG currents being Lie polynomials. The amplitudes $\mathcal{A}(Pn)$ are invariant under field redefinitions and gauge transformations, but the Berends-Giele currents $B^{\text{theory}}(P)$ are not invariant. For a coloured theory in the double copy, we now consider how the currents $B^{\text{theory}}(P)$ are related to b(P).

A BCJ numerator associates every Lie monomial Γ with a function $N_{\Gamma}^{\text{theory}} \in \mathcal{K}^{\text{theory}}$. Here $\mathcal{K}^{\text{theory}}$ is the space of functions of the kinematic data. For example, for the nonlinear sigma model, $\mathcal{K}^{\text{NLSM}}$ are functions of the Mandelstam invariants. For Yang Mills, \mathcal{K}^{YM} consists of functions that are also multilinear in the polarisation vectors of the gluons. As observed in [10], the statement of colour kinematics duality is that $\Gamma \mapsto N_{\Gamma}^{\text{theory}}$ defines a homomorphism

$$N^{\text{theory}}: \mathscr{L} \to \mathcal{K}^{\text{theory}}.$$
 (7.1)

Instead of considering BCJ numerators for *amplitudes*, we can look for maps, $\tilde{N}^{\text{theory}}$, which relate BG currents to b(P):

$$B^{\text{theory}}(P) = \tilde{N}^{\text{theory}}(b(P)).$$
(7.2)

In other words, we regard \tilde{N}_{Γ} as (off-shell) BCJ numerators for the BG currents of the theory. The numerators \tilde{N}_{Γ} may have free indices that N_{Γ} does not have (e.g. for YM, \tilde{N}_{Γ} has a free gluon polarization index). This almost trivial change of perspective has an interesting consequence.

Dropping the superscript 'theory' from now on, fix some gauge theory, and, assuming some gauge choices, let B(P) be the BG currents of the theory in some gauge. The results of §5 show that we can invert b(P) using (5.5) to write

$$\tilde{N}_{\Gamma} := B(\{\Gamma\}). \tag{7.3}$$

Here $\{\Gamma\}$ is only well-defined as an element of \mathscr{L}^* , but $B(\{\Gamma\})$ is well defined since, as we explain above, $B^{\text{theory}}(R \sqcup S) = 0$ for $R, S \neq \emptyset$. Moreover, $\Gamma \mapsto \tilde{N}_{\Gamma}$ is a homomorphism, because the S-bracket is Lie. The key point is that, given some set of B(P), the \tilde{N}_{Γ} defined by (7.3) are unique.

It might be helpful to describe (7.2) and (7.3) more explicitly in a basis. Using (5.17),

$$\tilde{N}_{\ell[P]} = B(\ell\{P\}) = \sum_{Q \in Basis} S^{\ell}(P|Q)B(Q), \qquad (7.4)$$

where $S^{\ell}(P|Q)$ is the generalized KLT matrix. If we multiply by s_P , contract free indices with the *n*th particle, and take the limit $s_P \to 0$, (7.4) becomes a well known formula for amplitude BCJ numerators, given in [42] (see also the discussion in §5 of [40]). Then (7.2) reads

$$N(b(P)) = \sum_{Q \in Basis} N_{\ell[Q]} \, b(P|Q) = \sum_{Q,R \in Basis} S^{\ell}(Q|R) \, B(R) \, b(P|Q) = B(P) \,. \tag{7.5}$$

Thus the existence of 'off-shell' numerators is generic and unique, given a choice of Berends-Giele currents.

This is in sharp contradistinction with the *on-shell* BCJ numerators for amplitudes. On-shell BCJ numerators are subject to a gauge freedom spanned by numerators of the form

$$N_{\Gamma}^{\text{gauge}} = \sum_{R,S} C_{R,S}(\{R,S\},\Gamma), \qquad (7.6)$$

for some arbitrary kinematic functions $C_{R,S} \in \mathcal{K}$. These contribute the following to the BG currents:

$$N_{\Gamma}^{\text{gauge}}(b(P)) = \sum_{R,S} C_{R,S} b(P|\{R,S\}) = \sum_{R,S} C_{R,S}(P,[b(R),b(S)]), \quad (7.7)$$

This contribution vanishes on-shell, because the RHS (7.7) has no $1/s_P$ pole, and so vanishes when multiplied by s_P , in the $s_P \to 0$ limit. It was this gauge freedom in a different guise that led to the original discovery of the BCJ relations in [3], where it was argued that there are (n-2)! - (n-3)! independent pure gauge numerators of this form. However, (7.7) shows that these no longer vanish off-shell. The off-shell numerators are therefore not subject to the freedom, (7.6), and are unique once a choice of Berends Giele formulation has been made.

BCJ numerators for amplitudes, N_{Γ} , are said to be *local* if they contain no poles in the Mandelstam variables.¹⁴ Local BCJ numerators are known for both the nonlinear sigma model (NLSM), [42,40] and for (super-)Yang-Mills [43,15,22,44,45,11] (see also [46] for theories with deformations $\alpha' F^3$ and ${\alpha'}^2 F^4$) see [5] for a review.

If the off-shell numerators of a theory are local, they restrict to give local on-shell numerators for the amplitudes of the theory.¹⁵ But, for a generic theory there is no reason

¹⁴ For a coloured theory, BCJ numerators can be obtained when the fundamental BCJ identities are satisfied by inverting on an (n-3)! basis, but this will lead to spurious poles in general.

¹⁵ An arbitrary set of local on-shell BCJ numerators for the theory may not be the restriction of the off-shell numerators, because of the gauge freedom, (7.6).

to expect that the unique *off-shell* numerators obtained from (7.3) will be local. Indeed, an obstruction to locality for Yang-Mills Berends-Giele currents in Lorenz gauge is identified in [15,22,26]. This led the authors to the introduction of 'BCJ gauge' in which local numerators are obtained.

