

Covariant color-kinematics duality, Hopf algebras, and permutohedraQu Cao^{1,6,*}, Jin Dong^{1,5,†}, Song He^{1,2,3,4,‡} and Yao-Qi Zhang^{1,5,§}¹CAS Key Laboratory of Theoretical Physics, Institute of Theoretical Physics,
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Based on the covariant color-kinematics duality, we investigate combinatorial and algebraic structures underlying their Bern-Carrasco-Johansson (BCJ) numerators of tree-level amplitudes in Yang-Mills-scalar (YMS) theory. The closed formulas for BCJ numerators of YMS amplitudes and the pure-YM ones exhibit nice quasishuffle Hopf algebra structures, and interestingly they can be viewed as summing over boundaries of all dimensions of a combinatorial permutohedron. In particular, the numerator with two scalars and $n - 2$ gluons contains Fubini number (\mathcal{F}_{n-2}) of terms in one-to-one correspondence with boundaries of a $(n - 3)$ -dimensional permutohedron, and each of them has its own spurious-pole structures and a gauge-invariant numerator (both depending on reference momenta). From such Hopf algebra or permutohedron structure, we derive new recursion relations for the numerators and intriguing “factorization” on each spurious pole/facet of the permutohedron. Similar results hold for general YMS numerators and the pure-YM ones. Finally, with a special choice of reference momenta, our results imply BCJ numerators in a heavy-mass effective field theory with two massive particles and $n - 2$ gluons/gravitons: we observe highly nontrivial cancellations in the heavy-mass limit, leading to new formulas for the effective numerators that resemble those obtained in recent works.

DOI: [10.1103/PhysRevD.107.026022](https://doi.org/10.1103/PhysRevD.107.026022)**I. INTRODUCTION**

Despite very different natures, gauge theories and gravity have deep connections; one of the oldest and the most prominent example is the double copy structure [1–3]. Originally it was discovered from Kawai-Lewellen-Tye relations [1] in string theory, and a modern realization of double copy has relied on the duality between color and kinematics for gauge theory amplitudes, where the Bern-Carrasco-Johansson (BCJ) kinematic numerators satisfy the same Jacobi relations as the color factors. The duality and double copy have led to tremendous progress in the

study of amplitudes both in gauge theory and gravity (see [4–6] and references therein). More recently, the authors of [7] have revealed a so-called covariant color kinematics (CCK) duality for a large class of theories including Yang-Mills theory (YM) and its coupling to biadjoint ϕ^3 [YM scalar (YMS)]. As a consequence, the duality implies new, closed-form expression for BCJ numerators of all tree-level amplitudes in YMS and YM theories. Previous works on BCJ numerators and kinematic algebras include [8–22] and references therein.

On the other hand, recent years have seen progress on revealing new geometric/combinatorial structures underlying scattering amplitudes, e.g., from the (all-loop) amplituhedron of supersymmetric Yang-Mills [23] to the associahedron for biadjoint ϕ^3 at tree level [24] (with extensions to string scattering [25]). It is natural to look for hints of such structures underlying YM and gravity amplitudes; instead of directly working with tree amplitudes, one may decompose the problem and ask a somewhat strange question as a first step: are there combinatorial structures underlying BCJ numerators?

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In this note, we take BCJ numerators from CCK duality [7] as inputs and present preliminary evidence for such structures: in addition to the more familiar quasishuffle Hopf algebras [26], we find hidden combinatorial permutohedra [27] for BCJ numerators. Any BCJ numerator can be written as the sum over all boundaries of a permutohedron (or terms from a quasishuffle product); for a codimension d boundary (length- d term), it contains a product of $d + 1$ factors each with a spurious pole and a gauge-invariant numerator. We will focus on the case with two scalars and $n - 2$ gluons, which corresponds to a $(n - 3)$ -dimensional permutohedron, and it has Fubini number \mathcal{F}_{n-2} boundaries with codimensions $d = 0, 1, \dots, n - 3$; each boundary is labeled by $d + 1$ subsets, and for each factor labeled by such a set both the numerator (which is gauge invariant in the gluons) and the (spurious pole) denominator are given by Lorentz products of momenta and polarizations, as well as the reference momenta. Apart from being the most illustrative BCJ numerators of YMS cases, we will also see that they give nice BCJ numerators in the heavy-mass effective theory (HEFT) [28–35] as well as decoupling limit into pure YM amplitudes. BCJ numerators in HEFT have attracted lots of interest recently for their roles in the computation of gravitational amplitudes for black-hole scattering and gravitational waves [36] (cf. [37–45] for some recent works). We will take the heavy-mass limit of YMs amplitude, and (as we have checked up to $n = 10$) highly nontrivial cancellations lead to a nice formula for BCJ numerators in HEFT that correspond to \mathcal{P}_{n-3} (one dimension lower).

Furthermore, our results imply new recursion relations and surprisingly, “factorization” properties of BCJ numerators on facets of permutohedra; all these can be extended to BCJ numerators of general YMS amplitudes, which in turn combine into a formula for the YM case as well. For the latter, we can then turn the logic around: since the BCJ numerators are manifestly gauge invariant in $n - 1$ gluons, by showing that all spurious poles indeed cancel in the amplitude based on such “factorizations,” it follows from the uniqueness theorem of [46] that they must give correct YM and gravity amplitude (after double copy) even without knowing the CCK duality.

Let us consider color-ordered YMS amplitude $A(1^\phi, 2, \dots, n - 1, n^\phi)$ with scalars $1^\phi, n^\phi$. Its expansion onto the Kleiss-Kuij basis [47] of bidual ϕ^3 amplitudes has BCJ master numerators as coefficients reads

$$A(1^\phi, 2, \dots, n - 1, n^\phi) = \sum_{\beta \in \mathcal{S}_{n-2}} K(1, \beta, n) A^{\phi^3}(1, \beta, n), \quad (1)$$

where the sum is over $(n - 2)!$ permutations of gluons and $A^{\phi^3}(1, \beta, n) \equiv m(1, 2, \dots, n | 1, \beta, n)$ denotes bidual ϕ^3 amplitudes with the first ordering fixed to be $(1, 2, \dots, n)$. Remarkably, the BCJ numerators from CCK duality $K(1, \beta, n)$ respect the Bose symmetry of all the

$n - 2$ gluons [7]: we only need a single numerator with the ordering chosen to be $\beta = (2, \dots, n - 1)$, and all others can be obtained by relabeling; they are also gauge invariant for the gluons, which becomes manifest since the dependence on polarizations is through Lorentz products of linearized field strengths $F_i^{\mu\nu} \equiv p_i^\mu \varepsilon_i^\nu - p_i^\nu \varepsilon_i^\mu$

$$[F_\sigma]^{\mu\nu} = [F_{\sigma_1} \cdot F_{\sigma_2} \cdots F_{\sigma_{|\sigma|}}]^{\mu\nu} \quad (2)$$

for an ordered subset σ . The price to pay for these desirable properties is the presence of $2^{n-2} - 1$ spurious poles, one for each nonempty subset $I \subset \{2, \dots, n - 1\}$:

$$D_I := p_I \cdot q_I, \quad \text{with} \quad p_I := \sum_{i \in I} p_i, \quad (3)$$

which depends on a reference momentum q_I . These numerators can be simplified with some choices of q_I , and the final amplitude is independent of them.

II. THE PERMUTOHEDRON AND ALGEBRA UNDERLYING BCJ NUMERATORS

In this section, we show that all the terms in a BCJ master numerator obtained from CCK duality for YMS amplitudes are in one-to-one correspondence with all boundaries of permutohedron \mathcal{P}_{n-2} , or equivalently terms from a quasishuffle product.

A. The (combinatorial) permutohedra and quasishuffle products

Following [7], we organize $K(1, 2, \dots, n)$ according to the spurious pole structure, which is isomorphic to the boundary structure of the permutohedron \mathcal{P}_{n-2} .

The permutohedron \mathcal{P}_{n-2} is an $(n - 3)$ -dimensional polytope [27], whose codimension d boundary Γ_d can be labeled by $d + 1$ consecutive subsets

$$\Gamma_d := \{I_0, I_1, \dots, I_d\}, \quad (4)$$

where $I_d \neq \emptyset$ and $I_d \subset I_{d-1} \subset \dots \subset I_0 = \{2, 3, \dots, n - 1\}$; the interior of \mathcal{P}_{n-2} can be viewed as its codimension 0 boundary, $\Gamma_0 := I_0$. \mathcal{P}_{n-2} and its boundaries have appeared in the context of cubic tree graphs from the worldsheet [48, 49]. Here each term of the BCJ numerator $K(1, 2, \dots, n)$ with $d + 1$ spurious poles corresponds to such a codimension d boundary, thus the numerator can be expanded in terms of boundaries of \mathcal{P}_{n-2}

$$K(1, 2, \dots, n) = \sum_{d=0}^{n-3} \sum_{\Gamma_d \in \partial^d \mathcal{P}_{n-2}} K_{\Gamma_d}(1, 2, \dots, n), \quad (5)$$

where we sum over all boundaries $\Gamma_d \in \partial^d \mathcal{P}_{n-2}$ with codimension $d = 0, \dots, n - 3$, and the contribution from Γ_d , $K_{\Gamma_d}(1, 2, \dots, n) \equiv K_{\Gamma_d}$ reads

$$K_{\Gamma_d} = \prod_{k=0}^d \frac{p_{1\Delta(I_k, I_{k+1})} \cdot F_{\tau_k} \cdot q_{I_k}}{D_{I_k}}. \quad (6)$$

It has $d + 1$ factors each with a denominator D_{I_k} of (3) and a numerator of the form $p_{1\Delta(I_k, I_{k+1})} \cdot F_{\tau_k} \cdot q_{I_k}$ for $k = 0, \dots, d$. To specify the ordered subset τ_k of the Lorentz product as in (2), we introduce an alternative form of (4) using ordered sets:

$$\begin{aligned} \Gamma_d &= \{\tau_0 \cup \tau_1 \cup \dots \cup \tau_d, \tau_1 \cup \dots \cup \tau_d, \dots, \tau_{d-1} \cup \tau_d, \tau_d\} \\ &\sim \{\tau_0, \tau_1, \dots, \tau_d\}, \end{aligned} \quad (7)$$

where the first line is equivalent to (4) but we use ordered sets $\tau_k = \text{Id}(I_k/I_{k+1})$ with $I_{d+1} \equiv \emptyset$. $\text{Id}(I)$ means sorting the subset I in numerical ordering [50]. Perhaps the most subtle point is that we also define $\Delta(I_k, I_{k+1}) := (\bar{I}_k)_{<\tau_{k,1}}$, which refers to the elements in the set $\bar{I}_k = \{2, 3, \dots, n-1\}/I_k$ that are numerically smaller than the first element $\tau_{k,1}$ of the ordered set τ_k .

For example, at $n = 5$, we have a boundary $\Gamma_2 = \{I_0 = \{2, 3, 4\}, I_1 = \{2, 4\}, I_2 = \{4\}\}$; equivalently, we have $\tau_0 = \{3\}, \tau_1 = \{2\}, \tau_2 = \{4\}$, thus we have a term

$$K_{234,2,4} = \frac{p_1 \cdot F_3 \cdot q_{234} p_1 \cdot F_2 \cdot q_{24} p_{123} \cdot F_4 \cdot q_4}{D_{234} D_{24} D_4}, \quad (8)$$

where we have used $\Delta(I_2, \emptyset) = (\bar{I}_2)_{<4} = \{2, 3\}$. A more nontrivial example for the latter is for $n = 9$, $\Delta(\{4, 5, 7, 8\}, \{4, 8\}) = \{2, 3, 6\}_{<5} = \{2, 3\}$.

