

Algebraic consistency and explicit construction of one-loop Bern-Carrasco-Johansson numerators of Yang-Mills and related theories

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We study the algebraic structure of one-loop Bern-Carrasco-Johansson numerators in Yang-Mills and related theories. Starting from the propagator matrix that connects color-ordered integrands to numerators, we identify the consistency conditions that ensure the existence of Jacobi-satisfying numerator solutions and determine the unique construction. The relation between one-loop numerators and forward-limit tree numerators is clarified, together with the additional physical conditions required for a consistent double-copy interpretation. We propose a two-step expansion strategy for obtaining explicit one-loop numerators. The Yang-Mills integrand is first decomposed into scalar-loop Yang-Mills-scalar building blocks, which are then expanded into biadjoint scalar integrands. We derive explicit results for up to three external gluons, showing how the kinematic consistency conditions uniquely determine the coefficients in each case. Similar results for Einstein-Yang-Mills and gravity amplitudes are also presented.

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I. INTRODUCTION

At tree level, the Bern-Carrasco-Johansson (BCJ) duality [1,2] states that color-ordered amplitudes $A(1, 2, \dots, n)$ can be expressed as a sum over cubic tree diagrams whose leaves are labeled by the external legs $1, 2, \dots, n-1$. Each diagram Γ contributes a term of the form

$$A(1, 2, \dots, n) = \sum_{\Gamma} \frac{N_{\Gamma}}{D_{\Gamma}}, \quad (1.1)$$

where D_{Γ} denotes the product of all propagators associated with the internal branches of the cubic tree, and N_{Γ} is a kinematic function depending on momenta and polarization vectors. The essential content of the BCJ duality is that the kinematic numerators N_{Γ} can be arranged to satisfy the same Jacobi identities as the color factors of Yang-Mills theory. In this way, the algebraic structure underlying gauge amplitudes mirrors that of the color algebra, allowing gravity amplitudes to be obtained through a “double copy” construction by replacing color factors with kinematic numerators.

At one-loop level, this organization naturally generalizes [1,2]: The integrand can be written as a sum over cubic one-loop diagrams, each diagram being a polygon whose vertices are decorated by cubic tree subgraphs with the

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same cyclic ordering of external legs. Schematically,

$$\mathcal{I}_n^{1\text{-loop}} = \sum_{\Gamma} \frac{N_{\Gamma}(\ell)}{D_{\Gamma}(\ell)}, \quad (1.2)$$

where the denominator $D_{\Gamma}(\ell)$ is the product of the Feynman propagators corresponding to all branches of the cubic one-loop diagram, and $N_{\Gamma}(\ell)$ is a loop-momentum-dependent kinematic numerator satisfying the Jacobi identities among neighboring graphs. The central question is then how to determine such numerators consistently, and in particular, how their existence constrains the analytic structure of the integrand.

In this work we focus on the algebraic consistency conditions that ensure the existence and uniqueness of such one-loop numerators, and on how these consistency principles can be used to construct explicit one-loop numerators for Yang–Mills and related theories. We also analyze the compatibility of these constructions with the Kawai–Lewellen–Tye (KLT) relations [3–5] at one loop. In this paper, we address the following three issues related to the problem of solving kinematic numerators and consequences on the integrands due to the numerator structure at one loop.

- (i) The first issue is how to solve numerators from integrands. Recall at tree level, the solution is based on the observation that Kleiss–Kuijff (KK) relations [6] and Jacobi identities happen to result in the same number of independent amplitudes and numerators, respectively [7]. So that given a KK satisfying theory, assuming the color-ordered amplitudes have been already computed from Feynman rules, the numerators can be determined from linear equations with equal number of known and unknown variables. Take the 4-point case as an example, a KK satisfying theory has 2 independent color-ordered amplitudes, as well as 2 independent numerators (the half-ladders [8]). The two sets are related by (1.3)

with the propagator matrix being the coefficients [9].

$$\begin{bmatrix} A(1234) \\ A(1324) \end{bmatrix} = \begin{bmatrix} \frac{1}{s} + \frac{1}{t} & \frac{-1}{t} \\ \frac{-1}{t} & \frac{1}{u} + \frac{1}{t} \end{bmatrix} \begin{bmatrix} N^{\text{tree}}(1234) \\ N^{\text{tree}}(1324) \end{bmatrix}. \quad (1.3)$$

The Mandelstam variables s , t and u are defined by $s = 2k_1 \cdot k_2$, $t = 2k_1 \cdot k_3$ and $u = 2k_1 \cdot k_4$, where k_i is the momentum of the particle fi . For massless theories, the propagator matrix is known to be singular and cannot be simply inverted. The kernel of this matrix corresponds to the BCJ relations of color-ordered amplitudes [10,11]. One then concludes that the necessary and sufficient condition for an arbitrary massless theory to be allowed a consistent numerator formulation is that the amplitudes should satisfy BCJ relations, in which case the kinematic numerators, regarded as unknowns, can be determined by inverting the propagator matrix (the momentum kernel [3,4,12]).

From this perspective it would be interesting¹ to see if a similar generalized argument can be used to determine the numerators from the integrand, where the cubic structure is assumed to reside at one loop level.²

This question motivates the first part of the present paper, in which we analyze the algebraic consistency conditions of the one-loop propagator matrix and demonstrate how these conditions ensure the existence and uniqueness of consistent numerators.

To further illustrate the problem, let us consider a 2-point integrand, which is the first nontrivial example. BCJ's formulation (1.2) demands that if the solution of numerators exists, the 2-point color-ordered integrand $\mathcal{I}_2$ needs to be expressible as the following sum over cubic diagrams.

$$\mathcal{I}_2(\ell, k_1, k_2) = \frac{1}{\ell^2} \frac{1}{(\ell + k_1)^2} \times \text{bubble}(\ell, \ell + k_1) + \frac{1}{\ell^2} \frac{1}{i\epsilon} \times \text{triangle}(\ell, \ell + k_1) + \frac{1}{(\ell + k_1)^2} \frac{1}{i\epsilon} \times \text{triangle}(\ell + k_1, \ell), \quad (1.4)$$

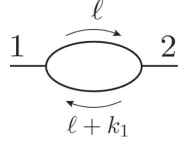
where ℓ is the loop momentum. The tree propagators in the second and the third terms have the form $\frac{1}{(k_1 + k_2)^2 + i\epsilon}$, which can be written as $\frac{1}{i\epsilon}$ due to momentum conservation.³ In view of the argument at tree level, let us rewrite the right-hand side of the equation in terms of basis numerators. At one loop a commonly used basis at n -point is the polygons attached with n external legs. In the 2-point case these are the bubble graphs with various loop momentum

¹This is especially so when the rank of propagator matrix has been revealed to be further reduced from those at tree level [13].