If a theory does not admit any set of local off-shell numerators, this would prevent it from participating in a KLT relation:

$$M = \sum_{P,Q \in Basis} S^{\ell}(P|Q)B(P)\tilde{B}(Q)$$
(7.8)

where $\tilde{B}(Q)$ might be another coloured theory. Since $S^{\ell}(P|Q)$ cancels one copy of b(P) in the product, locality of the numerators implies that the singularities of M arise only from one copy of b(P). In other words, M has singularities consistent with amplitude factorization. Without locality of the numerators, the singularity and factorisation structure of Mwould not be consistent, and so M would not come from a local field theory. The existence of local numerators is therefore what makes the theories in the BCJ web special.

If the off-shell numerators, (7.3), of a gauge theory are local, this implies that the theory satisfies the on-shell BCJ relations. Indeed,

$$B(\{P,Q\}) = N(b(\{P,Q\})).$$
(7.9)

If N is local, (7.9) will have no $1/s_{PQ}$ pole, since $b(\{P,Q\})$ has no $1/s_{PQ}$ pole. Then the partial amplitudes associated to B(P) satisfy

$$A^{\text{theory}}(\{P,Q\},n) = \lim_{s_{PQ}\to 0} s_{PQ}B^{\text{theory}}(\{P,Q\}) \cdot \epsilon_n = 0, \qquad (7.10)$$

which are the fundamental BCJ relations. Given this, it is reasonable conjecture the converse: that if a theory's partial amplitudes satisfy the BCJ relations, then there exists a field redefinition and gauge fixing of its Berends-Giele recursion so that it has *local* numerators. As discussed in [15], for (super)Yang-Mills the locality of the numerators following from Berends-Giele currents as in (7.3) is achieved in the so-called *BCJ gauge* [26]. This gauge is characterized by multiparticle fields labelled by planar binary trees satisfying generalized Jacobi identities and can be obtained via a standard finite gauge transformation of the gauge (super)fields [26,22].

The following subsections review particular examples.

7.2. Biadjoint scalar

For the biadjoint scalar theory,¹⁶ the numerators take values in $\mathcal{K}^{\text{Biadjoint}} = W$ i.e., in words Q representing colour orderings for the second Lie algebra:

$$N(Q)_{\Gamma}^{\text{Biadjoint}} = (Q, \Gamma).$$
(7.11)

If $\Gamma_1 + \Gamma_2 + \Gamma_3 = 0$ follows from the Jacobi identity, then $N_{\Gamma_1} + N_{\Gamma_2} + N_{\Gamma_3} = (Q, \Gamma_1 + \Gamma_2 + \Gamma_3) = 0$ follows immediately. This yields b(P|Q) = (Q, b(P)) as defined earlier.

Following [8], it was pointed out in [14] that this Berends-Giele multiparticle field b(iP|iQ) gives rise to an efficient algorithm to compute the inverse of the KLT matrix $S(P|Q)_i$, but no direct algebraic proof was given for this statement [13]¹⁷. This has now been proven in section 5.

The biadjoint amplitudes m(Pn|Qn) are then given by projecting the binary tree expansion b(Q) of (3.22) against P [13],

$$m(Pn|Qn) = \lim_{s_P \to 0} s_P(P, b(Q))) = \lim_{s_P \to 0} s_P b(P|Q).$$
(7.12)

The Kleiss-Kuijf relations follow from Ree's theorem (2.6) as $b(R \sqcup S | Q) = 0$ because b(Q) is a Lie polynomial, while the BCJ relations follow from the $\{,\}$ -bracket as discussed in section 4.2.

Example of biadjoint amplitudes are obtained from b(123) and b(1234):

$$m(1234|1234) = \frac{\langle 123, [[1,2],3] \rangle}{s_{12}} + \frac{\langle 123, [1,[2,3]] \rangle}{s_{23}} = \frac{1}{s_{12}} + \frac{1}{s_{23}},$$
(7.13)
$$m(12345|14235) = \frac{\langle 1234, [[[1,4],2],3] \rangle}{s_{14}s_{124}} + \frac{\langle 1234, [[1,[4,2]],3] \rangle}{s_{124}s_{24}} + \frac{\langle 1234, [[1,4],[2,3]] \rangle}{s_{14}s_{23}} + \frac{\langle 1234, [1,[4,2],3] \rangle}{s_{24}s_{234}} + \frac{\langle 1234, [1,[4,[2,3]]] \rangle}{s_{234}s_{23}} = -\frac{1}{s_{23}s_{234}},$$

where the expansion of b(123) and b(1234) can be found in (3.13).

¹⁶ This was an early example of the benefits of using combinatorial structures; biadjoint scalar tree amplitudes m(Pn|Qn) were obtained in [8] from planar binary trees. As shown in [14], the solution to the biadjoint scalar field equations yields a recursion for Berends-Giele currents b(P|Q) depending on two color orderings from which the amplitudes are obtained via the Berends-Giele amplitude formula. In [13], these double fields were reformulated as a map on the binary tree expansion (3.10), given by (3.20).

¹⁷ The statement that the KLT matrix is the inverse to the "biadjoint amplitudes" was argued on general grounds using intersection theory by Mizera [21]. The question in [13] was whether the two matrices $S(P|Q)_i$ and b(P|Q) defined by the precise recursive formulas given in [40] and [14] could be shown to be mutually inverse directly.