On the other hand, the boundaries of \mathcal{P}_{n-2} have a nice quasishuffle product interpretation. The quasishuffle product \star can be defined between two arbitrary generators $(\sigma_0, \sigma_1, \dots, \sigma_r)$ and $(\rho_0, \rho_1, \dots, \rho_s)$, where σ_i and ρ_j are sets with arbitrary lengths and can also be prompted to the quasishuffle Hopf algebra [26,34,35,51]. We summarize the definitions in Appendix A and here we just use the following result of the quasishuffle product $\hat{K}(2, \dots, n-1) \equiv (2)\star(3)\star\dots\star(n-1)$

$$\begin{aligned} \hat{K}(2, \dots, n-1) \\ = \sum_{d=0}^{n-3} \sum_{\tau \in \text{part}^{(d+1)}(2, \dots, n-1)} (-1)^{n+d-1} (\tau_0, \tau_1, \dots, \tau_d), \end{aligned} \quad (9)$$

where $\text{part}^{(d+1)}(2, \dots, n-1)$ denotes all the ordered partitions of $\{2, 3, \dots, n-1\}$ into $d+1$ nonempty subsets $(\tau_0, \tau_1, \dots, \tau_d)$ (each τ_i is sorted according to β). Terms on the rhs of (9) are in one-to-one correspondence with boundaries of \mathcal{P}_{n-2} as in (7), thus we can rewrite (5) in terms of the quasishuffle product

$$K(1, 2, \dots, n) = \langle \hat{K}(2, \dots, n-1) \rangle, \quad (10)$$

where we have defined a linear map $\langle \cdot \rangle$ from (6) for any partition $(\tau_0, \tau_1, \dots, \tau_d)$

$$\langle (\tau_0, \tau_1, \dots, \tau_d) \rangle = (-1)^{n+d-1} \prod_{k=0}^d \frac{p_{1\Delta(I_k, I_{k+1})} \cdot F_{\tau_k} \cdot q_{I_k}}{D_{I_k}}. \quad (11)$$

B. The counting and some examples

By definition, the permutohedron \mathcal{P}_m contains $m!$ vertices and $2^m - 2$ codimension one facets. More generally, the number of codimension d boundaries of this polytope is $(d+1)!S(m, d+1)$, where $S(m, d)$ is the second kind of Stirling number [52]. Algebraically, $S(m, d+1)$ also counts the number of ways to partition a set of m labeled objects into $d+1$ nonempty unlabeled subsets $\{\tau_0, \tau_1, \dots, \tau_d\}$ [52], so after considering the ordering between these sets, there are $(d+1)!S(m, d+1)$ terms in the summation for any d . The total number is the Fubini number \mathcal{F}_m , where $\mathcal{F}_m = \sum_{d=1}^m d!S(m, d)$ [53], thus the n -point BCJ numerator has \mathcal{F}_{n-2} terms. The explicit counting up to six-point is given in Table I.

Let us illustrate (5) and (6) with some examples. The most trivial case is $n = 3$, where the BCJ numerator corresponds to the zero-dimensional permutohedron \mathcal{P}_1 , which is just a point. It contains one term with $\Gamma_0 = \{I_0\} = \{2\}$, thus $K(1, 2, 3) = K_2(1, 2, 3) = \frac{p_1 \cdot F_2 \cdot q_2}{D_2}$, where we have used $\Delta(I_0, I_1) = \emptyset$, this is generally true since $\bar{I}_0 = \emptyset$.

For $n = 4$, the permutohedron \mathcal{P}_2 is a line segment, where the interior ($d = 0$) is labeled by $I_0 = \{23\}$, and the two vertices ($d = 1$) are labeled by $\{23, 2\}$ and $\{23, 3\}$; we show these three terms in Fig. 1.

Equivalently, in (9) the partition $\text{part}^{(1)}$ of $\{2, 3\}$ has $(\{\tau_0 = \{2, 3\}\})$ and $\text{part}^{(2)}$ has $(\tau_0 = \{2\}, \tau_1 = \{3\})$ and $(\tau_0 = \{3\}, \tau_1 = \{2\})$: they are nothing but the interior and the two vertices, according to (7).

Thus the BCJ numerator $K(1, 2, 3, 4)$ has three terms, $K_{23}, K_{23,2}$, and $K_{23,3}$, which read

TABLE I. Counting codimension- d boundaries of \mathcal{P}_{n-2} .

n	d				Total
	0	1	2	3	
3	1				1
4	1	2			3
5	1	6	6		13
6	1	14	36	24	75

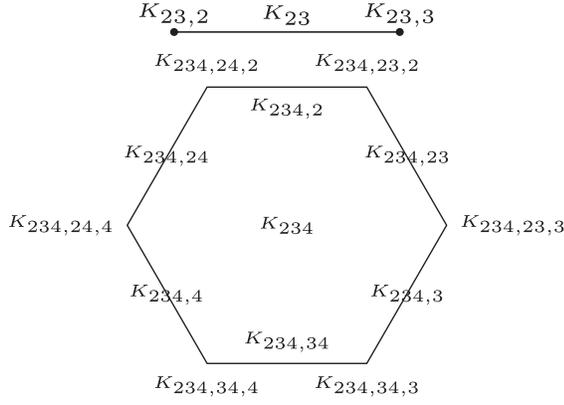


FIG. 1. Permutohedra \mathcal{P}_2 for $K(1, 2, 3, 4)$ (top) and \mathcal{P}_3 for $K(1, 2, 3, 4, 5)$ (bottom).

$$\begin{aligned} & \frac{p_1 \cdot F_{23} \cdot q_{23}}{D_{23}} + \frac{p_1 \cdot F_3 \cdot q_{23} p_1 \cdot F_2 \cdot q_2}{D_{23} D_2} \\ & + \frac{p_1 \cdot F_2 \cdot q_{23} p_{12} \cdot F_3 \cdot q_3}{D_{23} D_3}. \end{aligned} \quad (12)$$

Notice that the last term in the above equation is from the boundary $\{23, 3\}$, so the second factor in the numerator is $p_{1(\overline{\{3\}})_{<3}} \cdot F_3 \cdot q_3 = p_{12} \cdot F_3 \cdot q_3$. Meanwhile (12) shows that the four-point numerator $K(1, 2, 3, 4)$ has an overall pole $D_{I_0} = D_{23}$. This can be easily seen from (4) since the first set of any codimension d boundary Γ_d is always labeled by $I_0 = \{2, 3, \dots, n-1\}$.

Notice that (6) means each term in the BCJ numerator contains spurious poles, and the codimension d contribution will have $d+1$ spurious poles where D_{I_0} is an overall pole for every boundary. Except for the overall one, the simple poles can be written as D_I where I is a nonempty proper subset of $I_0 = \{2, 3, \dots, n-1\}$ and two simple poles D_I and D_J are compatible if and only if $I \subset J$ or $J \subset I$. For example, at five-point, except for the overall D_{234} , the simple poles are $D_2, D_3, D_4, D_{23}, D_{24}, D_{34}$, which correspond to the six codimension one boundaries of \mathcal{P}_3 , and the compatible double poles are

$$\{D_{23}D_2, D_{24}D_2, D_{23}D_3, D_{34}D_3, D_{24}D_4, D_{34}D_4\}, \quad (13)$$

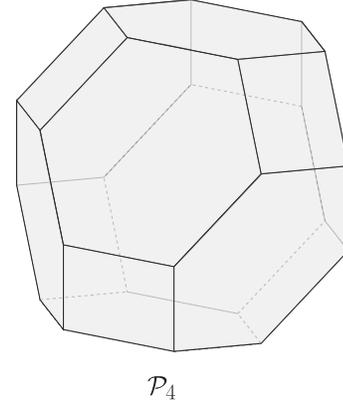


FIG. 2. The permutohedron \mathcal{P}_4 for $K(1, \dots, 6)$.

which correspond to six vertices of the hexagon \mathcal{P}_3 . We show the boundary contribution formally in Fig. 1. These 13 terms form a two-dimensional polytope \mathcal{P}_3 . These boundaries can also be realized in a quasishuffle product $\hat{K}(2, 3, 4)$, which will be discussed in Appendix B. To be precise, we give some explicit examples of different codimension here

$$\begin{aligned} K_{234} &= \frac{p_1 \cdot F_{234} \cdot q_{234}}{D_{234}}, \\ K_{234,23} &= \frac{p_1 \cdot F_4 \cdot q_{234} p_1 \cdot F_{23} \cdot q_{23}}{D_{234} D_{23}}, \\ K_{234,2} &= \frac{p_1 \cdot F_{34} \cdot q_{234} p_1 \cdot F_2 \cdot q_2}{D_{234} D_2}, \\ K_{234,23,2} &= \frac{p_1 \cdot F_4 \cdot q_{234} p_1 \cdot F_3 \cdot q_{23} p_1 \cdot F_2 \cdot q_2}{D_{234} D_{23} D_2}. \end{aligned} \quad (14)$$

The complete result for the BCJ numerator $K(1, 2, 3, 4, 5)$ is shown in the Appendix B.

Moreover, we emphasize that all the spurious poles are canceled in the final amplitude, and the amplitude does not depend on the reference momenta. The proof will be put into the following paper [54].

For $n=6$, \mathcal{P}_4 is a three-dimensional truncated octahedron shown in Fig. 2. As we have counted, it contains 14 codimension one boundaries (six squares and eight hexagons), 36 edges and $4! = 24$ vertices, thus 75 boundaries in total. Some terms with codimension $d=0, 1, 2, 3$ are

$$\begin{aligned} K_{2345} &= \frac{p_1 \cdot F_{2345} \cdot q_{2345}}{D_{2345}}, \\ K_{2345,234} &= \frac{p_1 \cdot F_5 \cdot q_{2345} p_1 \cdot F_{234} \cdot q_{234}}{D_{2345} D_{234}}, \\ K_{2345,234,23} &= \frac{p_1 \cdot F_5 \cdot q_{2345} p_1 \cdot F_4 \cdot q_{234} p_1 \cdot F_{23} \cdot q_{23}}{D_{2345} D_{234} D_{23}}, \\ K_{2345,234,23,2} &= \frac{p_1 \cdot F_5 \cdot q_{2345} p_1 \cdot F_4 \cdot q_{234} p_1 \cdot F_3 \cdot q_{23} p_1 \cdot F_2 \cdot q_2}{D_{2345} D_{234} D_{23} D_2}. \end{aligned} \quad (15)$$

III. NUMERATORS FOR GENERAL YMS AND PURE YM AMPLITUDES

More generally, the CCK duality has provided closed formulas for BCJ numerators of n -point YMS amplitude with $r \geq 2$ scalars [7]. It turns out that any such numerator corresponds to a permutohedron \mathcal{P}_{n-r} (with dimension $n - r - 1$): everything we have discussed above for $r = 2$ case still applies if we replace $\{2, 3, \dots, n - 1\}$ by the set of $n - r$ gluons. For example, in the other extreme with $r = n$ we can formally define $\mathcal{P}_0 := \mathcal{P}_\emptyset$ and the n -scalar numerator (of bi-adjoint ϕ^3 amplitude) is 1 or 0. For $r = n - 1$, we have the zero-dimensional \mathcal{P}_1 and the numerator with a single gluon i reads

$$K^{1\text{-gluon}}(1, \beta, n) = \frac{p_{1 \rightarrow i} \cdot F_i \cdot q_i}{D_i}, \quad (16)$$

where $1 \rightarrow i$ denotes all the scalars preceding i in $(1\beta n)$. We shall not repeat this for general cases but leave detailed discussions to a separate paper [54].