²Note however, for the purpose of calculating gravity amplitudes using double-copy, which is usually the motive for studying color-kinematics duality, one does not actually need to fully determine the numerators. The knowledge of the existence of kinematic numerators suffices [14].

³In most situations of this paper, the $i\epsilon$ is omitted for convenience.

values ℓ flowing from leg 1 toward 2.⁴



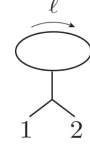
$$(1.5)$$

In this paper we symbolically represent this numerator by $N(\ell, 1, 2, -\ell)$, as a single cut from the above internal line yields a familiar half-ladder. We would like to emphasize this imaginary “cut” is merely a convenient way to understand the notation. The symbol $N(\ell, 1, 2, -\ell)$ represents the whole bubble numerator (1.5). Alternatively, one may introduce an imaginary cut from below. Therefore in this slightly redundant notation, the following two expressions

both represent the same bubble graph.

$$N(\ell, 1, 2, -\ell) = N(\ell + k_1, 2, 1, -(\ell + k_1)). \quad (1.6)$$

Using this notation, the Jacobi identity satisfied by the tadpole graph can be written as the following.



$$= N(\ell, 1, 2, -\ell) - N(\ell, 2, 1, -\ell). \quad (1.7)$$

And similarly for the other tadpole numerator. The 2-pt integrand $\mathcal{I}_2$ is then expressible symbolically as

$$\begin{aligned} \mathcal{I}_2(\ell, k_1, k_2) = & \frac{1}{\ell^2(\ell + k_1)^2} N(\ell, 1, 2, -\ell) + \frac{1}{\ell^2} \frac{1}{i\epsilon} (N(\ell, 1, 2, -\ell) - N(\ell - k_1, 1, 2, -(\ell - k_1))) \\ & + \frac{1}{(\ell + k_1)^2} \frac{1}{i\epsilon} (N(\ell, 1, 2, -\ell) - N(\ell + k_1, 1, 2, -(\ell + k_1))). \end{aligned} \quad (1.8)$$

From this equation we see that the problem of solving numerators at one loop is much more involved than its tree level counterpart (1.3). The above linear equation can be more or less rigorously solved by manually imposing periodic boundary conditions $\ell + Mk_1 \sim \ell$, for some large integer M [19,20]. At 2-point momentum conservation requires there is only one independent external momentum, therefore all shifted numerators can be labeled by the amount of shifting in the k_1 direction. Suppose if we further introduce shorthand notations for the integrand and the numerators, $\mathcal{I}_2(m) := \mathcal{I}_2(\ell + mk_1, k_1, k_2)$ and

$N(m) := N(\ell + mk_1, 1, 2, -(\ell + mk_1))$, and note that the integrand-numerator relation (1.8) takes the following form,

$$\begin{aligned} \mathcal{I}_2(m) = & A(m)N(m) + B(m)N(m+1) \\ & + C(m)N(m-1). \end{aligned} \quad (1.9)$$

Assuming again all integrands are known from Feynman rules, in principle the numerators can be determined from the $M \rightarrow \infty$ solution of the matrix equation

$$\begin{bmatrix} \mathcal{I}_2(0) \\ \mathcal{I}_2(1) \\ \mathcal{I}_2(2) \\ \vdots \\ \mathcal{I}_2(M-1) \end{bmatrix} = \begin{bmatrix} A(0) & B(0) & & & \\ C(1) & A(1) & B(1) & & \\ & C(2) & A(2) & B(2) & \\ & & \ddots & \ddots & \ddots \\ B(M-1) & & & & \end{bmatrix} \begin{bmatrix} N(0) \\ N(1) \\ N(2) \\ \vdots \\ N(M-1) \end{bmatrix} \quad (1.10)$$

The solution of this particular matrix problem is known in the mathematics literature [21,22].

However at 3-point we have two independent momenta, and the set of unknown variables $N(\ell + m_1 k_1 + m_2 k_2, \sigma, -(\ell + m_1 k_1 + m_2 k_2))$ form a two dimensional lattice [19,20]. One then needs to solve a corresponding $(M_1 \times M_2) \times (M_1 \times M_2)$ matrix problem and so on. It is preferably not to resort to such involved technique, even for the purpose of

⁴Note the convention for loop momentum used in this paper is slightly different from the one naturally inherited from string theory clarified in [15], and used in related problems, for example, in [16–18].

understanding the problem. Furthermore, it is difficult to check if a coefficient matrix of such a large dimension is singular, and whether the kernel of the matrix results in relations between color-ordered integrands like tree level.⁵ In Sec. II we show this difficulty can actually be circumvented by introducing physical conditions. This leads to a one loop generalization of the linear relation (2.12) between integrands and numerators. In Sec. II C we explain how the propagator matrix in this generalized linear relation is related to the original tree propagator matrix. Additionally, using a technique based on Sherman-Morrison formula [23], we explain in II D how the structure of the inverse propagator matrix (the momentum kernel) is affected by this generalization.

- (ii) The second issue concerns the relation between the numerator solutions solved from loop integrand and those solved from tree amplitudes, particularly the forward limit amplitudes. BCJ's integrand formulation (1.2) at one loop can be alternatively understood as a sum over various polygons with subtrees attached. It was observed by [17,24] that if we substitute the propagators of all n -gons appear in the integrand using the following partial fraction identity,

$$\frac{1}{\prod_{i=1}^n D_i} = \sum_{i=1}^n \frac{1}{D_i \prod_{j \neq i} (D_j - D_i)}, \quad (1.11)$$

the resulting integrand can be regrouped as a cyclic permutation sum of forward limit tree amplitudes [24–30]. Explicitly at 2-point this is done by replacing the propagator of the bubble graph in (1.8) by

$$\begin{aligned} \frac{1}{\ell^2(\ell + k_1)^2} &= \frac{1}{\ell^2[(\ell + k_1)^2 - \ell^2]} \\ &\quad - \frac{1}{(\ell + k_1)^2[(\ell + k_1)^2 - \ell^2]} \\ &= \frac{1}{\ell^2} \frac{1}{2\ell \cdot k_1} + \frac{1}{(\ell + k_1)^2} \frac{1}{(\ell + k_1) \cdot k_2}, \end{aligned}$$

and then regroup the first and the second term above with the first and the second tadpoles in (1.8) respectively, yielding

$$\begin{aligned} \mathcal{I}_2(\ell, k_1, k_2) &= \frac{1}{\ell^2} A_{\text{BCJ}}^{\text{tree}}(\ell, 1, 2, -\ell) + \frac{1}{(\ell + k_1)^2} \\ &\quad \times A_{\text{BCJ}}^{\text{tree}}(\ell + k_1, 2, 1, -(\ell + k_1)). \end{aligned} \quad (1.12)$$