7.3. NLSM

NLSM amplitudes can be studied by BG recursion [47], as above for biadjoint scalar theory. Although we do not prove it here, experimental evidence suggested the following formula for (off-shell) BCJ numerators for NLSM:

$$N_{\Gamma}^{\text{NLSM}} := \sum_{P \in Basis} (P, \Gamma) S^{\ell}(P|P), \quad \text{for } |\Gamma| = n$$
(7.14)

where $S^{\ell}(P|Q)$ is the generalized KLT matrix. It is clear that $\Gamma \mapsto N_{\Gamma}^{\text{NLSM}}$ is a homomorphism. In particular, if $\Gamma_1 + \Gamma_2 + \Gamma_3 = 0$ is a triple of Lie monomials that vanishes, then the corresponding numerators satisfy the BCJ numerator identity $N_{\Gamma_1} + N_{\Gamma_2} + N_{\Gamma_3} = 0$. We refer to [24] for an on-shell proof of (7.14) using CHY methods.

The NLSM amplitudes are computed from the correspondence (3.22),

$$A^{\text{NLSM}}(Pn) = \lim_{s_P \to 0} N^{\text{NLSM}}(s_P b(P)).$$
(7.15)

For example, at 4-points the numerators are

$$N^{\text{NLSM}}([[1,2],3]) = s_{12}(s_{23} + s_{13}),$$

$$N^{\text{NLSM}}([1,[2,3]]) = s_{12}(s_{23} + s_{13}) - s_{13}(s_{23} + s_{12}) = s_{23}(s_{12} - s_{13}),$$

$$N^{\text{NLSM}}([[1,3],2]) = s_{13}(s_{23} + s_{12}).$$
(7.16)

These satisfy

$$N^{\text{NLSM}}([[1,2],3]) - N^{\text{NLSM}}([1,[2,3]]) - N^{\text{NLSM}}([[1,3],2]) = 0.$$
(7.17)

Acting on b(123), we get

$$s_{123}N^{\text{NLSM}}(b(123)) = s_{12} + s_{23},$$
 (7.18)

which is the 4 point partial amplitude, $A^{\text{NLSM}}(1234)$. From the existence of the map (7.14), and the discussions in §4, it follows that the KK and BCJ relations are automatically satisfied by the NLSM amplitudes, as was proved in [48]. In [40], master BCJ numerators with fixed legs 1 and n of the NLSM amplitudes were observed in examples to be $N_{1|P|n} =$ $(-1)^{n/2}S(P|P)_1$ for even n. (7.14) has this as a special case.

7.4. Super-Yang-Mills

String theory OPEs (or supersymmetric BG recursion) can be used to recursively compute local SYM multiparticle superfields $\{A^{\Gamma}_{\alpha}, A^{\mu}_{\Gamma}, W^{\alpha}_{\Gamma}, F^{\mu\nu}_{\Gamma}\}, \mu, \nu = 1, ..., 10, \alpha = 1, ..., 16, in$ the BCJ gauge which are labelled by Lie monomials $\Gamma \in \mathscr{L}$ [6,26,22]. These can be taken to be the SYM numerators, i.e. $N^{SYM}_{\mu\Gamma} = A_{\mu\Gamma}$ etc.. As demonstrated in [26,22], the words labelling these superfields satisfy the same generalized Jacobi identities associated with the corresponding Lie monomial Γ . For example,

$$A^{\mu}_{[[1,2],[3,4]]} = A^{\mu}_{[[[1,2],3],4]} - A^{\mu}_{[[[1,2],4],3]}.$$
(7.19)

This leads to a proposal for local BCJ-satisfying numerators $N_{\mu}^{\rm SYM}$ from which SYM tree amplitudes arise from

$$\mathcal{A}^{\text{SYM}}(Pn) = A_n^{\mu} \lim_{s_P \to 0} s_P N_{\mu}^{\text{SYM}}(b(P)), \qquad (7.20)$$

where A_n^{μ} is the polarization vector of the *n*th particle while the action of N_{μ}^{SYM} on the Lie polynomials $\Gamma = [\Gamma_1, \Gamma_2]$ in (3.10) is given by

$$A_n^{\mu} N_{\mu\Gamma}^{\text{SYM}} := A_{n\mu} A_{[\Gamma_1, \Gamma_2]}^{\mu} , \qquad (7.21)$$

in terms of the $\theta = 0$ component of the local multiparticle superfield $A^{\mu}_{[\Gamma_1,\Gamma_2]}$ [6,22]. This representation *manifestly* satisfies the BCJ identities. For example, the five-point colorordered amplitudes in the Kleiss–Kuijf basis following from the maps (7.20) and (7.21) are given by

$$\mathcal{A}(12345) = \left(\frac{A^{\mu}_{[[[1,2],3],4]}}{s_{12}s_{45}} + \frac{A^{\mu}_{[1,[[2,3],4]]}}{s_{23}s_{51}} + \frac{A^{\mu}_{[[1,2],[3,4]]}}{s_{12}s_{34}} + \frac{A^{\mu}_{[[1,[2,3]],4]}}{s_{45}s_{23}} + \frac{A^{\mu}_{[1,[2,[3,4]]]}}{s_{51}s_{34}}\right)A_{5\mu}$$

together with the other 5 permutations of 2, 3, 4. It is straightforward to check that all BCJ numerator identities are manifestly satisfied. For example, comparing the above parametrization with the one in [3] leads to

$$n_3 = A^{\mu}_{[[1,2],[3,4]]} A^{\mu}_5, \qquad n_5 = A^{\mu}_{[1,[2,[3,4]]]} A^{\mu}_5, \qquad n_8 = A^{\mu}_{[[1,[4,3]],2]} A^{\mu}_5, \qquad (7.23)$$

from which the identity $n_3 - n_5 + n_8 = 0$ can easily be verified.