Moreover, since the pure YM amplitude can be expanded as a linear combination of these YMS ones [12,14,55–57], we obtain its BCJ numerators for free; the resulting numerator naively contains $2\mathcal{F}_{n-2}$ terms as derived in [7]. However, we can still organize the terms according to pole structures and immediately combine them in pairs as \mathcal{F}_{n-2} terms: the resulting numerator has the same form as the two-scalar case and corresponds to boundaries of permutohedron \mathcal{P}_{n-2} . By expanding $A^{\text{YM}}(1, 2, \dots, n)$ in exactly the same way as (1), each master BCJ numerator, e.g., $K^{\text{YM}}(1, 2, \dots, n)$ is given by a sum over boundaries of \mathcal{P}_{n-2} as in (5):

$$K^{\text{YM}}(1, 2, \dots, n) = \sum_{d=0}^{n-3} \sum_{\Gamma_d \in \partial^d \mathcal{P}_{n-2}} K_{\Gamma_d}^{\text{YM}}(1, 2, \dots, n),$$

where the contribution from each boundary is identical to (6) except for the $k = 0$ factor, which becomes

$$\frac{\varepsilon_n \cdot F_{1\tau_0} \cdot q_{I_0} + \varepsilon_1 \cdot F_{\tau_0} \cdot (\varepsilon_n p_{1n} \cdot q_{I_0} - q_{I_0} p_1 \cdot \varepsilon_n)}{D_{I_0}}. \quad (17)$$

Of course, similar to the YMS case, all spurious poles cancel in the final amplitude, which does not depend on q_I . Therefore we are free to choose them to simplify the expression (17). One such choice is $q_{I_0} = \varepsilon_n$, and the $k = 0$ factor (17) takes a simpler form

$$\frac{\varepsilon_n \cdot F_{1\tau_0} \cdot \varepsilon_n}{\varepsilon_n \cdot p_{23\dots n-1}} = - \frac{\varepsilon_n \cdot F_{1\tau_0} \cdot \varepsilon_n}{\varepsilon_n \cdot p_1}. \quad (18)$$

It is easy to see that the BCJ numerators become manifestly gauge invariant in particles $1, 2, \dots, n - 1$. For example, the BCJ numerator $K^{\text{YM}}(1, 2, 3, 4)$ reads

$$\frac{\varepsilon_4 \cdot F_{123} \cdot \varepsilon_4}{p_1 \cdot \varepsilon_4} - \frac{\varepsilon_4 \cdot F_{13} \cdot \varepsilon_4 p_1 \cdot F_2 \cdot q_2}{p_1 \cdot \varepsilon_4 D_2} - \frac{\varepsilon_4 \cdot F_{12} \cdot \varepsilon_4 p_{12} \cdot F_3 \cdot q_3}{p_1 \cdot \varepsilon_4 D_3}.$$

Furthermore, similar to the discussion in Sec. II A, BCJ numerators of YM amplitudes can also be interpreted in terms of quasishuffle products, and the only change is that in the linear map (11) the $k = 0$ factor is modified to (17).

Before ending the section, we mention the obvious double copy from YM to GR

$$M_n^{\text{GR}} = \sum_{\alpha, \beta} K^{\text{YM}}(1, \alpha, n) m(1, \alpha, n | 1, \beta, n) K^{\text{YM}}(1, \beta, n), \quad (19)$$

where we sum over a pair of permutations α, β of $\{2, 3, \dots, n - 1\}$, with m denoting biadjoint ϕ^3 amplitudes; if we replace YM by YMS with $1, n$ being scalars, it gives the amplitude with $n - 2$ gravitons and two scalars.

IV. RECURSIONS AND FACTORIZATIONS

In this section, we propose recursion relations and factorization properties (on spurious poles D_I) for the BCJ numerators, which are implied by the combinatorial and algebraic structure. The argument can be equally applied to both two-scalar YMS and pure YM numerators.

A. Recursion relations

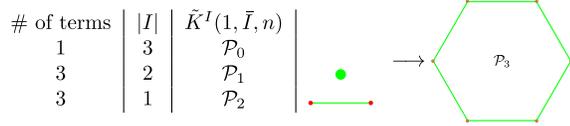
First, in quasishuffle product (9), one can collect the terms with the same τ_d and then apply the linear map (11) to obtain the following recursion relation,

$$K(1, 2, \dots, n) = \sum_{I \subset \{2, \dots, n-1\}} \frac{p_{1\Delta(I, \emptyset)} \cdot F_I \cdot q_I}{D_I} \tilde{K}^I(1, \bar{I}, n), \quad (20)$$

where the summation is over all the nonempty subsets of $\{2, 3, \dots, n - 1\}$. The definition of $\tilde{K}^I(1, \bar{I}, n)$ is slightly different from (6) in the denominator: it is given by the sum over boundaries of the permutohedron $\mathcal{P}_{\bar{I}}$ with vertices labeled by all permutations of set \bar{I} , and for each boundary $\Gamma_d = \{J_0 = \bar{I}, J_1, \dots, J_d\}$ where $J_d \subset J_{d-1} \dots \subset J_0$, we have a contribution

$$\tilde{K}_{\Gamma_d}^I = \prod_{k=0}^d \frac{p_{1\Delta(J_k, J_{k+1})} \cdot F_{\tau_k} \cdot q_{IJ_k}}{D_{IJ_k}}, \quad (21)$$

where $D_{IJ_k} = p_{IJ_k} \cdot q_{IJ_k}$, $\tau_k = \text{Id}(J_k/J_{k+1})$ with $J_{d+1} \equiv \emptyset$ and the complement of the set J_k appears in $\Delta(J_k, J_{k+1})$ is defined as \bar{I}/J_k . For $|I| = n - 2$ ($\bar{I} = \emptyset$), we define


 FIG. 3. Recursion relation at $n = 5$.

$\tilde{K}^I(1, n) = 1$. Formally, this numerator corresponds to the permutohedron \mathcal{P}_0 .

For example, the recursion relation of $K(2, 3, 4) \equiv K(1, 2, 3, 4, 5)$ [58] reads

$$\begin{aligned}
 K(2, 3, 4) &= \frac{p_1 \cdot F_{234} \cdot q_{234}}{D_{234}} + \frac{p_1 \cdot F_{23} \cdot q_{23}}{D_{23}} \tilde{K}^{23}(4) \\
 &+ \frac{p_1 \cdot F_{24} \cdot q_{24}}{D_{24}} \tilde{K}^{24}(3) + \frac{p_{12} \cdot F_{34} \cdot q_{34}}{D_{34}} \tilde{K}^{34}(2) \\
 &+ \frac{p_1 \cdot F_2 \cdot q_2}{D_2} \tilde{K}^2(3, 4) + \frac{p_{12} \cdot F_3 \cdot q_3}{D_3} \tilde{K}^3(2, 4) \\
 &+ \frac{p_{123} \cdot F_4 \cdot q_4}{D_4} \tilde{K}^4(2, 3). \quad (22)
 \end{aligned}$$

Geometrically, the recursion relation (20) tells us how the codimension one boundaries of permutohedron are glued together. In the above five-point example, the term with $|I| = 3$ in the first line has only one pole and corresponds to the interior (codimension 0 boundary) of \mathcal{P}_3 , depicted in Fig. 3. For the three terms with $|I| = 2$ in the second line, each factor $\tilde{K}^I(1, \bar{I}, n)$ corresponds to a zero-dimensional permutohedron; on the other hand, each term is mapped to a codimension one boundary of \mathcal{P}_3 without vertices. For the remaining three terms with $|I| = 1$ in the last line, each $\tilde{K}^I(1, \bar{I}, n)$ corresponds to a one-dimensional permutohedron and it is mapped to a codimension one boundary with two vertices.

B. Factorization properties on spurious poles

Next, we move to certain intriguing factorization properties of the BCJ numerator on spurious poles. Combinatorially, any codimension one boundary of the permutohedron \mathcal{P}_{n-2} is the product of two lower-dimensional permutohedra $\mathcal{P}_I \times \mathcal{P}_{\bar{I}}$. Remarkably, we find that on any pole $D_I = 0$, the residue of the BCJ numerator factorizes into the product of a $(|I| + 2)$ -point numerator and a $(n - |I|)$ -point numerator. Unlike the usual factorization on the physical poles of the amplitude, these factorizations on the spurious poles stem from the combinatorial picture without any known physical origin. Explicitly

$$\text{Res}_{|D_I=0} K(1, 2, \dots, n) = D_I K(1, \text{Id}(I), P) \tilde{K}^I(1, \text{Id}(\bar{I}), n), \quad (23)$$

where $P \equiv \bar{I}n$ denotes an effective scalar. For the definition of $\Delta(I_k, J_{k+1})$ in $K(1, \text{Id}(I), P)$, the complement of the set

I_k is still defined as $\bar{I}_k = \{2, 3, \dots, n-1\}/I_k$ while for $\Delta(J_k, J_{k+1})$ in $\tilde{K}^I(1, \text{Id}(\bar{I}), n)$ the complement of J_k is defined as \bar{I}/J_k . The factor $D_I K(1, \text{Id}(I), P)$ in (23) means that the overall pole D_I of $K(1, \text{Id}(I), P)$ is excluded. The factorization properties (23) can be proved directly by plugging in the definitions on both sides.

For instance, at six points as shown in Fig. 2, there are 14 codimension one boundaries $D_I = 0$ including eight poles with $|I| = 1$ or 3 corresponding to hexagons and six poles with $|I| = 2$ corresponding to squares. On any of the hexagon boundary, i.e., when $D_I = 0$ with $|I| = 1$ or 3, the residue factorizes into $\mathcal{F}_3 = 13$ terms (times $\mathcal{F}_1 = 1$ term). Similarly when $D_I = 0$ with $|I| = 2$, the residue factorizes differently, e.g., as $D_{23} K(1, 2, 3, 456) \times \tilde{K}^{23}(1, 4, 5, 6)$ when $D_{23} = 0$ (the square is the product of two line segments $\mathcal{P}_{\{23\}} \times \mathcal{P}_{\{45\}}$).

Algebraically, the quasishuffle algebra can be prompted to a bialgebra by introducing the coproduct map [26], and one can show the factorization properties from the coproduct. Similar to [34,35], we can also define the antipode map to make the bialgebra a quasishuffle Hopf algebra. Acting on the BCJ numerators, the antipode map does nothing but changes its overall sign. The detail is given in the Appendix A.

We expect the factorization properties of BCJ numerators to be the key for showing the cancellation of spurious poles in the amplitude. Such properties also suggest certain positive geometries (rather than just combinatorics) underlying these BCJ numerators, and we leave further investigations to future works.

V. HEAVY-MASS EFFECTIVE FIELD THEORY

In this section, we study YMS amplitudes and their BCJ numerators in the HEFT, which are obtained by taking the heavy-mass limit for a pair of massive scalars with momenta [33–35]

$$p_1^\mu = m v^\mu, \quad p_n^\mu = -m v^\mu - k^\mu, \quad (24)$$

where $v^2 = 1$ and we are interested in the limit $m \rightarrow \infty$; in other words, we will study the expansion in $1/m$ of the BCJ numerators which we denote as $K_H(1, 2, \dots, n)$, as well as that of ϕ^3 amplitudes, which combine to give the resulting HEFT amplitude $A^H(1, 2, \dots, n)$ at the leading order in $1/m$. Here k^μ is at the same order as gluon momenta, which stay finite at $\mathcal{O}(m^0)$ as $m \rightarrow \infty$.