Here by forward limit tree amplitude we mean that if we construct color-order tree amplitudes using

BCJ's formula (1.1) for tree amplitude, formally writing down tree numerators, identifying external legs according to the forward limit, and additionally, replacing the tree numerator $N^{\text{tree}}(\ell, \sigma(1), \sigma(2), \dots, \sigma(n), -\ell)$ formally just written down by their corresponding symbols introduced to denote polygon basis numerators,⁶ $N(\ell, \sigma(1), \sigma(2), \dots, \sigma(n), -\ell)$, then the forward limit tree amplitudes such as $A_{\text{BCJ}}^{\text{tree}}(\ell, 1, 2, -\ell)$ obtained after regrouping will be identical to the ones we just wrote down through this procedure. Graphically speaking, these can be understood as welding two parallel legs of the forward limit tree amplitude. All propagators appear in these tree amplitudes are just linear in loop momentum ℓ , which is formally identical to tree propagator in a massless theory. Here we introduce subscripts $A_{\text{BCJ}}^{\text{tree}}$ to indicate these are built from the cubic formulation of BCJ and contain numerators, regarded as unknowns, which is not to be confused with amplitudes built from Feynman rules that generically carry more than cubic structure.

The fact that these forward limit tree amplitudes appear in the integrand decomposition (1.12) bear such remarkable resemblance to tree amplitudes however, seem to suggest that they could be identified their values with the actual forward limit tree amplitudes obtained from Feynman rules, which we shall denote as $A_{\text{Feyn}}^{\text{tree}}$ in the following. In view of the linear relation (1.3) between tree amplitudes and numerators, this is equivalent to suggesting that we identify polygon basis numerators, $N(\ell, \sigma(1), \sigma(2), \dots, \sigma(n), -\ell)$ such as (1.5) and tree numerators in the same theory with both ends welded together. Therefore the existence of numerator solution at one loop requires the existence of numerator solution at tree level, which seems to be a reasonable requirement.

A few questions then arise. One naturally wonders the relation between the numerator solutions obtained from the knowledge of forward limit amplitudes just described, and the numerator solutions obtained directly from integrands (mentioned in (i) and will be explained in Sec. II). Additionally one may ask when such a solution exists. We will show in Sec. III that more conditions need to be met to guarantee a solution built from the welded forward limit tree numerators, in addition to requiring tree amplitudes of the same theory to satisfy BCJ relations. We shall see that, for nonlinear sigma model (NLSM), these conditions happen to be met, and therefore yields a consistent set of kinematic numerators (part of the verification detail will be

⁵See [16,18], however, for discussions long this line of thought.

⁶As discussed for instance in [24,27,29,31], where the tree-level and forward-limit structures are treated in the same sense.

given in Appendix A). The fact that NLSM satisfies the extra conditions is not surprising, as the theory has a natural cubic action that satisfies the Jacobi identity [32]. For the same reason this is also true for self-dual Yang-Mills theory in general dimensions [33]. From this perspective, a physically interesting BCJ structure seems to require stronger conditions than the bypassing method of (i). In Sec. III we will also explain the inconsistency caused by identifying polygon basis numerators with the welded forward limit tree numerators in the case when these extra conditions are violated.

Another question is how or whether the one loop numerators related to the welded forward limit tree numerators, in the case when extra conditions are not met, so that we cannot simply identify the two. In Sec. III A we will write down the relation between these two numerators, therefore for a generic theory, one can calculate one loop numerators if tree level numerators are already known, and vice versa.

- (iii) The third issue concerns compatibility between the Kawai-Lewellen-Tye (KLT) [3–5] relation, the double-copy formulation of BCJ, and related expressions of gravity integrands. Specifically, we find that at one loop level, starting from a double-copy formulation of the gravity integrand, suppose if we order integrands by the method explained in Sec. II C, the resulting KLT formula either contain graphs with miss-aligned loop momenta ℓ , or that one copy of the integrand carries an extra difference term Δ_ℓ ,

$$\tilde{\mathcal{I}}_{GR}(\ell, 12) = (\mathcal{I}_{YM}(\ell, 12) + \Delta_\ell) S[1|1]_\ell \tilde{\mathcal{I}}_{YM}(\ell, 12), \quad (1.13)$$

where $\Delta_\ell = f(\ell) - f(\ell + c)$. The reverse is also true. Starting from a KLT formula with the loop momenta in both of the gauge theory integrands defined in the conventional way, one obtains a double-copy formula with the loop momenta of the two copies related by a shift. Therefore cautions must be made when reproducing gravity integrands using this approach. We discuss this issue in Sec. IV.⁷

Additionally, we present in Appendix A a symmetry property of the nonlinear sigma model numerator, which supplement the discussion in Sec. III. A 3-point example solving the numerators using the method explained in Sec. A is presented in Appendix B.

Beside analysing general BCJ structure at one loop level, in this paper we present explicit numerator formulas at one loop level for Yang-Mills-scalar (YMS) and related theories [pure Yang-Mills (YM), gravity, and Einstein-Yang-Mills

(EYM)]. The practical problems we tackle in this paper are the following.

- (a) We shall see in Sec. II that, at least for the low-point cases we have checked explicitly, the propagator matrices we derive using the bypassing method mentioned above (issue (i)) is full-rank.⁸ So that given a color-ordered integrand, in principle one should be able to solve the numerators by inverting the propagator matrix, and such a solution is unique.⁹ Inverting the propagator matrix, however, could be a rather formidable task in practical calculations. In this paper we present an alternative, constructive approach to this problem, specifically tailored for the YMS theory. This part of the discussions, presented in Secs. VII to VII C, runs in parallel with the general discussion given in Secs. II to II D [issue (i)].

Recall that at tree level, in the special case when only one gluon participates the scattering with an arbitrary number of biadjoint scalars, the color-ordered amplitudes are built from cubic Feynman graphs only [35], which naturally define a Jacobi satisfying set of numerators [36,37]. Take the 1-gluon and 3-scalar amplitudes for example, equation (1.3) in this case can be written as the following.

$$A^{\text{YMS}}(1^s, 2^g, 3^s, 4^s) = \sum_{\sigma \in S_2} m(1^s, 2^g, 3^s, 4^s | 1^s \sigma 4^s) N^{\text{tree}}(1^s \sigma 4^s), \quad (1.14)$$

where we used superscripts to indicate particle species. The biadjoint scalars carry two copies of the color factors, so that when stripped off one copy, they contribute one color factor to the BCJ numerator. On the other hand a gluon carries only one copy of the color factor, therefore after stripping off contributes just a kinematic factor. Explicitly, in our example these are

$$N^{\text{tree}}(1^s, 2^g, 3^s, 4^s) = N^{(K)}(1234) N^{(C)}(1234) = e_2 \cdot k_1 f^{134}, \quad (1.15)$$

$$N^{\text{tree}}(1^s, 3^s, 2^g, 4^s) = N^{(K)}(1324) N^{(C)}(1324) = e_2 \cdot (k_1 + k_3) f^{134}. \quad (1.16)$$

⁸This phenomenon—that algebraic relations implied by the Jacobi identity impose stricter constraints at one loop than at tree level—is not isolated. In fact, as the loop order increases, it becomes increasingly difficult to construct numerators that satisfy exact Jacobi identities. Starting from two loops, various contact-term contributions that integrate to zero must be introduced in order to build numerators obeying generalized forms of Jacobi relations [13,14].