7.4.1. Non-local vs local BCJ numerators from Berends-Giele in the Lorenz vs BCJ gauge

As an example of the definition of BCJ-satisfying numerators (7.3) and its (non)locality properties, consider the Berends-Giele current of standard Yang-Mills theory [12] for the color-ordered five-point amplitude. As shown in [15], the standard Berends-Giele current $J^{\mu}(1234)$ of [12] can be written in terms of multiparticle fields $\hat{A}^{\mu}_{[\Gamma_1,\Gamma_2]}$ in the Lorenz gauge

$$s_{1234}J^{\mu}(1234) = \frac{\hat{A}^{\mu}_{[[[1,2],3],4]}}{s_{12}s_{45}} + \frac{\hat{A}^{\mu}_{[1,[[2,3],4]]}}{s_{23}s_{51}} + \frac{\hat{A}^{\mu}_{[[1,2],[3,4]]}}{s_{12}s_{34}} + \frac{\hat{A}^{\mu}_{[[1,[2,3]],4]}}{s_{45}s_{23}} + \frac{\hat{A}^{\mu}_{[1,[2,[3,4]]]}}{s_{51}s_{34}}, \quad (7.24)$$

where $\hat{A}^{\mu}_{[\Gamma_1,\Gamma_2]}$ are the recursive multiparticle vector potential

$$\hat{A}^{[\Gamma_1,\Gamma_2]}_{\mu} = -\frac{1}{2} \left[\hat{A}^{\Gamma_1}_{\mu} (k^{\Gamma_1} \cdot \hat{A}^{\Gamma_2}) + \hat{A}^{\Gamma_1}_{\nu} \hat{F}^{\Gamma_2}_{\mu\nu} - (\Gamma_1 \leftrightarrow \Gamma_2) \right]$$
(7.25)

and $F^{\Gamma_2}_{\mu\nu}$ are the local multiparticle field-strengths defined similarly [26,22], see for example §4.3 of [22] for the difference between A^{μ}_{Γ} and \hat{A}^{μ}_{Γ} .

Using the prescription (7.3) to obtain BCJ-satisfying numerators one gets, for example

$$N^{\mu}_{[[1,2],[3,4]]} = J^{\mu}(\{\{1,2\},\{3,4\}\}), \qquad N^{\mu}_{[[1,[4,3]],2]} = J^{\mu}(\{\{1,\{4,3\}\},2\})$$

$$N^{\mu}_{[1,[2,[3,4]]]} = J^{\mu}(\{1,\{2,\{3,4\}\}\}), \qquad (7.26)$$

leading to

$$\begin{split} N^{\mu}_{[[1,2],[3,4]]} &= s_{12}s_{34} \Big(J^{\mu}(1234)s_{23} - J^{\mu}(1243)s_{24} - J^{\mu}(2134)s_{13} + J^{\mu}(2143)s_{14} \Big) , \quad (7.27) \\ N^{\mu}_{[1,[2,[3,4]]]} &= s_{23}s_{34} \Big(J^{\mu}(1234)s_{12} - J^{\mu}(1324)s_{13} - J^{\mu}(1342)s_{13} + J^{\mu}(1432)s_{14} \Big) \\ &\quad + s_{24}s_{34} \Big(J^{\mu}(1423)s_{14} + J^{\mu}(1432)s_{14} - J^{\mu}(1243)s_{12} - J^{\mu}(1342)s_{13} \Big) , \\ N^{\mu}_{[[1,[4,3]],2]} &= s_{13}s_{34} \Big(J^{\mu}(1432)s_{23} - J^{\mu}(1342)s_{24} - J^{\mu}(4312)s_{12} + J^{\mu}(4132)s_{23} \Big) \\ &\quad + s_{14}s_{34} \Big(J^{\mu}(1432)s_{23} - J^{\mu}(3142)s_{24} - J^{\mu}(1342)s_{24} + J^{\mu}(3412)s_{12} \Big) . \end{split}$$

It is easy to see that the BCJ numerator relation $n_3 - n_5 + n_8 = 0$ is satisfied by the above representations as $N^{\mu}_{[[1,2],[3,4]]} - N^{\mu}_{[1,[2,[3,4]]]} + N^{\mu}_{[[1,[4,3]],2]} = 0$ due to the shuffle symmetry $J^{\mu}(R \sqcup S) = 0$ (note that the numerators follow from contraction with the polarization A^{μ}_5 , e.g. $n_3 = N^{\mu}_{[[1,2],[3,4]]}A^{\mu}_5$). For example, the terms proportional to $s_{14}s_{24}s_{34}$ are given by

$$-J^{\mu}(1342) - J^{\mu}(1423) - J^{\mu}(1432) - J^{\mu}(3142) = -J^{\mu}(3 \sqcup 142) = 0.$$
 (7.28)

All the other BCJ numerator relations can be similarly verified.

It can be checked by explicitly computing the BG currents in Lorenz gauge that the numerators (7.27) are *not* local. But when the Berends-Giele currents are computed in the BCJ gauge, the right-hand side of (7.27) do become local expressions. Indeed, using $A^{\mu}_{[\Gamma_1,\Gamma_2]}$ in the BCJ gauge (instead of $\hat{A}^{\mu}_{[\Gamma_1,\Gamma_2]}$ in (7.24)), the linear combinations in (7.27) yield:

$$N^{\mu}_{[[1,2],[3,4]]} = A^{\mu}_{[[1,2],[3,4]]} \qquad N^{\mu}_{[[1,[4,3]],2]} = A^{\mu}_{[[1,[4,3]],2]}$$

$$N^{\mu}_{[1,[2,[3,4]]]} = A^{\mu}_{[1,[2,[3,4]]]}$$
(7.29)

To see this note that in the BCJ gauge $A^{\mu}_{[\Gamma_1,\Gamma_2]}$ satisfies the same relations as the Lie monomial $[\Gamma_1,\Gamma_2]$ so (7.29) follow from the property $\Gamma = b(\{\Gamma\})$ proved in (5.1).