A. Heavy limit of YMS amplitudes

We will make a particular choice of the reference momenta: $q_I = v$ for all I , which dramatically simplifies formulas for BCJ numerators and give rise to poles similar to HEFT numerators in [34]. In fact, for $n = 4$ such a choice reduces the BCJ numerator to one term, since $v \cdot F_a \cdot v$ vanishes for a single particle a

$$K_H(1, 2, 3, 4) = \frac{p_1 \cdot F_{23} \cdot v}{p_{23} \cdot v} = -\frac{2m^2}{k^2} v \cdot F_{23} \cdot v, \quad (25)$$

where in the second equality we have used $v \cdot k = -k^2/(2m)$, which is implied by the on-shell condition $p_n^2 = m^2$. Notice that $K_H(1, 3, 2, 4) = K_H(1, 2, 3, 4)$, thus the amplitude $A^H(1, 2, 3, 4)$ becomes

$$\begin{aligned} & \left(\frac{1}{s_{12}} + \frac{1}{s_{23}} \right) K_H(1, 2, 3, 4) - \frac{1}{s_{23}} K_H(1, 3, 2, 4) \\ &= -\frac{m v \cdot F_{23} \cdot v}{k^2 v \cdot p_2}. \end{aligned} \quad (26)$$

Physically, the final HEFT amplitude has the leading order $\mathcal{O}(m)$ [33]. In the above example, we can see that the numerators are at $\mathcal{O}(m^2)$, and the sum of the leading contribution of ϕ^3 amplitudes at $\mathcal{O}(m^0)$, say $1/s_{23}$ times the corresponding numerators vanishes. Therefore, the sum of the contribution of ϕ^3 amplitudes at the next order, i.e., $1/s_{12}$ from $A^{\phi^3}(1, 2, 3, 4)$ times the numerator produces the HEFT amplitude as the first nonvanishing order. This is also the case for $n = 5$. However, for higher n , the numerator contains some additional terms with higher power of m . To obtain the leading order contribution of HEFT final amplitude, we expand the numerators and the ϕ^3 amplitudes in m^{-1} . Note the overall pole $D_{23\dots n-1} = v \cdot k$ for BCJ numerators is proportional to m^{-1} , we first collect the numerator according to its superficial order of m^{-1} , i.e., terms with $(i-1)p_1$ s in the numerator,

$$K_H(1, 2, \dots, n) = \sum_{i=2}^{\lfloor n/2 \rfloor} K_H^{(i)}(1, 2, \dots, n), \quad (27)$$

where the upper bound of the summation is $\lfloor n/2 \rfloor$ since $p_1 \cdot F_a \cdot v = 0$ implies that the numerator should contain as many $p_1 \cdot F_{ab} \cdot v$ as possible to have the highest power of p_1 . In the above expansion, $K_H^{(i)} \equiv K_H^{(i)}(1, 2, \dots, n)$ refers to terms with the superficial order $\mathcal{O}(m^i)$. For example, at six points we have the following terms for $K_H^{(2)}$ and $K_H^{(3)}$, respectively:

$$\frac{p_1 \cdot F_{23} \cdot v p_{23} \cdot F_5 \cdot v p_{23} \cdot F_4 \cdot v}{v \cdot k v \cdot p_{45} v \cdot p_4},$$

$$\frac{p_1 \cdot F_{25} \cdot v p_1 \cdot F_{34} \cdot v}{v \cdot k v \cdot p_{34}}.$$

In fact, as explained in Appendix C, the actual order of $K_H^{(i)}$ is $\mathcal{O}(m^2)$ for $i = 2$ and $\mathcal{O}(m^{i-1})$ otherwise.

In the HEFT amplitude, we sum over all cubic graphs relevant at leading order, and for each graph with its propagator structure, its numerator is given by the corresponding commutator of $K_H^{(i)}$ [59]. Nicely we observe that

certain commutators of $K_H^{(i)}$ actually vanish, and the end result is that only $K_H^{(2)}$ contributes to the amplitude at the leading order. We have checked such vanishing results up to $n = 10$, but we do not have an all- n proof at the moment.

In fact, such vanishing results are better than what we need here, i.e., only $K_H^{(2)}$ contributes to gauge-theory amplitudes at leading order. We have checked up to $n = 10$ that the stronger vanishing results actually ensure that only $K_H^{(2)}$ contributes to gravity amplitude, which is at order $\mathcal{O}(m^2)$, as obtained by double copy in HEFT. We leave more details in the Appendix C with a proof of the simplest case. As a result of this conjecture, the amplitude is given by

$$A^H(1, 2, \dots, n) = \sum_{\Theta^1} \frac{K_H^{(2)}(1, \Theta^1, n)}{d_{\Theta^1}}, \quad (28)$$

where the summation is over nested commutators of depth $n-4$ (“codepth” 1) of the ordered set $(2, 3, \dots, n-1)$. For instance, at five points, we sum over $\Theta^1 = ([2, 3], 4)$, $(2, [3, 4])$; d_{Θ^1} denotes the propagator denominator corresponding to the cubic tree associated with Θ^1 [two subtrees on the scalar line $(1n)$]:

Moreover, it is easy to show (see Appendix C for details) that the effective BCJ numerator $K_H^{(2)}(1, 2, \dots, n)$ contains \mathcal{F}_{n-3} terms, and its pole structure corresponds to the permutohedron $\mathcal{P}_{\{34\dots n-1\}}$, which means that

$$K_H^{(2)}(1, 2, \dots, n) = \sum_{d=0}^{n-2} \sum_{\Gamma_d \in \partial^d \mathcal{P}_{n-3}} K_{H,\Gamma_d}^{(2)}(1, 2, \dots, n). \quad (29)$$

For the boundary $\Gamma_d = \{I_0, I_1, \dots, I_d\} \in \partial^d \mathcal{P}_{\{34\dots n-1\}}$, where $I_d \subset I_{d-1} \subset \dots \subset I_0 = \{3, 4, \dots, n-1\}$ and $I_d \neq \emptyset$, the contribution is

$$\begin{aligned} K_{H,\Gamma_d}^{(2)} &= \frac{m v \cdot F_{\tau_0} \cdot v}{p_{23\dots n-1} \cdot v} \prod_{k=1}^d \frac{p_{\Delta(I_k, I_{k+1})} \cdot F_{\tau_d} \cdot v}{v \cdot p_{I_k}}, \\ &= -\frac{2m^2 v \cdot F_{\tau_0} \cdot v}{k^2} \prod_{k=1}^d \frac{p_{\Delta(I_k, I_{k+1})} \cdot F_{\tau_d} \cdot v}{v \cdot p_{I_k}}, \end{aligned} \quad (30)$$

where in the calculation of $\Delta(I_k, I_{k+1})$, the complement set of I_k is still taken to be $\{2, 3, \dots, n-1\}/I_k$. For $n = 4$, there is no commutator in Θ^1 and the result is (26). For $n = 5$, the amplitude becomes

$$A^H(1, 2, 3, 4, 5) = \frac{1}{s_{12}} \frac{K_H^{(2)}(1, 2, [3, 4], 5)}{s_{34}} + \frac{1}{s_{123}} \frac{K_H^{(2)}(1, [2, 3], 4, 5)}{s_{23}}, \quad (31)$$

where $K_H^{(2)}(1, 2, 3, 4, 5)$ is given by

$$-\frac{2m^2}{k^2} \left(v \cdot F_{234} \cdot v + \frac{v \cdot F_{24} \cdot v p_2 \cdot F_3 \cdot v}{v \cdot p_3} + \frac{v \cdot F_{23} \cdot v p_{23} \cdot F_4 \cdot v}{v \cdot p_4} \right).$$

Let us give a final example for $n = 6$ amplitude

$$\begin{aligned} & \frac{1}{s_{12}} \left(\frac{K_H^{(2)}(1, 2, [[3, 4], 5], 6)}{s_{34}s_{345}} + \frac{K_H^{(2)}(1, 2, [3, [4, 5]], 6)}{s_{45}s_{345}} \right) \\ & + \frac{1}{s_{123}} \frac{K_H^{(2)}(1, [2, 3], [4, 5], 6)}{s_{23}s_{45}} \\ & + \frac{1}{s_{1234}} \left(\frac{K_H^{(2)}(1, [[2, 3], 4], 5, 6)}{s_{23}s_{234}} + \frac{K_H^{(2)}(1, [2, [3, 4]], 5, 6)}{s_{34}s_{234}} \right). \end{aligned} \quad (32)$$

It is interesting to notice the numerators we present here only differ from those in [34] denoted by $N(1, 2, \dots, n)$ by an overall prefactor

$$K_H^{(2)}(1, 2, \dots, n) = (-1)^n (n-2) \frac{2m}{k^2} v \cdot p_2 N(1, 2, \dots, n). \quad (33)$$

It is highly nontrivial, however, that these two sets of effective BCJ numerators give the same HEFT amplitude. In [34], the expression involves the sum of cubic graphs corresponding to nested commutators of depth $n-3$ of the ordered set $(2, 3, \dots, n-1)$, thus the propagator denominator contains an overall factor $s_{23\dots n-1}$, which in our case is replaced by different $s_{1\sigma}$ for different terms. In addition, the numerator of [34] for each cubic graph is given by a nested commutator of $N(1, 2, \dots, n)$, thus the number of terms in it is twice as ours. Nevertheless, we have analytically checked up to $n=10$ that the amplitude (28) agrees with [34]. Moreover, we have checked that although they look very different, the HEFT gravity amplitude via double copy also agrees with that in [34], and we expect both agreements to hold for all n .

B. Decoupling into pure YM

Given the explicit result of the n -point heavy mass BCJ numerators, the $(n-1)$ -point pure YM BCJ numerators, as well as the amplitudes, can be easily obtained via the decoupling limit: $mv \rightarrow \varepsilon_n, p_{23\dots n-1}^2 \rightarrow 0$ to obtain the BCJ

numerator $K'^{\text{YM}}(2, 3, \dots, n)$ [33,34]. Under this kinematics, the overall factor k^2 vanishes, which we ignore in the decoupling limit. For instance, the three-point BCJ numerator is given by $K'^{\text{YM}}(2, 3, 4) = -2\varepsilon_4 \cdot F_{23} \cdot \varepsilon_4$. Therefore, the three-point amplitude is

$$\begin{aligned} A^{\text{YM}}(2, 3, 4) &= -\frac{\varepsilon_4 \cdot F_{23} \cdot \varepsilon_4}{\varepsilon_4 \cdot p_2}, \\ &= \varepsilon_4 \cdot \varepsilon_2 p_2 \cdot \varepsilon_3 - \varepsilon_2 \cdot \varepsilon_3 p_2 \cdot \varepsilon_4 - \varepsilon_4 \cdot \varepsilon_3 p_3 \cdot \varepsilon_2. \end{aligned} \quad (34)$$

For the four-point YM amplitude, the numerator $K'^{\text{YM}}(2, 3, 4, 5)$ reads

$$\begin{aligned} & -2 \left(\varepsilon_5 \cdot F_{234} \cdot \varepsilon_5 + \frac{\varepsilon_5 \cdot F_{24} \cdot \varepsilon_5 p_2 \cdot F_3 \cdot \varepsilon_5}{p_3 \cdot \varepsilon_5} \right. \\ & \left. + \frac{\varepsilon_5 \cdot F_{23} \cdot \varepsilon_5 p_{23} \cdot F_4 \cdot \varepsilon_5}{p_4 \cdot \varepsilon_5} \right). \end{aligned}$$

Note that $K'^{\text{YM}}(2, 3, \dots, n)$ also manifests the gauge invariance of particles $2, 3, \dots, n-1$. Moreover, it is related to the BCJ numerator given in Sec. III via

$$K'^{\text{YM}}(2, 3, \dots, n) = 2\varepsilon_n \cdot p_2 K^{\text{YM}}(2, 3, \dots, n)|_{q_1 \rightarrow \varepsilon_n}.$$

These numerators, accompanied by different ϕ^3 amplitudes, produce the same YM amplitude.