⁹By uniqueness here we mean with respect to this particular integrand, which is in general defined up terms that vanish after the loop integration.

⁷While preparing this manuscript, we became aware of a related work [34] that happens to overlap with this part of our work.

At higher points the kinematic dependent part of the BCJ numerator generalizes to a product of the polarization with a sum of momenta that appear on one side of the gluon, defined by the color order, $\epsilon \cdot X = \epsilon \cdot (\sum_{\text{all momenta on the left}} k_i)$ [36,37]. In this paper we shall denote the kinematic dependent part of the numerator $N^{(K)}(\sigma)$ as $C(\sigma)$, to be consistent with the notation used in [38–40]. The color dependent part of the BCJ numerator $N^{(C)}$ is given by the usual half-ladder, with the structure constant at the position corresponds to the gluon replaced by a Kronecker delta, $N^{(C)}(1^s, \dots, i^g, \dots, n^s) = f^{12*} f^{3*} \dots \delta^{**} \dots f^{*n-1, n}$. More than one Feynman graph contribute to a numerator when more gluons are involved, but rules were developed to write down directly the BCJ numerators from Feynman graphs [36,39–41]. In particular it was argued that gauge invariance to a large extent fixes the kinematic part of the YMS numerators, so that ansatz can also be introduced to simplify the calculation [36,42–44]. Other powerful methods were developed to write down the tree YMS numerators using fusion rules [45–51], string theory [52], and Cachazo-He-Yuan formula [53–57], see, e.g., [58–60]. Remarkably, it was observed by [36,50,51] that at tree level the pure Yang-Mills numerators can be actually derived from knowledge of YMS numerators, making them of great practical interest.

In view of the both rather simple numerator formulas and their application values at tree level, we feel the YMS theory could be a worthy investigating case

for the one loop numerator problem. Especially that the tree numerator formulas rely heavily on a language based on the symbol $X = \sum_{\text{all momenta on the left}} k_i$, defined as the momentum sum on one side of the gluon insertion position, which is apparently a tree topology concept. One naturally wonders how are the YMS numerator formulas generalized to one loop level. And indeed, we shall see in Sec. VII A that such a language generalizes to one loop level, with the color-stripped numerator for a single gluon insertion given by exactly the same formula.

$$C(\ell; 1, \alpha) = \epsilon_p \cdot X_p(\ell; 1, \alpha) \quad (1.17)$$

And we have a naturally generalized definition for the symbol X^μ appropriate for the one loop topology. The two and three gluon cases are also found to be given by the same formulas as at tree level, but with the symbols X^μ replaced by the generalized ones, and are proved in Secs. VII B and VII C, respectively.

As for the problem concerning computing pure YM numerators using YMS numerators, at tree level this relies on factorizing the gluon numerator into a subtree [50,51], which is also a topology dependent technique. In Sec. V we use an identity written down by [29,31,61,62] as a substitute, which relates the color-ordered integrands of pure YM with YMS ones, and we explain how to construct YM numerator at one loop using the YMS numerators. Explicitly, we obtain the pure YM numerator formulas for the 2-, 3-point cases as the following.¹⁰

$$\begin{aligned} N^{\text{YM}}(\ell; 1, 2) &= (D-2) \left[(\epsilon_1)_\mu (\epsilon_2)_\nu - \frac{\epsilon_1 \cdot \epsilon_2}{k_1 \cdot k_2} (k_1)_\mu (k_2)_\nu \right] \ell^\mu (\ell + k_1)^\nu + \text{Tr}[F_1 \cdot F_2], \\ N^{\text{YM}}(\ell; 1, 2, 3) &= (D-2) \left[(\epsilon_1)_\mu (\epsilon_2)_\nu (\epsilon_3)_\tau - \frac{\epsilon_1 \cdot \epsilon_2}{k_1 \cdot k_2} (k_1)_\mu (k_2)_\nu (\epsilon_3)_\tau - \frac{\epsilon_1 \cdot \epsilon_3}{k_1 \cdot k_3} (k_1)_\mu (\epsilon_2)_\nu (k_3)_\tau - \frac{\epsilon_2 \cdot \epsilon_3}{k_2 \cdot k_3} (\epsilon_1)_\mu (k_2)_\nu (k_3)_\tau \right] \\ &\quad \times \ell^\mu (\ell + k_1)^\nu (\ell + k_1 + k_2)^\tau + \text{Tr}[F_2 \cdot F_3] \epsilon_1 \cdot \ell + \text{Tr}[F_1 \cdot F_3] \epsilon_2 \cdot (\ell + k_1) \\ &\quad + \text{Tr}[F_1 \cdot F_2] \epsilon_3 \cdot (\ell + k_1 + k_2) - \text{Tr}[F_1 \cdot F_2 \cdot F_3] \epsilon_1 \cdot \ell \epsilon_2 \cdot (\ell + k_1) \epsilon_3 \cdot (\ell + k_1 + k_2), \end{aligned} \quad (1.18)$$

where ϵ_i^μ , k_i^μ respectively denote the polarization vector and momentum of i . The $F_i^{\mu\nu} = k_i^\mu \epsilon_i^\nu - \epsilon_i^\mu k_i^\nu$ refers to the strength tensor of i , while $\text{Tr}[F_1 \cdot F_2 \cdot \dots \cdot F_j]$ denote the cyclic contraction of strength tensors $F_1^{\mu_1 \mu_2} F_2^{\mu_2 \mu_3} \dots F_j^{\mu_j \mu_1}$. The other numerator $N(\ell; 1, 3, 2)$ with three gluons is directly obtained from $N(\ell; 1, 2, 3)$ via exchanging the roles of 2 and 3. Moreover, numerators with more than three gluons can also be decomposed by splitting the gluon set into two ordered sets corresponding to scalars and gluons. In this situation, our YMS results with 1 to 3 gluons provide the exact expressions of the corresponding terms in this decomposition.