7.5. Z-theory and the open superstring

In order to upgrade the discussion in the previous subsection to the open superstring with α' corrections we will exploit the non-abelian Z-theory method to evaluate α' expansions of open string disk integrals. Recall that the string disk integrals are computed via the Berends-Giele method as

$$Z(P,n|Q,n) = \lim_{s_P \to 0} s_P b^{\alpha'}(P|Q)$$
(7.30)

where the Berends-Giele currents are computed using the equations of motion of the nonabelian Z-theory [49]. One can promote the setup of [49] to the theory of free Lie algebras by assuming the existence of α' corrections to the Catalan expansion (3.10) and defining

$$b^{\alpha'}(P|Q) = (b^{\alpha'}(P), Q)$$
(7.31)

which together with (7.30) implies that Z-theory admits a free Lie algebra representation. Using the explicit expressions of $b^{\alpha'}(P|Q)$ up to ${\alpha'}^7$ order from [49] one can show that they indeed admit a Lie-polynomial form,

$$s_{P}b^{\alpha'}(P) = \sum_{XY=P} [b^{\alpha'}(X), b^{\alpha'}(Y)]$$

$$+ {\alpha'}^{2} \zeta_{2} \sum_{XYZ=P} k_{X} \cdot k_{Y} [b^{\alpha'}(X), [b^{\alpha'}(Z), b^{\alpha'}(Y)]]$$

$$- {\alpha'}^{2} \zeta_{2} \sum_{XYZ=P} k_{Y} \cdot k_{Z} [[b^{\alpha'}(X), b^{\alpha'}(Y)], b^{\alpha'}(Z)]$$

$$+ {\alpha'}^{2} \zeta_{2} \sum_{XYZW=P} [[b^{\alpha'}(X), b^{\alpha'}(Y)], [b^{\alpha'}(W), b^{\alpha'}(Z)]]$$

$$- {\alpha'}^{2} \zeta_{2} \sum_{XYZW=P} [[b^{\alpha'}(X), b^{\alpha'}(Z)], [b^{\alpha'}(W), b^{\alpha'}(Y)]] + \mathcal{O}(\alpha'^{3})$$
(7.32)

and so on.

It is important to emphasize that the symmetries of the "domain" P and integrand Q are different, in particular $b^{\alpha'}(P|Q) \neq b^{\alpha'}(Q|P)$. The integrand Q satisfies shuffle symmetry as $b^{\alpha'}(P|R \sqcup S) = \langle b^{\alpha'}(P), R \sqcup S \rangle = 0$ because $b^{\alpha'}(P)$ is a Lie polynomial. The shuffle symmetries of the domain P are twisted by the monodromies of the disk integrals as explained in [49].

Finally, our proposal for obtaining bosonic¹⁸ open superstring disk amplitudes including α' corrections is to replace the recursion b(P) from (3.10) by its α' -corrected $b^{\alpha'}(P)$ from (7.32),

$$\mathcal{A}^{\text{string}}(P,n) = \lim_{s_P \to 0} s_P N^{\text{SYM}}_{\mu}(b^{\alpha'}(P)) A^{\mu}_n.$$
(7.33)

This proposal has been explicitly verified for the bosonic components of the disk amplitudes up to seven points and up to ${\alpha'}^3$ [50]. While the SYM amplitudes in the field-theory limit $\alpha' \to 0$ are correctly obtained using the analogous map N_{μ}^{SYM} in the Lorenz gauge, the higher α' orders of the string disk amplitude (7.33) require the BCJ gauge as in the map (7.21).

8. Conclusions

We have seen that there is much nontrivial structure in the amplitudes of coloured theories that can be formulated in the language of Lie polynomials and their dual. These impact quite generally on the study of tree-level scattering amplitudes for the theories encompassed by the double copy [5]. Important outstanding questions concern the locality of numerators and the existence and role of the kinematic algebras that should underpin them. We have seen that off-shell Berends-Giele numerators are unique up to the choices of Berends-Giele recursion itself. Since numerators are unique within a Berends-Giele framework, the locality of the corresponding numerators is a determined question. However, this question of their locality in the off-shell regime is subject to the choices involved in field redefinition and gauge; we have seen that they are not local for SYM in Lorenz gauge, but that a BCJ gauge can be found. A reasonable conjecture is that a Berends-Giele framework can be found with local numerators for any such theory that factorizes and whose amplitudes satisfy the BCJ relations.

¹⁸ Fermionic amplitudes require corrections following from a Dirac term $\sim k_P^m W_P \gamma^m W_n$ [15].

An ongoing topic of research is the identification of the kinematic algebra for a given theory, see [5] and references therein. For a given theory, take some set of BG current, B(P). Then these B(P), then we can implicitly define a kinematic bracket $\{,\}_{\mathcal{K}}$ on the associated off-shell numerators N_{Γ_1} and N_{Γ_2} by imposing the relation

$$N_{[\Gamma_1,\Gamma_2]} = B(\{[\Gamma_1,\Gamma_2]\}) = \{B(\{\Gamma_1\}), B(\{\Gamma_2\})\}_{\mathcal{K}} = \{N_{\Gamma_1}, N_{\Gamma_2}\}_{\mathcal{K}},$$
(8.1)

where $\{, \}_{\mathcal{K}}$ is the antisymmetric operation, implicitly defined by (8.1) on the image of N. It is a Lie bracket on the image of N, because N is a homomorphism. Imposing linearity in Mandelstam variables, the definition (8.1) implies an off-shell BCJ-like relation,

$$B(\{P,Q\}) = \{B(P), B(Q)\}_{\mathcal{K}},\tag{8.2}$$

where $\{,\}_{\mathcal{K}}$ is extended to act on the B(P) as

$$\{B(P), B(Q)\}_{\mathcal{K}} := \sum \frac{(P, \Gamma_1)}{s_{\Gamma_1}} \frac{(Q, \Gamma_2)}{s_{\Gamma_2}} \{N_{\Gamma_1}, N_{\Gamma_2}\}_{\mathcal{K}}.$$
(8.3)