VI. CONCLUSIONS AND OUTLOOK

In this note, we established a correspondence between BCJ numerators from covariant color-kinematics duality and the combinatorial permutohedra, which are closely related to the quasishuffle Hopf algebra. This apply to all YMS amplitudes, but the most interesting case is that, with two scalars whose numerators share the same combinatorial structure as the pure YM ones, each term is mapped to a boundary of \mathcal{P}_{n-2} ; the contribution from each boundary is almost identical in these two cases, except that we need to modify one factor to take into account the remaining two gluons. We also found nice recursion relations and factorization properties implied by this picture. Finally, based on highly nontrivial cancellations which are needed for both YMS and gravity amplitudes (via double copy) in HEFT, we conjectured a compact formula for their effective numerators; they become closely related to permutohedra \mathcal{P}_{n-3} , which, while producing the same amplitude, differ by an overall factor from the numerators in [34,35].

There are numerous open questions for further investigations. First, as we will present in [54], it is interesting to see how lower-dimensional permutohedra for general YMS numerators combine into \mathcal{P}_{n-2} , which corresponds to the pure YM ones; we also find interesting combinatorial structures underlying BCJ numerators of amplitudes in

nonlinear sigma model etc. Moreover, the somewhat miraculous cancellations that simplify these numerators in HEFT still remain to be proven, which would also be important to establish the correct double copy in HEFT. Since the final amplitudes are independent of reference momenta, all the spurious poles must cancel, which still calls for a direct understanding (without relying on the CCK duality); such an understanding could connect this combinatorial picture (especially the factorizations) to the uniqueness theorem for YM amplitude [46,60] and YMS ones via the universal expansion [57]. Last but not least, it is tempting to ask this: Could we combine the permutohedra for BCJ numerators with the associahedra for biadjoint ϕ^3 amplitudes and obtain a unified geometric understanding of gluon and graviton scattering?

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APPENDIX A: REVIEW OF THE PERMUTOHEDRA AND HOPF ALGEBRAS

1. The permutohedra

The permutohedron \mathcal{P}_m refers to an $(m-1)$ -dimensional polytope, whose vertices are labeled by the $m!$ permutations of $(1, 2, 3, \dots, m)$. Two permutations are connected by an edge if and only if they differ in only two places, and the numbers on these places are neighbors [52]. For example, the \mathcal{P}_1 is just a point, and the \mathcal{P}_2 is just a line whose vertices can be labeled as $\{12\}$ and $\{21\}$.

For $m=3$, the permutohedron is a hexagon and \mathcal{P}_4 is a truncated octahedron, as shown in Fig. 4.

It is also easy to translate the traditional label of vertices of permutohedron to our convention. In our problem, the vertices of \mathcal{P}_{n-2} should correspond to the permutations of $\{2, 3, \dots, n-1\}$ denoted by $p = p_1 p_2 \dots p_{n-2}$. For any vertex p , we put it into a set $\{\text{Id}(p_1, p_2, \dots, p_{n-2}), \text{Id}(p_1, p_2, \dots, p_{n-3}), \dots, p_1\}$. Then each codimension $n-2$ boundary is labeled by the intersection of two vertices. For example, for the \mathcal{P}_2 as shown in the left side of Fig. 5, the two vertices are now labeled by $\{23, 2\}$ and $\{23, 3\}$, and the codimension 0 line is just $\{23, 2\} \cap \{23, 3\} = \{23\}$. More generally, the codimension d boundary can be labeled by the intersection of two codimension $d+1$ boundaries, which is labeled by $d+1$ sets. The slightly nontrivial example \mathcal{P}_3 is also shown in Fig. 5.

In this new notation, the codimension 0 boundary is always labeled by $I_0 \equiv \{2, 3, \dots, n-1\}$ and the codimension one boundaries are labeled as $\{I_0, I_1\}$, where I_1 is a nonempty proper subset of I_0 , so there are $2^{n-2} - 2$ codimension one boundaries in total. For example, for the permutohedron \mathcal{P}_4 , the codimension one boundaries include eight hexagons (with $|I_1| = 1$ or 3) and six squares (with $|I_1| = 2$). Two codimension one boundaries $\{I_0, I_1\}$ and $\{I_0, I'_1\}$ are adjacent if and only if the $I_1 \subset I'_1$ or $I_1 \supset I'_1$. As a codimension two boundary, the intersection of the above two boundaries is just $\{I_0, I_1, I'_1/I_1\}$ if $I_1 \subset I'_1$ and similar if $I_1 \supset I'_1$. It is easy to notice that the boundary structure of \mathcal{P}_{n-2} is just the same as the pole structure in our n -point BCJ numerator.

Combinatorially, each codimension one boundary of the permutohedron \mathcal{P}_{n-2} , say $\{I_0, I_1\}$ is the product of two permutohedra $\mathcal{P}_{I_1} \times \mathcal{P}_{I_1^c}$, which we refer to as ‘‘combinatorial factorization.’’ For example, on a codimension one boundary of \mathcal{P}_4 , say $\{2345, 2\}$, the permutohedron factorizes into $\mathcal{P}_{\{2\}} \times \mathcal{P}_{\{345\}}$, which is just a hexagon; on another

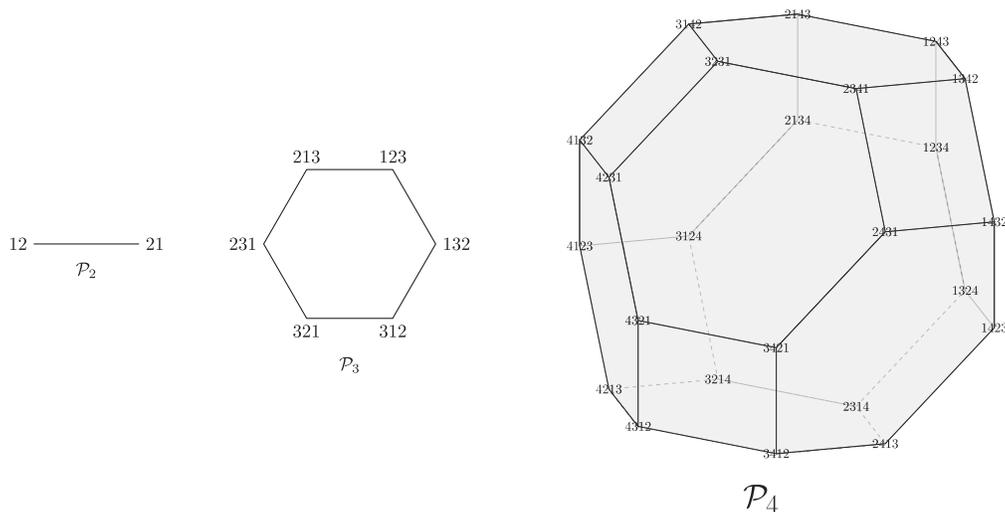
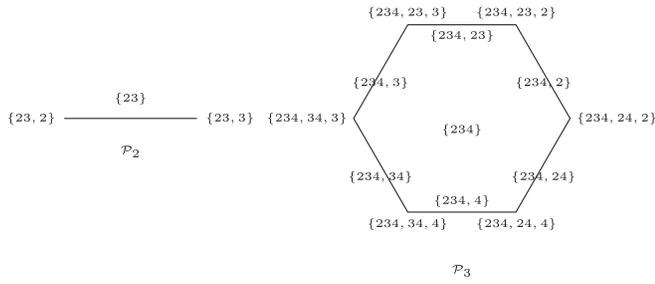


FIG. 4. Permutohedra \mathcal{P}_2 , \mathcal{P}_3 , and \mathcal{P}_4 .


 FIG. 5. \mathcal{P}_2 and \mathcal{P}_3 in our convention.

codimension one boundary $\{2345, 23\}$, it factorizes into $\mathcal{P}_{\{23\}} \times \mathcal{P}_{\{45\}}$, i.e., the product of two line segments, which is a square. Let us also list all the codimension one boundaries of \mathcal{P}_5 . Denoted as $\{23456, I_1\}$, when $|I_1| = 1$ or 4 , the boundary is just the truncated octahedron \mathcal{P}_4 ; when $|I_1| = 2$ or 3 , the boundary becomes a line segment times a hexagon which is a hexagonal prism. More generally, we can see that boundaries corresponding to $|I_1| = a$ and $|I_1| = n - 2 - a$ have the same shape.

2. Hopf algebras

The quasishuffle algebra consists of a vector space V of generators, which are denoted as $(\sigma_0, \sigma_1, \dots, \sigma_r)$. To begin, we introduce some standard nomenclature for generators: we will refer to generators with a single subset (σ_0) as “letters,” those with multiple subsets $\sigma \equiv (\sigma_0, \sigma_1, \dots, \sigma_r)$ as “words.” The quasishuffle product between two generators can be defined recursively as

$$\begin{aligned} & (\sigma_0, \sigma_1, \dots, \sigma_r) \star (\rho_0, \rho_1, \dots, \rho_s) \\ &= \sigma_0 [(\sigma_1, \dots, \sigma_r) \star (\rho_0, \rho_1, \dots, \rho_s)] \\ & \quad + \rho_0 [(\sigma_0, \sigma_1, \dots, \sigma_r) \star (\rho_1, \dots, \rho_s)] \\ & \quad - (\sigma_0 \rho_0) [(\sigma_1, \dots, \sigma_r) \star (\rho_1, \dots, \rho_s)], \end{aligned} \quad (\text{A1})$$

where we also defined an identity element \mathbb{I} for the quasishuffle product

$$\begin{aligned} \mathbb{I}(\sigma_0) \cdots (\sigma_r) &= (\sigma_0) \cdots (\sigma_r) \mathbb{I} = (\sigma_0) \cdots (\sigma_r), \\ \mathbb{I} \star (\sigma_0) \cdots (\sigma_r) &= (\sigma_0) \cdots (\sigma_r) \star \mathbb{I} = (\sigma_0) \cdots (\sigma_r). \end{aligned} \quad (\text{A2})$$

For example, the quasishuffle product between two letters is

$$(2) \star (3) = (2, 3) + (3, 2) - (23), \quad (\text{A3})$$

and the product between a letter with a word is

$$\begin{aligned} (2, 3) \star (4) &= (2)[(3) \star (4)] + (4, 23) - (24, 3), \\ &= (2, 3, 4) + (2, 4, 3) - (2, 34) \\ & \quad + (4, 23) - (24, 3). \end{aligned} \quad (\text{A4})$$

From (A1), the quasishuffle product between two generators can also be written out explicitly

$$\begin{aligned} & (\sigma_0, \sigma_1, \dots, \sigma_r) \star (\rho_0, \rho_1, \dots, \rho_s) \\ &= \sum_{\substack{\tau_{\{\sigma\}} = (\sigma_0, \sigma_1, \dots, \sigma_r) \\ \tau_{\{\rho\}} = (\rho_0, \rho_1, \dots, \rho_s)}} (-1)^{d-r-s} (\tau_0, \tau_1, \dots, \tau_d), \end{aligned} \quad (\text{A5})$$

where the σ_i or ρ_i are now any subsets of $\{2, 3, \dots, n-1\}$. The notation $\tau_{\{\sigma\}}$ means that we restrict the partition τ onto the subset $\{\sigma\} = \cup_{i=0}^r \sigma_i$, for example $(234, 56, 78)|_{\{2,4,6\}} = (24, 6)$.

Here, we give the $n = 4$ example for the BCJ numerators from the linear map of the quasishuffle product (10). The BCJ numerators $K(1, 2, 3, 4) = \langle \hat{K}(2, 3) \rangle$ can be mapped from the quasishuffle product (A3) via the rule (11), which is the same as the result shown in (12).