In order to answer the aforementioned problems for YMS theory, in this paper we present a set of organization principles that regroups Feynman graphs contributing to the color-ordered integrand. Entries of the propagator matrix factorizes in each of these

¹⁰The factors $\frac{\epsilon_i \cdot \epsilon_j}{k_i \cdot k_j}$ ($i \neq j$, $i, j = 1, 2, 3$) in the two and three point numerators $N^{\text{YM}}(\ell; 1, 2)$ and $N^{\text{YM}}(\ell; 1, 2, 3)$ seem to be singular due to momentum conservation and the massless conditions of external particles. Nevertheless, these terms are of the form $\frac{0}{0}$ when the biajoint scalar integrands in the decomposition formulas are taken into account. In fact, the final result after division is finite.

groups, so that the remaining coefficient is identified as the unique numerator solution to this color-ordered integrand.

$$\mathcal{I}^{\text{YMS}}(\ell, 123\dots n) = \sum_{\sigma \in S_{n-1}} N(1\sigma)\tilde{M}(1\sigma|123\dots n). \quad (1.19)$$

- (b) The next problem runs parallel to the issue (ii) in the case of YMS. We determine the one loop numerator solutions for the one, two and three gluon cases for the YMS theory in Secs. VII to VII C, which because of the propagator matrix being full-rank, is unique for the color-ordered integrand defined by the Feynman rules. On the other hand tree numerator solutions are known to be nonunique [1]. A natural question is whether the numerator solution (1.15), and its multiple-gluon formula given by the graphic rules derived in [36,38,39,41,58–60] for tree level numerators correspond to this unique solution. Namely, suppose if we write down the half-ladder numerators based on the rules given by [36,38–41,58–60], taking the forward limit and then have their both sides welded, would the resulting numerators be the same as the n -gons obtained in (a)? In Sec. VIII we see that the answer is affirmative. The welded tree numerators naturally define a loop dependent formula compatible with the consistency condition (1.6) and are therefore the unique solution. Alternatively, one can see the tree numerator formulas when welded are identical to the loop ones computed in Secs. VII to VII C. Finally we

briefly remark in Sec. IX on the gravity and EYM cases where we do not have a color-ordered integrand nor Feynman rules.

II. EFFECTIVE NUMERATORS AND PROPAGATOR MATRIX AT ONE LOOP

A. Existence of a solution and a 2-point example

Strictly speaking, the problem of solving kinematic numerators at one loop is mathematically defined by the infinite matrix relation (1.10) explained in the introduction. The technically challenging problem however, can be circumvented by solving for a physically equivalent set of kinematic numerators instead. A way out is to note that adding arbitrary difference terms related by a constant shift in the loop momentum effectively give the same 1-loop amplitude, a technique frequently employed in earlier study of the integrand behavior under the influence of a BCJ formulation [16,18].

$$\begin{aligned} A_{1\text{-loop}} &= \int d^D \ell \mathcal{I}_n(\ell) \\ &= \int d^D \ell \mathcal{I}_n(\ell) + f(\ell) - f(\ell + c). \end{aligned} \quad (2.1)$$

Assuming that our integrand is color-ordered with respect to some loop momentum independent color factors (this assumption will change when we discuss gravity integrands in Sec. IV). In the 2-point example we add difference terms and consider the following shifted integrand.

$$\begin{aligned} \tilde{\mathcal{I}}_2(\ell, k_1, k_2) &= \left[\frac{1}{\ell^2(\ell + k_1)^2} + \frac{1}{\ell^2} \frac{1}{i\epsilon} + \frac{1}{(\ell + k_1)^2} \frac{1}{i\epsilon} \right] N(\ell, 1, 2, -\ell) - \left[\frac{1}{\ell^2} \frac{1}{i\epsilon} \right] N(\ell - k_1, 1, 2, -(\ell - k_1)) \\ &+ \left(\underbrace{\left[\frac{1}{\ell^2} \frac{1}{i\epsilon} \right] N(\ell - k_1, 1, 2, -(\ell - k_1))}_{f(\ell)} - \underbrace{\left[\frac{1}{(\ell + k_1)^2} \frac{1}{i\epsilon} \right] N(\ell, 1, 2, -\ell)}_{f(\ell + k_1)} \right) \\ &- \left[\frac{1}{(\ell + k_1)^2} \frac{1}{i\epsilon} \right] N(\ell + k_1, 1, 2, -(\ell + k_1)) \\ &+ \left(\underbrace{\left[\frac{1}{(\ell + k_1)^2} \frac{1}{i\epsilon} \right] N(\ell + k_1, 1, 2, -(\ell + k_1))}_{g(\ell)} - \underbrace{\left[\frac{1}{\ell^2} \frac{1}{i\epsilon} \right] N(\ell, 1, 2, -\ell)}_{g(\ell - k_1)} \right) \end{aligned} \quad (2.2)$$

The difference terms were added deliberately to cancel the “misaligned” numerators appearing in the equation, leaving

$$\tilde{\mathcal{I}}_2(\ell, k_1, k_2) = \frac{1}{\ell^2(\ell + k_1)^2} N(\ell, 1, 2, -\ell). \quad (2.3)$$

Comparing with the tree level argument, we see that for this effective integrand at 2-point the number of independent numerator is just 1, and the propagator matrix is just the factor $1/\ell^2(\ell + k_1)^2$, which inverts to give the generalization of the momentum kernel in this case, $\ell^2(\ell + k_1)^2$.

Addressing (i): The derivation above allows us to answer the questions raised in (i) in the introduction, specifically for this 2-point case. We see from Eq. (2.3) in the sense of writing an effective integrand (up to terms that vanishes upon integration) in terms of the BCJ formulation (1.2), the method discussed in this section always permits a solution for the basis numerator (1.5), regardless of whether the same theory gives BCJ satisfying amplitudes at tree level. Note that Eq. (2.3) is enough to determine all numerators: Here we have assumed the integrand $\mathcal{I}_2(\ell, k_1, k_2)$, given by Feynman rules, is a known function of the polarizations, external and loop momenta, so that numerator $N(\ell, 1, 2, -\ell)$ at every ℓ is solved from the integrand $\mathcal{I}_2(\ell, k_1, k_2)$ at that specific value of ℓ . Additionally, the set of all numerators written symbolically with the other order, $N(\ell, 2, 1, -\ell)$, are actually the same

set with the original order due to the nature of this notation. Namely, from (1.6) we see that

$$N(\ell, 2, 1, -\ell) = N(\ell - k_1, 1, 2, -(\ell - k_1)). \quad (2.4)$$

Since these together determine all basis numerators and nothing more, all numerators appearing at 2-point are solved.