(See [51] for an off-shell BCJ relation for NLSM, but which is not obviously of the form (8.2).) It is highly nontrivial to find a BG formulation that gives local numerators for NLSM and YM. But if a particular choice of gauge is known to give local off-shell numerators, then (8.1) expresses these local numerators as nested bracketings with respect to $\{ , \}_{\mathcal{K}}$. In this situation, it would therefore be reasonable to call $\{ , \}_{\mathcal{K}}$ the "kinematic algebra" of the theory; a clear goal in the subject is to find an intrinsic definition of such a bracket on \mathcal{K} . However, even given a local Lie bracket $\{ , \}_{\mathcal{K}}$ on the N_{Γ} , there is no guarantee that this bracket admits a consistent extension to a Lie bracket

$$\{ , \}_{\mathcal{K}} : \mathcal{K}_P \times \mathcal{K}_Q \to \mathcal{K}_{PQ},$$

$$(8.4)$$

on the whole of the kinematic spaces \mathcal{K}_P .

There are many other directions to explore. Intermediate steps in the calculations of α' expansion method from [52] can be described by the same combinatorics as the contact terms in the equation of motion for QV_P [53], therefore they should profit from framing the results in terms of the contact term map acting on Lie polynomials. Given that the Drinfeld associator itself is a *Lie series* this connection promises to reveal more synergies between mathematical ideas and scattering amplitudes. Similarly, the Berends-Giele formulation of the non-abelian Z-theory to compute α' corrections to string disk integrals [49] induces α'

corrections to the recursion (3.10) of planar binary trees as seen in (7.32). It is natural to ask whether the recursion (7.32) itself is generated recursively from purely combinatorial methods. The appearance of factors of $k_X \cdot k_Y$ suggest that the *S*-bracket may play a role. The combinatorial understanding of the Drinfeld method discussed in [54] is an encouraging development in this direction.

Given that the field-theory KLT matrix $S^{\ell}(P|Q)_i$ is the inverse of the biadjoint Berends-Giele double current b(iR|iS) as in (5.28), it is natural to look for the inverse of the α' -corrected double current $b^{\alpha'}(P|Q)$ from [49] to obtain α' corrections to the KLT matrix. Note that these corrections will not coincide with those in the string theory KLT matrix since odd and multiple zeta values are absent from the latter (see e.g. [19,55]) but must be present in the former.

Similarly, the structures studied in this paper can be realized in the context of the CHY formulae, ambitwistor strings and the geometry of $\mathcal{M}_{0,n}$. Much is already well known, for example [56,57,10], but more appears in [24]. A particular challenge is to better understand numerators from this perspective.

Again another challenge is to take these insights to higher loops. Tree level colour factors are labelled by Lie monomials, and partial tree amplitudes are labelled by permutations. This is just the leading order avatar of the more general story, at arbitrary orders in the perturbation series, in which colour factors are associated to ribbon graphs, and partial amplitudes are labelled by marked surfaces with boundary (possibly with punctures and nontrivial genus). The results in the present paper are essentially all derived from the Jacobi identity satisfied by Lie monomials. More generally, colour factors labelled by ribbon graphs at higher order satisfy analogous identities; again more appears in [24].

The maps and techniques discussed in this paper show that free Lie algebras permeate the theory of scattering amplitudes. They also raise the expectations that many more elegant results are yet to be discovered.

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Appendix A. Berends-Giele recursion for Yang–Mills in the free Lie algebra

Here we repeat the discussion of section 3 replacing the biadjoint scalar by Yang-Mills. Consider pure Yang–Mills theory in d-dimensions with the Lagrangian

$$\mathcal{L}_{YM} = \frac{1}{4} \operatorname{tr}(\mathbb{F}_{\mu\nu} \mathbb{F}^{\mu\nu}), \qquad \mathbb{F}_{\mu\nu} := -[\nabla_{\mu}, \nabla_{\nu}].$$
(A.1)

The trace is over the generators t^a of a Lie algebra, \mathfrak{g} , the covariant derivative is given by $\nabla_{\mu} = \partial_{\mu} - \mathbb{A}_{\mu}$ and $\mathbb{A}_{\mu} = \mathbb{A}^a_{\mu} t^a$ is the gluon potential. In the Lorenz gauge, $\partial_{\mu} \mathbb{A}^{\mu} = 0$, the field equation $[\nabla_{\mu}, \mathbb{F}^{\mu\nu}] = 0$ becomes

$$\Box \mathbb{A}^{\nu}(x) = [\mathbb{A}_{\mu}(x), \partial^{\mu} \mathbb{A}^{\nu}(x)] + [\mathbb{A}_{\mu}(x), \mathbb{F}^{\mu\nu}(x)].$$
(A.2)