As we mentioned in the main text, the quasishuffle product $(2) \star (3) \star \dots \star (n-1)$ gives the sum over all the ordered partitions of $\{2, 3, \dots, n-1\}$ into $d+1$ nonempty subsets with $d = 0, 1, \dots, n-3$ [see Eq. (9)]. When $d = n-3$, the ordered partition gives the $(n-2)!$ permutations of $\{2, 3, \dots, n-1\}$; when $d = 1$, it gives has $2^{n-2} - 2$ terms. Generally, the unordered partition of $n-2$ labels $\{2, 3, \dots, n-1\}$ into $d+1$ nonempty subsets is given by the second kind of Stirling number $S(n-2, d+1)$ [52]. For example, $S(n-2, n-2) = 1$ and $S(n-2, 2) = 2^{n-3} - 1$. After considering the ordering between these sets, there are $(d+1)!S(n-2, d+1)$ ordered partitions with length $d+1$. Since the partitions are related to the boundaries of permutohedron via (7), $(d+1)!S(n-2, d+1)$ also counts the codimension d boundaries of permutohedron \mathcal{P}_{n-2} . Thus, the total number of partitions with length $1, 2, \dots, n-2$ is the Fubini number $\mathcal{F}_{n-2} = \sum_{d=1}^{n-2} d!S(n-2, d)$ [53], which is also the total number of all codimension boundaries of \mathcal{P}_{n-2} .

To make the quasishuffle algebra a bialgebra, we can also define the coproduct $\delta: V \rightarrow V \otimes V$ as a linear map, which satisfies [26,34,35]

$$\begin{aligned} \delta((\sigma_0)) &= \mathbb{I} \otimes (\sigma_0) + (\sigma_0) \otimes \mathbb{I}, \\ \delta((\sigma_0, \sigma_1, \dots, \sigma_s) \star (\rho_0, \rho_1, \dots, \rho_t)) \\ &= \delta((\sigma_0, \sigma_1, \dots, \sigma_s)) \star \delta((\rho_0, \rho_1, \dots, \rho_t)). \end{aligned} \quad (\text{A6})$$

The definition of the coproduct can also be extended to be consistent with the tensor product as $(A \otimes B) \star (C \otimes D) = (A \star C) \otimes (B \star D)$. Additionally, the unit element of coalgebra ϵ can be defined as

$$\epsilon(\mathbb{I}) = \mathbb{I}, \quad \epsilon(\sigma) = 0. \quad (\text{A7})$$

To illustrate, we give an example of the coproduct:

$$\begin{aligned} \delta(2\star 3) &= \mathbb{I} \otimes [(2, 3) + (3, 2) - (23)] \\ &+ (2) \otimes (3) + (3) \otimes (2) \\ &+ [(2, 3) + (3, 2) - (23)] \otimes \mathbb{I}. \end{aligned} \quad (\text{A8})$$

From this example, we can see that the coproduct of the specific quasishuffle $(2\star 3\star \dots \star n - 1)$, which is defined as $\hat{K}(2, 3, \dots, n - 1)$ and can be written in terms of the tensor product of lower-point ones. Generally, we have

$$\delta(\hat{K}(2, 3, \dots, n - 1)) = \sum_{I \subset \{2, 3, \dots, n-1\}} \hat{K}(I) \otimes \hat{K}(\bar{I}), \quad (\text{A9})$$

where the summation runs over all subsets of $\{2, 3, \dots, n - 1\}$, which is allowed to be the empty set, and we define $\delta(\emptyset) = \mathbb{I}$.

Notice that each term in the coproduct of the BCJ numerator factorizes into the product of two lower-point numerators in the sense of (23), so it motivates us to define a replacement rule C for tensor products as

$$C(\hat{K}(I) \otimes \hat{K}(\bar{I})) = K(1, \text{Id}(I), P)\tilde{K}^I(1, \text{Id}(\bar{I}), n), \quad (\text{A10})$$

where σ and ρ are words. Then the factorization property (23) can be written in the language of coproduct

$$\text{Res}_{|D_I=0} K(1, 2, \dots, n) = \text{Res}_{|D_I=0} C\delta(\hat{K}(2, 3, \dots, n - 1)). \quad (\text{A11})$$

We can also promote the bialgebra to be a Hopf algebra by defining the antipode map $S: V \rightarrow V$ [26,34,35], which satisfies $\star(\mathbb{I} \otimes S)\delta((\sigma)) = \star(S \otimes \mathbb{I})\delta((\sigma)) = \epsilon(\sigma)\mathbb{I}$, where $\star(\sigma_0 \otimes \sigma_1) \equiv \sigma_0 \star \sigma_1$. To be explicit, it can be defined recursively

$$\begin{aligned} S(\mathbb{I}) &:= \mathbb{I}, \\ S((\sigma_1, \sigma_2, \dots, \sigma_r)) &:= - \sum_{i=0}^{r-1} S((\sigma_1, \sigma_2, \dots, \sigma_i)) \\ &\quad \star S((\sigma_{i+1}, \sigma_{i+2}, \dots, \sigma_r)). \end{aligned} \quad (\text{A12})$$

When acting on the $\hat{K}(2, 3, \dots, n - 1)$, it trivially gives

$$S\hat{K}(2, 3, \dots, n - 1) = (-1)^n \hat{K}(2, 3, \dots, n - 1). \quad (\text{A13})$$

Thus the antipode only changes the numerator $\hat{K}(2, 3, \dots, n - 1)$ by an overall sign. So there is no useful interpretation of the antipode map.

APPENDIX B: EXPLICIT BCJ NUMERATORS FOR FIVE POINTS

For completeness, we provide another explicit example for the five-point BCJ numerator of YMS amplitude, which corresponds to all boundaries of \mathcal{P}_3

$$\begin{aligned} &K(1, 2, 3, 4, 5) \\ &= \frac{1}{D_{234}} \left(\frac{p_1 \cdot F_{234} \cdot q_{234}}{D_{234}} + \frac{p_1 \cdot F_{34} \cdot q_{234} p_1 \cdot F_2 \cdot q_2}{D_2} + \frac{p_1 \cdot F_{24} \cdot q_{234} p_{12} \cdot F_3 \cdot q_3}{D_3} + \frac{p_1 \cdot F_{23} \cdot q_{234} p_{123} \cdot F_4 \cdot q_4}{D_4} \right. \\ &+ \frac{p_1 \cdot F_4 \cdot q_{234} p_1 \cdot F_{23} \cdot q_{23}}{D_{23}} + \frac{p_1 \cdot F_3 \cdot q_{234} p_1 \cdot F_{24} \cdot q_{24}}{D_{24}} + \frac{p_1 \cdot F_2 \cdot q_{234} p_{12} \cdot F_{34} \cdot q_{34}}{D_{34}} \\ &+ \frac{p_1 \cdot F_4 \cdot q_{234} p_1 \cdot F_3 \cdot q_{23} p_1 \cdot F_2 \cdot q_2}{D_{23} D_2} + \frac{p_1 \cdot F_4 \cdot q_{234} p_1 \cdot F_2 \cdot q_{23} p_{12} \cdot F_3 \cdot q_3}{D_{23} D_3} \\ &+ \frac{p_1 \cdot F_3 \cdot q_{234} p_{13} \cdot F_4 \cdot q_{24} p_1 \cdot F_2 \cdot q_2}{D_{24} D_2} + \frac{p_1 \cdot F_3 \cdot q_{234} p_1 \cdot F_2 \cdot q_{24} p_{123} \cdot F_4 \cdot q_4}{D_{24} D_4} \\ &\left. + \frac{p_1 \cdot F_2 \cdot q_{234} p_{12} \cdot F_4 \cdot q_{34} p_{12} \cdot F_3 \cdot q_3}{D_{34} D_3} + \frac{p_1 \cdot F_2 \cdot q_{234} p_{12} \cdot F_3 \cdot q_{34} p_{123} \cdot F_4 \cdot q_4}{D_{34} D_4} \right). \end{aligned} \quad (\text{B1})$$

It contains 13 terms, or the Fubini number \mathcal{F}_3 . These 13 terms can also be realized by quasishuffle product $2\star 3\star 4$ evaluated as (9) acted by the linear map (11): in the same order as the above equation, the partitions are $(\{234\})$, $(\{34\}, \{2\})$, $(\{24\}, \{3\})$, $(\{23\}, \{4\})$, $(\{4\}, \{23\})$, $(\{3\}, \{24\})$, $(\{2\}, \{34\})$, $(\{4\}, \{3\}, \{2\})$,

$(\{4\}, \{2\}, \{3\})$, $(\{3\}, \{4\}, \{2\})$, $(\{3\}, \{2\}, \{4\})$, $(\{2\}, \{4\}, \{3\})$, $(\{2\}, \{3\}, \{4\})$.

The five-point YM numerator $K^{\text{YM}}(1, 2, 3, 4, 5)$ is almost the same as (B1) except that with our special choice, in each term the factor $p_1 \cdot F_{\tau_0} \cdot q_{234}$ is changed to $\epsilon_5 \cdot F_{\tau_0} \cdot \epsilon_5$ and the overall pole D_{234} is changed to $\epsilon_5 \cdot p_{234} = -\epsilon_5 \cdot p_1$.

APPENDIX C: DETAILS OF THE EFFECTIVE NUMERATORS IN HEAVY LIMIT AND DOUBLE COPY

1. Effective BCJ numerators for HEFT

Recall in (27) that we expand K_H into $K_H^{(i)}$ by counting the power of p_1 ; therefore we have a good control of the maximal power of the heavy mass m . For $n = 4, 5$, the expansion is trivial since we have one and three terms all

contribute to $K_H^{(2)}(1, 2, 3, 4)$ and $K_H^{(2)}(1, 2, 3, 4, 5)$, respectively, as given in Sec. V. For $n = 6$, the following term with explicit factor m^2 will contribute to $K_H^{(2)}(1, 2, \dots, 6)$:

$$-\frac{2m^2 v \cdot F_{23} \cdot v p_{23} \cdot F_5 \cdot v p_{23} \cdot F_4 \cdot v}{k^2 v \cdot p_{45} v \cdot p_4}. \quad (C1)$$

Meanwhile $K_H^{(3)}(1, 2, \dots, 6)$ is given by

$$-\frac{2m^3}{k^2} \left(\frac{v \cdot F_{25} \cdot v v \cdot F_{34} \cdot v}{v \cdot p_{34}} + \frac{v \cdot F_{25} \cdot v v \cdot F_{34} \cdot v}{v \cdot p_{25}} + \frac{v \cdot F_{24} \cdot v v \cdot F_{35} \cdot v}{v \cdot p_{24}} + \frac{v \cdot F_{24} \cdot v v \cdot F_{35} \cdot v}{v \cdot p_{35}} + \frac{v \cdot F_{23} \cdot v v \cdot F_{45} \cdot v}{v \cdot p_{23}} + \frac{v \cdot F_{23} \cdot v v \cdot F_{45} \cdot v}{v \cdot p_{45}} \right). \quad (C2)$$

Importantly, the actual power of m for $K_H^{(i)}$ is 2 for $i = 2$ and $i - 1$ for $2 < i \leq \lfloor n/2 \rfloor$ since for the latter cases the expressions are proportional to an addition $v \cdot k \propto m^{-1}$ after collecting terms carefully. For instance, (C2) can be rewritten as

$$-\frac{2m^3}{k^2} v \cdot k \left(\frac{v \cdot F_{25} \cdot v v \cdot F_{34} \cdot v}{v \cdot p_{34} v \cdot p_{25}} + \frac{v \cdot F_{24} \cdot v v \cdot F_{35} \cdot v}{v \cdot p_{24} v \cdot p_{35}} + \frac{v \cdot F_{23} \cdot v v \cdot F_{45} \cdot v}{v \cdot p_{23} v \cdot p_{45}} \right) \quad (C3)$$