B. Solving higher-point numerators

The method explained through a 2-point example discussed in Sec. II A generalizes to higher points in a straightforward manner. At n -point the basis numerators are n -gons with n external legs attached, and our nomenclature is likewise redundant.

$$\begin{aligned} N(\ell, \sigma(1), \sigma(2), \sigma(3), \dots, \sigma(n), -\ell) &= N(\ell + k_{\sigma(1)}, \sigma(2), \sigma(3), \dots, \sigma(n), \sigma(1), -(\ell + k_{\sigma(1)})) \\ &= N(\ell + k_{\sigma(1)} + k_{\sigma(2)}, \sigma(3), \dots, \sigma(n), \sigma(1), \sigma(2), -(\ell + k_{\sigma(1)} + k_{\sigma(2)})) \\ &= \dots \end{aligned} \quad (2.5)$$

where $\sigma \in S_n$ is understood to be any of the permutations. Starting from the knowledge of all color-ordered integrands, which we assume to be already computed from Feynman rules, one solves numerators using BCJ's formula (1.2). More specifically, one uses the redundancy

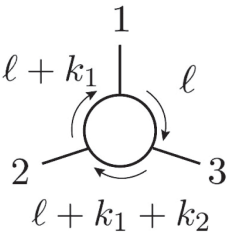
of the nomenclature to fix, for example, $\sigma(1) = 1$, leaving $(n-1)!$ independent numerators for each ℓ . In addition one note that BCJ's formula (1.2) for integrands also satisfy the same symmetry as our nomenclature for numerators,

$$\begin{aligned} \mathcal{I}_n(\ell, \sigma(1), \sigma(2), \sigma(3), \dots, \sigma(n)) &= \mathcal{I}_n(\ell + k_{\sigma(1)}, \sigma(2), \sigma(3), \dots, \sigma(n), \sigma(1)) \\ &= \dots \end{aligned} \quad (2.6)$$

as well as the explicit integrands obtained by (not necessarily cubic) Feynman rules. (We neglect the proof of this, as it can be readily checked in the lower-point cases.) Therefore we have the same number of independent equations and unknowns. Shifting terms in the integrand properly as in the 2-point example shown in Sec. II A and

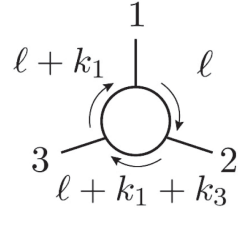
we obtain an $(n-1)! \times (n-1)!$ matrix equation, where the basis numerators can be solved from.

For concreteness we list the result for 3-point. The calculation details can be found in Appendix B. At 3-point we have the following two independent numerators and the corresponding consistency conditions for their notations.



$$\begin{aligned} &= N(\ell, 123, -\ell) \\ &= N(\ell + k_1, 231, -(\ell + k_1)) \\ &= N(\ell + k_1 + k_2, 312, -(\ell + k_1 + k_2)) \end{aligned} \quad (2.7)$$

and



$$\begin{aligned}
 &= N(\ell, 132, -\ell) \\
 &= N(\ell + k_1, 321, -(\ell + k_1)) \\
 &= N(\ell + k_1 + k_3, 213, -(\ell + k_1 + k_3))
 \end{aligned} \tag{2.8}$$

The above two sets are related by the following relabeling transformations, respectively.

$$\begin{array}{ll}
 OP_1: & \ell \rightarrow \ell + k_1 \quad \text{and} \quad OP_2: \quad \ell \rightarrow \ell + k_1 \\
 & k_1 \rightarrow k_2 \quad \quad \quad k_1 \rightarrow k_3 \\
 & k_2 \rightarrow k_3 \quad \quad \quad k_2 \rightarrow k_1 \\
 & k_3 \rightarrow k_1 \quad \quad \quad k_3 \rightarrow k_2
 \end{array} \tag{2.9}$$

Using the method just explained leads to a linear relation between shifted integrands and the numerators,

$$\begin{aligned}
 \begin{bmatrix} \tilde{\mathcal{I}}_3(\ell, 123) \\ \tilde{\mathcal{I}}_3(\ell, 132) \end{bmatrix} &= \begin{bmatrix} \tilde{M}(23|23) & \tilde{M}(23|32) \\ \tilde{M}(32|23) & \tilde{M}(32|32) \end{bmatrix} \\
 &\times \begin{bmatrix} N(\ell, 123, -\ell) \\ N(\ell, 132, -\ell) \end{bmatrix}, \tag{2.10}
 \end{aligned}$$

where the propagator matrix $\tilde{M}(\alpha|\beta)$ is given by (B4) in the Appendix. We invert the propagator matrix to solve $N(\ell, 123, -\ell)$ and $N(\ell, 132, -\ell)$ for all values of ℓ . Other orderings actually refer the same set of numerators through (2.7) and (2.8), and we have obtained all the basis numerators. We see again in this example the numerator solution exists regardless of whether the same theory has tree level solutions.

C. n -point propagator matrix and its relation to forward limit tree propagator matrices

At higher points the method discussed in Secs. II A and II B would be rather complicated, as it requires considerable

graphical manipulations on BCJ's formula (1.2). In this section we present a formally different, but more easily generalized, method to obtain the same numerator solution. The argument presented in this section also explains the relation between the one loop generalized propagator matrix described in Secs. II A, II B and the forward limit of the conventional tree propagator matrix $m(\alpha|\beta)$ defined in [55].

Note a subtlety here: We will not try to identify forward limit amplitudes defined by Feynman rules, $A_{\text{Feyn}}^{\text{tree}}$, with any object in the current section. Such identification is the main issue raised by (ii) in the introduction and will be discussed in Sec. III. The method presented here is only due to the knowledge of the cubic structure in $A_{\text{BCJ}}^{\text{tree}}$, and the fact that integrands can be expanded in terms of $A_{\text{BCJ}}^{\text{tree}}$, which was explained in the introduction.

The following derivation will be rather straightforward. But to avoid unnecessarily complicated notations, let us first use the 3-point case to demonstrate the idea. Instead of the graphical decomposition (1.2), we consider the forward limit decomposition of the integrand explained in the introduction. At 3-point, this is given by

$$\begin{aligned}
 \mathcal{I}_3(\ell, 123) &= \frac{1}{\ell^2} A_{\text{BCJ}}^{\text{tree}}(\ell, 1, 2, 3, -\ell) + \frac{1}{(\ell + k_1)^2} A_{\text{BCJ}}^{\text{tree}}(\ell + k_1, 2, 3, 1, -(\ell + k_1)) \\
 &+ \frac{1}{(\ell + k_1 + k_2)^2} A_{\text{BCJ}}^{\text{tree}}(\ell + k_1 + k_2, 3, 1, 2, -(\ell + k_1 + k_2)). \tag{2.11}
 \end{aligned}$$