We now define a perturbative solution \mathbb{A} that takes values in \mathscr{L} rather than some given Lie algebra L. (A.2) leads to the following iteration for $\mathbb{A}_{\leq n}$, with values in $\mathscr{L}_{\leq n}$:

$$\begin{aligned} \mathbb{A}_{\leq n+1}^{\nu} &= \mathbb{A}_{1}^{\nu} + \operatorname{proj}_{\mathscr{L}_{\leq n+1}} \Box^{-1} \left([\mathbb{A}_{\leq n}^{\mu}(x), \partial_{\mu} \mathbb{A}_{\leq n}^{\nu}(x)] + [\mathbb{A}_{\leq n\mu}(x), \mathbb{F}_{\leq n}^{\mu\nu}(x)] \right), \quad (A.3) \\ \mathbb{F}_{\leq n+1}^{\mu\nu} &= \operatorname{proj}_{\mathscr{L}_{\leq N+1}} 2\partial^{[\mu} \mathbb{A}_{\leq n+1}^{\nu]} - [\mathbb{A}_{\leq n}^{\mu}, \mathbb{A}_{\leq n}^{\nu}]. \end{aligned}$$

where $\operatorname{proj}_{\mathscr{L}_{\leq n+1}}$ projects onto the $\mathscr{L}_{\leq n+1}$ part. The recursion is seeded by

$$\mathbb{A}_{1}^{\mu} = \sum_{i \in \mathbb{N}} e_{i}^{\mu} \exp(ik_{i} \cdot x) i \tag{A.4}$$

where the letter *i* replaces the usual generator $t_i^a \in \mathfrak{g}$ and e_i^{μ} is the polarization vector of the *i*th gluon. Note that \Box^{-1} acts on momentum eigenstates $\exp(ik \cdot x)$ to give $-1/k^2$.

To obtain the amplitude, define the multi-particle field \mathbb{A}_{n-1}^{μ} , which is the degree n-1 part of $\mathbb{A}_{\leq n-1}^{\mu}$:

$$\mathbb{A}_{n-1}^{\mu} := \operatorname{proj}_{\mathscr{L}_{n-1}} \mathbb{A}_{\leq n-1}^{\mu}.$$
(A.5)

In terms of \mathbb{A}_{n-1}^{μ} , the \mathscr{L} -valued version of the amplitude is

$$\mathcal{A}_n = s_{12...n-1} e^{-ik_{12...n-1} \cdot x} e_{n\mu} \mathbb{A}_{n-1}^{\mu}, \qquad (A.6)$$

where e_n^{μ} is the polarization of the *n*th gluon. The colour polarizations $t_1, \ldots, t_n \in \mathfrak{g}$ define the map $\mathbf{t} : \mathscr{L} \to \mathfrak{g}$, and the YM amplitude is then given by $t_n^a \mathbf{t}(\mathcal{A}_n)^a$. The partial tree amplitudes are given by

$$\mathcal{A}_n(P,n) := (P, \mathcal{A}_n), \tag{A.7}$$

for permutations P.

The Berends-Giele current for an ordering P is

$$J_P^{\mu} := (P, \mathbb{A}^{\mu}) \exp(-ik_P \cdot x), \tag{A.8}$$

where the factor of $\exp(-ik_P \cdot x)$ removes the x-dependence in $(P, \mathbb{A}^{\mu}_{|P|})$. J^{μ}_{P} is linear in each e_i with $i \in P$, with coefficients that depend only on the momenta. Taking inner products (A.3) with a word P gives the YM Berends-Giele recursion relation:

$$J_{P}^{\mu} = \frac{1}{s_{P}} \sum_{XY=P} \left[J_{X}^{\mu} (k_{X} \cdot J_{Y}) + J_{X}^{\nu} \mathcal{F}_{Y}^{\mu\nu} - (X \leftrightarrow Y) \right],$$
(A.9)
$$\mathcal{F}_{Y}^{\mu\nu} = k_{Y}^{\mu} J_{Y}^{\nu} - k_{Y}^{\nu} J_{Y}^{\mu} - \sum_{RS=Y} \left(J_{R}^{\mu} J_{S}^{\nu} - J_{R}^{\nu} J_{S}^{\mu} \right)$$

where J_i^{μ} for a letter *i* is equal to the polarization vector e_i^{μ} of the *i*-th gluon. Here again we have used the following deconcatenation identity,

$$(P, \Gamma) = \sum_{XY=P} (X, \Gamma_1)(Y, \Gamma_2) - (X, \Gamma_2)(Y, \Gamma_1), \qquad (A.10)$$

for a word P, and a Lie monomial $\Gamma = [\Gamma_1, \Gamma_2]$.

Since $\mathbb{A}_n \in \mathscr{L}$, it follows from Ree's theorem that

$$J^m_{R\sqcup S} = 0, \qquad (A.11)$$

cf. the discussions in [41] and [26]. In terms of J_P^{μ} , the YM partial tree amplitudes are [12]

$$\mathcal{A}^{\rm YM}(Pn) = s_P J_P \cdot J_n \,, \tag{A.12}$$

which is equivalent to the earlier definition, (A.7).

Appendix B. The main property of the S bracket

This appendix proves the following proposition, from §4.2:

Proposition. For $P, Q \in \mathscr{L}^*$, the S bracket satisfies

$$b(\{P,Q\}) = [b(P), b(Q)], \qquad (B.1)$$

i.e., b maps the S-bracket to the Lie bracket.