On the other hand, we also expand ϕ^3 amplitudes according to the order of m^{-1} ,

$$A^{\phi^3}(1, \beta, n) = \sum_{j=0}^{n-3} A^{\phi^3, (j)}(1, \beta, n), \quad (C4)$$

where $A^{\phi^3, (j)}(1, \beta, n)$ denoted terms with the order $\mathcal{O}(m^{-j})$. For instance, at $n = 6$ and $j = 2, 3$ we have

$$A^{\phi^3, (2)}(1, 2, \dots, 6) = \frac{1}{s_{12} s_{34} s_{1234}} + \frac{1}{s_{23} s_{123} s_{1234}} + \frac{1}{s_{12} s_{45} s_{123}},$$

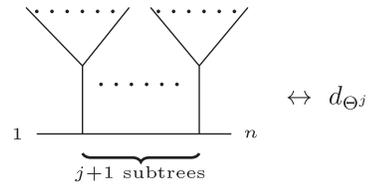
$$A^{\phi^3, (3)}(1, 2, \dots, 6) = \frac{1}{s_{12} s_{123} s_{1234}}. \quad (C5)$$

Therefore the amplitudes are expressed by

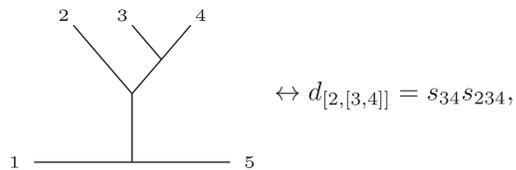
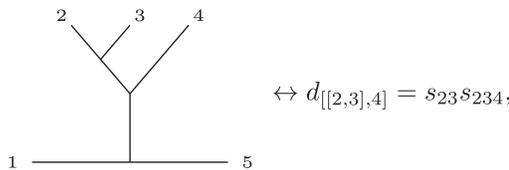
$$A^H(1, 2, \dots, n) = \sum_{\beta \in \mathcal{S}_{n-2}} A^{\phi^3}(1, \beta, n) K_H(1, \beta, n),$$

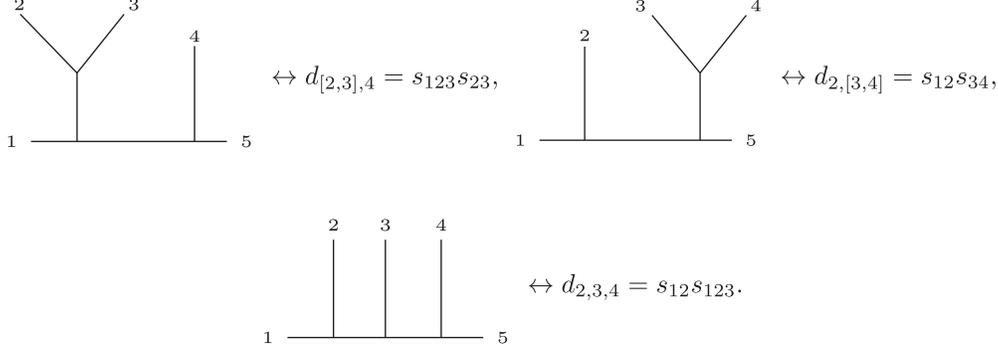
$$= \sum_{j=0}^{n-3} \sum_{\Theta^j} \sum_{i=2}^{\lfloor n/2 \rfloor} \frac{K_H^{(i)}(1, \Theta^j, n)}{d_{\Theta^j}}. \quad (C6)$$

Here, each term in the summation is at order $\mathcal{O}(m^{i-j})$ for $i = 2$ and $\mathcal{O}(m^{i-1-j})$ otherwise. We define a nested commutator of depth r of an ordered set to be r mutually compatible commutators acting on the ordered set; and we use Θ^j for $j = 0, 1, \dots, n-3$ to represent nested commutator of depth $n-3, n-4, \dots, 0$ of the ordered set $(2, 3, \dots, n-1)$. For examples, for $n = 5$ with $j = 0, 1, 2$ we sum over $\Theta^0 = ([2, 3], 4]$, $\Theta^1 = ([2, [3, 4]])$ and $\Theta^2 = (2, [3, 4])$. Moreover, d_{Θ^j} is the propagator denominator corresponding to the cubic graph associated with Θ^j :



For $n = 5$, d_{Θ^j} s involved in the summation are given by





Notice that the correct order of the amplitude $A^H(1, 2, \dots, n)$ is $\mathcal{O}(m^1)$, therefore physically one expects the contribution to higher power of m vanishes. We have checked this fact up to $n = 10$. Moreover, we have observed that the only contribution to the leading order of amplitudes is $i = 2$ and $j = 1$, which means

$$K_H^{(2)}(\Theta^0) = 0 \quad \text{and} \quad K_H^{(i)}(1, \Theta^{i-2}, n) = 0 \quad \text{for } 2 < i \leq \lfloor n/2 \rfloor. \quad (\text{C7})$$

Note that

$$K_H^{(i)}(1, \Theta^j, n) = 0 \Rightarrow K_H^{(i)}(1, \Theta^a, n) = 0 \quad \text{for } a < j, \quad (\text{C8})$$

since $K_H^{(i)}(1, \Theta^a, n)$ is nothing but the linear combination of those with $j > a$. Therefore, Eq. (C7) already ensures the vanishing of $\mathcal{O}(m^h)$ with $h > 1$. In addition, the general conjecture, which is even stronger than (C7) and confirmed up to ten points, reads

$$K_H^{(i)}(1, \Theta^{2(i-2)}, n) = 0 \quad \text{for } 2 \leq i \leq \lfloor n/2 \rfloor. \quad (\text{C9})$$

We now give a proof of the simplest case of conjecture (C9), say $i = n/2$ for even n , for which we have

$$K_H^{(n/2)}(1, 2, \dots, n) = \sum_{\tau \in \text{part}(n/2), |\tau_k|=2} \prod_{k=0}^{n/2-1} \frac{p_1 \cdot F_{\tau_k} \cdot v}{D_{I_k}}, \quad (\text{C10})$$

where we sum over the ordered partition of $(2, \dots, n-1)$ into $n/2$ sets with each set contains two elements. The above expression is invariant under the permutation on any two labels, therefore

$$K_H^{(n/2)}(1, \Theta^{n-4}, n) = 0, \quad (\text{C11})$$

which completes the proof.

In summary, the effective BCJ numerator contributing to the leading order of the amplitude $A^H(1, 2, \dots, n)$ is $K_H^{(2)}$, where the power of m is only contributed from the overall pole $v \cdot k = -\frac{k^2}{2m}$ and the factor $mv \cdot F_{\tau_0} \cdot v$ in numerator (6). This fact is equivalent to the boundary (4) does not contain particle 2 except for the I_0 . The proof is straightforward. Whenever there is a $I_k (k \neq d)$, which consists of 2 and a I_{k+1} does not consist of 2, then $\Delta(I_k, I_{k+1}) = \bar{I}_k|_{<2} = \emptyset$, which means that this boundary at least contributes to the superficial order of $\mathcal{O}(m^3)$, unless $|\tau_k| = 1$ for which this term vanishes. Similarly, for the remaining $I_d \supset \{2\}$ case, $\Delta(I_d, \emptyset)$ also becomes an empty set, and this boundary will either contribute to at least superficial order $\mathcal{O}(m^3)$ or vanishes.

Therefore, the remained pole structure contains two parts of contribution. The pole structure of the first part is related to $\mathcal{P}_{\{34\dots n-1\}}$ with an additional overall pole $D_{23\dots n-1}$, which implies that there are \mathcal{F}_{n-3} terms. The other part is also corresponded to $\mathcal{P}_{\{34\dots n-1\}}$, but does not have the pole $D_{34\dots n-1}$. So naively there are $2\mathcal{F}_{n-3}$ terms contributing to order $\mathcal{O}(m^1)$. However, for the first part which contains pole $D_{34\dots n-1}$, the numerator of each term must include a factor $mv \cdot F_2 \cdot v$ and hence vanishes. Consequently, we obtain the expression of the effective BCJ numerator (29) in the heavy limit and the leading order of amplitude is given by (28).

2. Double copy

It is quite interesting that the vanishing properties (C9) are precisely sufficient to ensure the leading order of amplitude for heavy scalars coupled to gravitons also only receives the contribution from $K_H^{(2)}$. Consider the double copy of (C6)

$$\begin{aligned} M_n^H &= \sum_{\alpha, \beta \in \mathcal{S}_{n-2}} K_H(1, \alpha, n) m(1, \alpha, n | 1, \beta, n) K_H(1, \beta, n), \\ &= \sum_{j=0}^{n-3} \sum_{\Theta^j} \sum_{i, i'=2}^{\lfloor n/2 \rfloor} \frac{K_H^{(i)}(1, \Theta^j, n) K_H^{(i')}(1, \Theta^j, n)}{d_{\Theta^j}}, \end{aligned} \quad (\text{C12})$$

where Θ^j for $j = 0, 1, \dots, n-3$ is the nested commutators of depth $n-3, n-2, \dots, 0$ of the unordered set $\{2, 3, \dots, n-1\}$ and d_{Θ^j} is the corresponding propagator denominator. Note that with the support of (C8), the conjecture (C9) implies

$$K_H^{(i)}(1, \Theta^j, n) K_H^{(i')}(1, \Theta^j, n) = 0 \quad \text{for } i + i' - j - 2 = 2 \quad \text{with } i, i' \neq 2, \quad (\text{C13})$$

$$K_H^{(2)}(1, \Theta^j, n) K_H^{(i')}(1, \Theta^j, n) = 0 \quad \text{for } i' - j + 1 = 2 \quad \text{with } i' \neq 2, \quad (\text{C14})$$

which would have contributed at $\mathcal{O}(m^2)$. Therefore, the amplitude is simplified into

$$M_n^H = \sum_{\Theta^1} \frac{K_H^{(2)}(1, \Theta^1, n)^2}{d_{\Theta^1}} + \sum_{\Theta^2} \frac{K_H^{(2)}(1, \Theta^2, n)^2}{d_{\Theta^2}}, \quad (\text{C15})$$

Importantly, the above two contributions are at the same order $\mathcal{O}(m^2)$, where for the first part, i.e., the contribution from summing over Θ^1 , one needs to collect terms in pair on the support of (C9) to organize the result in explicit $\mathcal{O}(m^2)$. For $n = 4$, there would be no contribution from the second part and the amplitude reads

$$M_4^H = \frac{K_H^{(2)}(1, 2, 3, 4)^2}{s_{12}} + \frac{K_H^{(2)}(1, 3, 2, 4)^2}{s_{13}} = \frac{2mv \cdot k K_H^{(2)}(1, 2, 3, 4)^2}{s_{12}s_{13}}, \quad (\text{C16})$$

where we have used $K_H^{(2)}(1, 2, 3, 4) = K_H^{(2)}(1, 3, 2, 4)$. A more nontrivial case is for $n = 5$, the result is given by

$$\begin{aligned} & \frac{1}{s_{34}} \left(\frac{K_H^{(2)}(2, [3, 4])^2}{s_{12}} + \frac{K_H^{(2)}([3, 4], 2)^2}{s_{134}} \right) + \frac{1}{s_{24}} \left(\frac{K_H^{(2)}(3, [2, 4])^2}{s_{13}} + \frac{K_H^{(2)}([2, 4], 3)^2}{s_{124}} \right) + \frac{1}{s_{23}} \left(\frac{K_H^{(2)}(4, [2, 3])^2}{s_{14}} + \frac{K_H^{(2)}([2, 3], 4)^2}{s_{123}} \right) \\ & + \frac{K_H^{(2)}(2, 3, 4)^2}{s_{12}s_{123}} + \frac{K_H^{(2)}(3, 2, 4)^2}{s_{13}s_{123}} + \frac{K_H^{(2)}(2, 4, 3)^2}{s_{12}s_{124}} + \frac{K_H^{(2)}(4, 2, 3)^2}{s_{14}s_{124}} + \frac{K_H^{(2)}(3, 4, 2)^2}{s_{13}s_{134}} + \frac{K_H^{(2)}(4, 3, 2)^2}{s_{14}s_{134}}, \end{aligned} \quad (\text{C17})$$

where we have omitted the scalar labels 1 and 5 in $K_H^{(2)}$. Note that for two terms in each pair in the first line, the numerators are equal, which is the part of the conjecture (C9) with $i = 2, j = 0$. Therefore, by collecting terms in pairs the first line gives rise to an additional $v \cdot k$ and we have the amplitude consistently at $\mathcal{O}(m^2)$. This argument works for general n with each pair corresponding to cubic graphs with two identical subtrees placed reversely on the scalar line.