Recall that the amplitudes $A_{\text{BCJ}}^{\text{tree}}$ should be understood as the color-ordered tree amplitudes formally written down using the tree cubic formula (1.1), with the two parallel legs of every numerator welded together, and then replaced by their corresponding counterparts appear in the one loop integrand (the n -gons), according to the nomenclature

suggestion, $N^{\text{tree}}(\ell, \sigma(1), \sigma(2), \dots, \sigma(n), -\ell) \rightarrow N(\ell, \sigma(1), \sigma(2), \dots, \sigma(n), -\ell)$. This replacement implies a natural correspondence between the actual tree basis numerators (the half-ladders) $N^{\text{tree}}(\ell, \sigma(1), \sigma(2), \dots, \sigma(n), -\ell)$ and the n -gons $N(\ell, \sigma(1), \sigma(2), \dots, \sigma(n), -\ell)$, so that the amplitudes $A_{\text{BCJ}}^{\text{tree}}$ can be expanded in exactly the same way as real

tree amplitudes, such as (1.3). At 3-point this allows us to expand all $A_{\text{BCJ}}^{\text{tree}}$ in Eq. (2.11) into $3!$ unknown variables $N(\ell, \sigma(1), \sigma(2), \sigma(3), -\ell)$. Schematically, we have the following linear relation.

$$\begin{aligned}
 \underbrace{\begin{bmatrix} \mathcal{I}_3(\ell, 123) \\ \mathcal{I}_3(\ell, 132) \\ \mathcal{I}_3(\ell, 213) \\ \boxed{\mathcal{I}_3(\ell, 231)} \\ \mathcal{I}_3(\ell, 312) \\ \mathcal{I}_3(\ell, 321) \end{bmatrix}}_{3!=6\text{permutations}} &= \begin{bmatrix} \frac{1}{\ell^2} m(\ell 123 | \ell 123) & \dots \\ \vdots & \\ \square & \square \square \square \square \square \end{bmatrix} \begin{bmatrix} N(\ell, 123, -\ell) \\ N(\ell, 132, -\ell) \\ N(\ell, 213, -\ell) \\ \boxed{N(\ell, 231, -\ell)} \\ N(\ell, 312, -\ell) \\ N(\ell, 321, -\ell) \end{bmatrix} \\
 &+ \begin{bmatrix} \frac{1}{(\ell+k_1)^2} m(\ell+k_1, 231 | \ell+k_1, 231) & \dots \\ \vdots & \\ \square & \square \square \square \square \square \end{bmatrix} \begin{bmatrix} N(\ell+k_1, 123, -(\ell+k_1)) \\ N(\ell+k_1, 132, -(\ell+k_1)) \\ \vdots \\ \boxed{N(\ell+k_1, 231, -(\ell+k_1))} \\ N(\ell+k_1, 321, -(\ell+k_1)) \end{bmatrix} \\
 &+ \dots
 \end{aligned} \tag{2.12}$$

The coefficient $m(\alpha|\beta)$ appeared are apparently the same tree propagator matrix entries [55] from our discussion above.

For the same reason mentioned in (i) in the introduction, the solution to such a matrix equation alone cannot be determined, as it involves more unknown variables related by shiftings. Solving them requires more matrix equations involving shifted integrands, which in turn leads to more unknown variables. The problem cannot be rigorously

solved unless we introduce boundary conditions and take infinite limits. However let us focus on the row of the matrix equation index by permutation (231) [highlighted in (2.12)]. Observe that when loop momentum takes the value $\ell+k_1$, this equation is actually formally identical to the first row indexed by id = (123). A quick way to see this is to note that it came from the numerator expansion of the following equation, the right-hand side of which is by itself invariant under the symmetry transformation OP_1 of (2.9).

$$\begin{aligned}
 \mathcal{I}_3(\ell, 231) &= \frac{1}{\ell^2} A_{\text{BCJ}}^{\text{tree}}(\ell, 2, 3, 1, -\ell) + \frac{1}{(\ell+k_2)^2} A_{\text{BCJ}}^{\text{tree}}(\ell+k_2, 3, 1, 2, -(\ell+k_2)) \\
 &+ \frac{1}{(\ell+k_2+k_3)^2} A_{\text{BCJ}}^{\text{tree}}(\ell+k_2+k_3, 1, 2, 3, -(\ell+k_2+k_3))
 \end{aligned} \tag{2.13}$$

The left-hand side of the equation, $\mathcal{I}_3(\ell, 123)$, on the other hand, belong to the known variables where we solve the numerators from, presumably given by Feynman rules of the theory of interest, and satisfies the same symmetry $\mathcal{I}_3(\ell, 123) = \mathcal{I}_3(\ell+k_1, 231)$ by construction. This identification, together with the symmetry assumption (2.7) of the nomenclature of the numerators allows us to completely remove the redundant line. A similar argument also

identifies the line index by (312) with id = (123). Similarly, lines indexed by (321) and (213) with (132), reducing the problem to a 2×2 matrix equation.

More explicitly, let us focus on just the first row of the matrix equation (2.12) that come from the $\frac{1}{\ell^2} A_{\text{BCJ}}^{\text{tree}}(\ell, 1, 2, 3, -\ell)$ term in (2.11). There are three terms related by cyclic permutation of the external legs,

$$\begin{aligned}
 \frac{1}{\ell^2} A_{\text{BCJ}}^{\text{tree}}(\ell, 1, 2, 3, -\ell) &= \frac{1}{\ell^2} m(\ell, 123, -\ell | \ell, 123, -\ell) N(\ell, 123, -\ell) + \frac{1}{\ell^2} m(\ell, 123, -\ell | \ell, 231, -\ell) N(\ell, 231, -\ell) + \dots \\
 &+ \frac{1}{\ell^2} m(\ell, 123, -\ell | \ell, 312, -\ell) N(\ell, 312, -\ell) + \dots
 \end{aligned} \tag{2.14}$$

Equation (2.1) allows us to trade individual terms in the integrand with shifted ones plus terms that vanished after the integration, by which we shift these three individual terms by the appropriate amount so that they can be related by the symmetry operation OP_1 of (2.9). Consistency of the nomenclature then allows us to identify all three numerators symbolically as $N(\ell, 123, -\ell)$.

$$\begin{aligned} \tilde{\mathcal{I}}_3(\ell, 123) &= \left(\frac{1}{\ell^2} m(\ell 123 | \ell 123) N(\ell, 123, -\ell) \right) + \dots \\ &\times \left(\frac{1}{(\ell + k_1)^2} m(\ell + k_1, 123, -(\ell + k_1) | \ell + k_1, 231, -(\ell + k_1)) \underbrace{N(\ell + k_1, 231, -(\ell + k_1))}_{=N(\ell, 123, -\ell)} \right) + \dots \\ &+ \left(\frac{1}{(\ell + k_1 + k_2)^2} m(\ell + k_1 + k_2, 123, -(\ell + k_1 + k_2) | \ell + k_1 + k_2, 312, -(\ell + k_1 + k_2)) \right. \\ &\times \left. \underbrace{N(\ell + k_1 + k_2, 312, -(\ell + k_1 + k_2))}_{=N(\ell, 123, -\ell)} \right) + \dots \end{aligned} \quad (2.15)$$

Repeating the same manipulation reduces the unknowns in all rows of the matrix equation (2.12) to $3!/3 = 2$.