The proof uses the following definitions. The deconcatenation coproduct $\delta : W \to W \otimes W$ is defined on words P by

$$\delta(P) = \sum_{XY=P} X \otimes Y.$$
(B.2)

Write $\delta'(P)$ to be as above but with the sum restricted to non-empty words X, Y. Further, write

$$\delta_{\wedge}(P) = \sum_{XY=P} X \otimes Y - Y \otimes X, \qquad (B.3)$$

and similarly for δ'_{\wedge} . Finally, define the S-bracket to act on $\mathscr{L}^* \otimes \mathscr{L}^*$ as

$$\{X \otimes Y, Q\} = X \otimes \{Y, Q\}, \qquad \{P, X \otimes Y\} = \{P, X\} \otimes Y.$$
(B.4)

Lemma. The deconcatenation of the S-bracket is

$$\delta'\{P,Q\} \sim \{\delta_{\wedge}P,Q\} + \{P,\delta_{\wedge}Q\} + s_{P,Q}P \otimes Q.$$
(B.5)

Proof. First note that for non-empty X, Y

$$\delta'(XY) = \delta'(X) \cdot (e \otimes Y) + (X \otimes e) \cdot \delta'(Y), +X \otimes Y, \qquad (B.6)$$

where e is the empty word. So

$$\delta'\{P,Q\} = \delta'r^*(P) \star \ell^*(Q) + r^*(P) \star \delta'\ell^*(b) + \sum_{P=XiY,Q=ZjW} s_{ij}(X \sqcup \overline{Y})i \otimes j(Z \sqcup W), \quad (B.7)$$

where we have used the explicit formulas for ℓ^* and r^* of (2.19). The KK relations give $XiY \sim i(\overline{X} \sqcup Y) \sim (X \sqcup \overline{Y})i$, so the third term in (B.7) sums to $s_{P,Q}P \otimes Q$. The deconcatenation of ℓ^* and r^* can be evaluated using (2.19). For example, the deconcatenation of a single term in (2.19) is

$$\delta(i\overline{X}\sqcup Y) = \sum_{X=X_1X_2} \sum_{Y=Y_1Y_2} i\overline{X}_2 \sqcup Y_2 \otimes \overline{X}_1 \sqcup Y_2.$$
(B.8)

Total shuffles vanish in \mathscr{L}^* . So, in $\mathscr{L}^* \otimes \mathscr{L}^*$,

$$\delta(i\overline{X}\sqcup Y) = \sum_{Y=Y_1Y_2} i\overline{X}\sqcup Y_2 \otimes Y_2 + \sum_{X=X_1X_2} i\overline{X}_2\sqcup Y \otimes \overline{X}_1.$$
(B.9)

This can be used to find that

$$\delta'(\ell^*(P)) = (\ell^* \otimes 1) \circ \delta'_{\wedge}(P), \tag{B.10}$$

and a similar identity for $r^*(Q)$.

Proof. (of the proposition) When P, Q are single letters, (B.1) follows directly. Note that BG recursion can be written as

$$b(P) = \frac{1}{s_P} \sum_{X,Y} (X \otimes Y, \delta'(P)) [b(X), b(Y)], \qquad (B.11)$$

for any homogeneous $P \in \mathscr{L}^*$. Substituting $\{P, Q\}$ for P into this recursion, the lemma gives that

$$s_{PQ}b(\{P,Q\}) = \sum_{X,Y} (X \otimes Y, \{\delta'_{\wedge}P,Q\} + \{P,\delta'_{\wedge}(Q)\} + s_{P,Q}P \otimes Q) \ [b(X),b(Y)],$$

$$= s_{P,Q}[b(P),b(Q)] + \sum_{P=XY} [b(X),b(\{Y,Q\})] - (X \leftrightarrow Y) + \sum_{Q=XY} [b(\{P,X\}),b(Y)] - (X \leftrightarrow Y).$$

(B.12)

By induction, write $b({Y,Q}) = [b(Y), B(Q)]$ in the second last line to find

$$\sum_{P=XY} [b(X), [b(Y), b(Q)] - (X \leftrightarrow Y) = \sum_{P=XY} [[b(X), b(Y)], b(Q)] = s_P[b(P), b(Q)],$$
(B.13)

using the Jacobi identity followed by BG recursion. The same argument applied to the third line shows that the RHS of (B.12) is [b(P), b(Q)] multiplied by s_{PQ} .

Appendix C. The KLT matrix formula

This appendix obtains again the standard formula for the KLT matrix,

$$S^{\ell}(1A|1B) = \prod_{i=2}^{n} s_{i,A_i(AB)},$$
(C.1)

where $A_i(AB)$ is the subset of $\{1, 2, 3, ..., n\}$ containing all letters that both precede *i* in 1*B* and follow *i* in 1*A*. We explicitly compute $S^{\ell}(12...n|1A)$ by expanding $\ell[12...n]$, which is in spirit similar to the argument in [16].

The main idea is to iteratively apply the main property of the S-bracket:

$$[b(P), k] = b(\{P, k\}), \tag{C.2}$$

for a letter k. Using the formula for $\{P, k\}$ (equation (4.10)), this gives

$$[\dots [[1, 2]3] \dots, n] = s_{12}[\dots [b(12), 3] \dots, n]$$

= $s_{12}s_{1,3}[\dots [b(132), 4] \dots, n]$
+ $s_{12}s_{12,3}[\dots [b(123), 4] \dots, n]$
= \dots (C.3)

The RHS is the nested sum,

$$s_{12}\left(\sum_{12=A_2B_2}s_{2,A_2}\left(\ldots\left(\sum_{A_{n-1}nB_{n-1}-A_nB_n}s_{n,A_n}b(A_nnB_n)\right)\ldots\right)\right)\right).$$
 (C.4)

Here all the words A_i begin with the letter 1 and by convention $s_{i,A} = 0$ when A is empty. $S^{\ell}(12...n|1A)$ is the coefficient of b(1A) in (C.4). Reversing the order of the summations gives this coefficient as

$$S^{\ell}(12...n|1A) = \prod_{i=2}^{n} \left(\sum_{C_i = A_i i B_i} s_{i,A_i} \right)$$
(C.5)

where C_i is the word 1A with the letters $1, \ldots, i-1$ removed. In other words, A_i is a word in the letters j such that j < i in the ordering 1A and i < j in the ordering $12 \ldots n$.

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