Moreover, the amplitude (C15) can be simplified further, e.g., for (C17), the first pair in the first line reads

$$\frac{1}{s_{34}} \frac{(s_{12} + s_{134}) K_H^{(2)}(2, [3, 4])^2}{s_{12}s_{134}} = \frac{1}{s_{34}} \frac{(2mv \cdot k + s_{34}) K_H^{(2)}(2, [3, 4])^2}{s_{12}s_{134}}. \quad (\text{C18})$$

Similar operations can be applied to the remaining two pairs, and one can check that the amplitude is then given by

$$M_5^H = 2mv \cdot k \left(\frac{K_H^{(2)}(2, [3, 4])^2}{s_{12}s_{134}s_{34}} + \frac{K_H^{(2)}(3, [2, 4])^2}{s_{13}s_{124}s_{24}} + \frac{K_H^{(2)}([2, 3], 4)^2}{s_{14}s_{123}s_{23}} \right), \quad (\text{C19})$$

where the second line of (C17) has been canceled. The analogous cancellation has also been observed at higher points, which leads to the conjecture of a more compact version of (C15)

$$M_n^H = 2mv \cdot k \sum_g \frac{K_H^{(2)}(1, \Theta^0(I), \Theta^0(\bar{I}), n)^2}{s_{1I}s_{1\bar{I}}d_{\Theta^0(I)}d_{\Theta^0(\bar{I})}}, \quad (\text{C20})$$

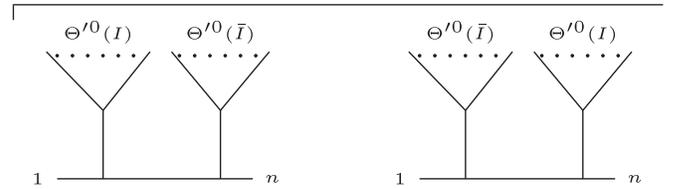


FIG. 6. Cubic graphs with two identical subtrees placed reversely on the scalar line.

where we sum over the cubic graphs g corresponding to half of the possible Θ^1 s; i.e., each graph is either of two graphs with two identical subtrees (contain legs I and \bar{I}) where the subtrees are placed reversely on the scalar line (see Fig. 6). We also define $\Theta^0(I)$ to be the nested commutator of depth $|I| - 1$ of the unordered set I and

$d_{\Theta^0(I)}$ to be the corresponding propagator denominator; for each term in the summation, $\Theta^0(I)$ and $\Theta^0(\bar{I})$ are given by the subtrees of the graph g . The above expression contains $(2n - 7)!!$ terms, which is equal to the number of terms in an $(n - 1)$ -point amplitude of gravitons scattering (without heavy scalars).

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- [1] H. Kawai, D. C. Lewellen, and S. H. H. Tye, *Nucl. Phys.* **B269**, 1 (1986).
- [2] Z. Bern, J. J. M. Carrasco, and H. Johansson, *Phys. Rev. D* **78**, 085011 (2008).
- [3] Z. Bern, J. J. M. Carrasco, and H. Johansson, *Phys. Rev. Lett.* **105**, 061602 (2010).
- [4] Z. Bern, J. J. Carrasco, M. Chiodaroli, H. Johansson, and R. Roiban, *arXiv:1909.01358*.
- [5] Z. Bern, J. J. Carrasco, M. Chiodaroli, H. Johansson, and R. Roiban, *J. Phys. A* **55**, 443003 (2022).
- [6] T. Adamo, J. J. M. Carrasco, M. Carrillo-González, M. Chiodaroli, H. Elvang, H. Johansson, D. O’Connell, R. Roiban, and O. Schlotterer, in 2022 Snowmass Summer Study (2022), *arXiv:2204.06547*.
- [7] C. Cheung and J. Mangan, *J. High Energy Phys.* **11** (2021) 069.
- [8] C. R. Mafra, O. Schlotterer, and S. Stieberger, *J. High Energy Phys.* **07** (2011) 092.
- [9] T. Bargheer, S. He, and T. McLoughlin, *Phys. Rev. Lett.* **108**, 231601 (2012).
- [10] F. Cachazo, S. He, and E. Y. Yuan, *J. High Energy Phys.* **07** (2014) 033.
- [11] S. He, R. Monteiro, and O. Schlotterer, *J. High Energy Phys.* **01** (2016) 171.
- [12] C.-H. Fu, Y.-J. Du, R. Huang, and B. Feng, *J. High Energy Phys.* **09** (2017) 021.
- [13] F. Teng and B. Feng, *J. High Energy Phys.* **05** (2017) 075.
- [14] Y.-J. Du and F. Teng, *J. High Energy Phys.* **04** (2017) 033.
- [15] S. He, O. Schlotterer, and Y. Zhang, *Nucl. Phys.* **B930**, 328 (2018).
- [16] A. Edison and F. Teng, *J. High Energy Phys.* **12** (2020) 138.
- [17] S. He, L. Hou, J. Tian, and Y. Zhang, *J. High Energy Phys.* **08** (2021) 118.
- [18] R. Monteiro and D. O’Connell, *J. High Energy Phys.* **07** (2011) 007.
- [19] R. Monteiro and D. O’Connell, *J. High Energy Phys.* **03** (2014) 110.
- [20] C. Cheung and C.-H. Shen, *Phys. Rev. Lett.* **118**, 121601 (2017).
- [21] G. Chen, H. Johansson, F. Teng, and T. Wang, *J. High Energy Phys.* **11** (2019) 055.
- [22] A. Edison, S. He, H. Johansson, O. Schlotterer, F. Teng, and Y. Zhang, *arXiv:2211.00638*.
- [23] N. Arkani-Hamed and J. Trnka, *J. High Energy Phys.* **10** (2014) 030.
- [24] N. Arkani-Hamed, Y. Bai, S. He, and G. Yan, *J. High Energy Phys.* **05** (2018) 096.
- [25] N. Arkani-Hamed, S. He, and T. Lam, *J. High Energy Phys.* **02** (2021) 069.
- [26] M. E. Hoffman, *J. Algebr. Comb.* **11**, 49 (2000).
- [27] Wikipedia, Permutohedron—Wikipedia, the free encyclopedia, <http://en.wikipedia.org/w/index.php?title=Permutohedron&oldid=1067270212> (2022).
- [28] H. Georgi, *Phys. Lett. B* **240**, 447 (1990).
- [29] M. E. Luke and A. V. Manohar, *Phys. Lett. B* **286**, 348 (1992).
- [30] M. Neubert, *Phys. Rep.* **245**, 259 (1994).
- [31] A. V. Manohar and M. B. Wise, *Heavy Quark Physics*, Cambridge Monographs on Particle Physics, Nuclear Physics and Cosmology (Cambridge University Press, Cambridge, England, 2000).
- [32] P. H. Damgaard, K. Haddad, and A. Helset, *J. High Energy Phys.* **11** (2019) 070.
- [33] A. Brandhuber, G. Chen, G. Travaglini, and C. Wen, *J. High Energy Phys.* **07** (2021) 047.
- [34] A. Brandhuber, G. Chen, H. Johansson, G. Travaglini, and C. Wen, *Phys. Rev. Lett.* **128**, 121601 (2022).
- [35] A. Brandhuber, G. R. Brown, G. Chen, J. Gowdy, G. Travaglini, and C. Wen, *J. High Energy Phys.* **12** (2022) 101.
- [36] A. Brandhuber, G. Chen, G. Travaglini, and C. Wen, *J. High Energy Phys.* **10** (2021) 118.
- [37] D. A. Kosower, B. Maybee, and D. O’Connell, *J. High Energy Phys.* **02** (2019) 137.
- [38] Z. Bern, C. Cheung, R. Roiban, C.-H. Shen, M. P. Solon, and M. Zeng, *Phys. Rev. Lett.* **122**, 201603 (2019).
- [39] T. Damour, *Phys. Rev. D* **102**, 024060 (2020).
- [40] Z. Bern, J. Parra-Martinez, R. Roiban, M. S. Ruf, C.-H. Shen, M. P. Solon, and M. Zeng, *Phys. Rev. Lett.* **126**, 171601 (2021).
- [41] P. Di Vecchia, C. Heissenberg, R. Russo, and G. Veneziano, *J. High Energy Phys.* **07** (2021) 169.
- [42] E. Herrmann, J. Parra-Martinez, M. S. Ruf, and M. Zeng, *J. High Energy Phys.* **10** (2021) 148.
- [43] N. E. J. Bjerrum-Bohr, P. H. Damgaard, L. Planté, and P. Vanhove, *J. High Energy Phys.* **08** (2021) 172.
- [44] N. E. J. Bjerrum-Bohr, L. Planté, and P. Vanhove, *J. High Energy Phys.* **03** (2022) 071.
- [45] G. U. Jakobsen, G. Mogull, J. Plefka, and J. Steinhoff, *Phys. Rev. Lett.* **128**, 011101 (2022).

- [46] N. Arkani-Hamed, L. Rodina, and J. Trnka, *Phys. Rev. Lett.* **120**, 231602 (2018).
- [47] R. Kleiss and H. Kuijf, *Nucl. Phys.* **B312**, 616 (1989).
- [48] X. Gao, S. He, and Y. Zhang, *J. High Energy Phys.* **11** (2017) 144.
- [49] S. He, G. Yan, C. Zhang, and Y. Zhang, *J. High Energy Phys.* **08** (2018) 040.
- [50] For $K(1, \beta, n)$, everything stays the same except that in (7) the definition of τ_i s become $\tau_k = \beta(I_k/I_{k+1})$, i.e., any subset I is sorted according to β ordering.
- [51] G. Chen, G. Lin, and C. Wen, [arXiv:2208.05519](https://arxiv.org/abs/2208.05519).
- [52] Wikipedia, Stirling numbers of the second kind—Wikipedia, the free encyclopedia, <http://en.wikipedia.org/w/index.php?title=Stirling%20numbers%20of%20the%20second%20kind&oldid=1116823918> (2022).
- [53] I. Mezo, *Combinatorics and Number Theory of Counting Sequences (1st ed.)* (Chapman and Hall/CRC, London, 2019).
- [54] Q. Cao, J. Dong, and Y.-Q. Zhang (to be published).
- [55] C. S. Lam and Y.-P. Yao, *Phys. Rev. D* **93**, 105008 (2016).
- [56] C. Cheung, C.-H. Shen, and C. Wen, *J. High Energy Phys.* **02** (2018) 095.
- [57] J. Dong, S. He, and L. Hou, *Phys. Rev. D* **105**, 105007 (2022).
- [58] Here we have omitted the labels of the scalar particles 1 and n in the numerators K and \tilde{K} .
- [59] Z. Bern and T. Dennen, *Phys. Rev. Lett.* **107**, 081601 (2011).
- [60] L. Rodina, *J. High Energy Phys.* **09** (2019) 084.