Since the derivation above is straightforward, we write the integrand-numerator relation at generic n -point directly. At n -point we have the following symmetry transformation that associates cyclic permutations of the external legs with specific shift of loop momentum ℓ , for all ordering $(\rho(1), \rho(2), \dots, \rho(n))$ of the external legs.

$$\begin{aligned} \ell &\rightarrow \ell + k_{\rho(1)} \\ k_{\rho(1)} &\rightarrow k_{\rho(2)} \\ \vdots &\quad \quad \quad \vdots \\ k_{\rho(n)} &\rightarrow k_{\rho(1)} \end{aligned} \quad (2.16)$$

The numerators are assumed to be invariant under such symmetry,

$$\begin{aligned} &N(\ell, \rho(1), \rho(2), \dots, \rho(n), -\ell) \\ &= N(\ell + k_{\rho(1)}, \rho(2), \dots, \rho(n), \rho(1), -(\ell + k_{\rho(1)})). \end{aligned} \quad (2.17)$$

This allows us to reduce the basis to $n!/n = (n-1)!$ numerators. We may choose to fix $\rho(1) = 1$. Together with the same symmetry of the integrands yields an $(n-1)! \times (n-1)!$ matrix equation relating the integrands and the numerators.

$$\mathcal{I}_n(\ell, 1, \rho) = \sum_{\sigma \in S_{n-1}} \tilde{M}(\rho|\sigma) N(\ell, 1, \sigma, -\ell). \quad (2.18)$$

The manipulation explained above shows that the contribution from a single forward limit tree amplitude is

$$\begin{aligned} \frac{1}{\ell^2} A(\ell, 1, \rho(2), \rho(3), \dots, \rho(n), -\ell) &\sim \sum_{\sigma \in S_{n-1}} \left(\frac{1}{\ell^2} m(\ell, 1, \rho(2), \rho(3), \dots, \rho(n), -\ell | \ell, 1, \sigma(2), \sigma(3), \dots, \sigma(n), -\ell) \right. \\ &+ \frac{1}{(\ell + k_1)^2} m(\ell + k_1, 1, \rho(2), \rho(3), \dots, \rho(n), -(\ell + k_1) | \ell \\ &+ k_1, \sigma(2), \sigma(3), \dots, \sigma(n), 1, -(\ell + k_1)) + \frac{1}{(\ell + k_1 + k_{\sigma(2)})^2} m(\ell + k_1 \\ &+ k_{\sigma(2)}, 1, \rho(2), \rho(3), \dots, \rho(n), -(\ell + k_1 + k_{\sigma(2)}) | \ell + k_1 \\ &+ k_{\sigma(2)}, \sigma(3), \dots, \sigma(n), 1, \sigma(2), -(\ell + k_1 + k_{\sigma(2)})) \dots \left. \right) \\ &\times N(\ell, 1, \sigma(2), \sigma(3), \dots, \sigma(n), -\ell). \end{aligned} \quad (2.19)$$

Reading off the coefficient, and we conclude that the (ρ, σ) -entry of the (effective) propagator matrix $\tilde{M}(\rho|\sigma)$ at n -point is

$$\begin{aligned}
\tilde{M}(\rho|\sigma) = & \sum_{(\bar{1}, \bar{\rho}) \in \text{cyclic perm. of } (1, \rho)} \left(\frac{1}{\ell^2} m(\ell, \bar{1}, \bar{\rho}(2), \bar{\rho}(3), \dots, \bar{\rho}(n), -\ell | \ell, 1, \sigma(2), \sigma(3), \dots, \sigma(n), -\ell) \right. \\
& + \frac{1}{(\ell + k_1)^2} m(\ell + k_1, \bar{1}, \bar{\rho}(2), \bar{\rho}(3), \dots, \bar{\rho}(n), -(\ell + k_1) | \ell + k_1, \sigma(2), \sigma(3), \dots, \sigma(n), 1, -(\ell + k_1)) \\
& + \frac{1}{(\ell + k_1 + k_{\sigma(2)})^2} m(\ell + k_1 + k_{\sigma(2)}, \bar{1}, \bar{\rho}(2), \bar{\rho}(3), \dots, \bar{\rho}(n), -(\ell + k_1 + k_{\sigma(2)}) | \ell + k_1 \\
& \left. + k_{\sigma(2)}, \sigma(3), \dots, \sigma(n), 1, \sigma(2), -(\ell + k_1 + k_{\sigma(2)})) \dots \right) \quad (2.20)
\end{aligned}$$

where the cyclic sum $(\bar{1}, \bar{\rho})$ comes from the fact that integrand is a cyclic sum of the forward limit terms of the form (2.19).

D. Momentum kernel and the Sherman-Morrison formula

As already mentioned in the introduction, the Jacobi identities impose increasingly stringent algebraic constraints on kinematic numerators as the loop order grows. At tree level, there exist infinitely many possible sets of numerators related by generalized gauge transformations, while beyond two loops these constraints can no longer be satisfied diagram by diagram without introducing contact-term contributions that integrate to zero [13,14]. At one loop, however, we are in the fortunate situation where the corresponding propagator matrix happens to be nonsingular, allowing us to determine the numerators uniquely from the integrand. We note that, when regarded as a function of loop momentum ℓ , the propagator matrices at 2- and 3-points given in Eqs. (2.3) and (B4) respectively, are nonsingular except at a few poles and therefore can be regularized using the method described by [63]. It is then interesting to see if the inverse propagator matrix present any general features, considering the fact that at tree level, momentum kernels are actually simpler than propagator matrices in the sense that one can write down an analytic formula at arbitrary n -point. Regarding this problem, we find the propagator matrices derived from the shifting technique explained in Sec. II however, are rather complicated beyond 3-point, even though a few general features can indeed be identified. We use the Sherman-Morrison formula [23] (which is a special case of the Woodbury matrix identity) to analyze the problem, which we briefly explain in the following.

Starting with a matrix A with known inverse matrix A^{-1} , let us consider a perturbation of the original matrix A given by

$$A + \alpha uv^T \quad (2.21)$$

where α is a numerical parameter. u, v are column vectors. The Sherman-Morrison formula is an explicit formula for

the inverse of the perturbed matrix $A + \alpha uv^T$.

$$(A + \alpha uv^T)^{-1} = A^{-1} - \frac{\alpha A^{-1} u v^T A^{-1}}{1 + \alpha v^T A^{-1} u} \quad (2.22)$$

To see how the formula works, let us consider the special case where A is a diagonal matrix $\text{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)$ with an apparent inverse, and that u, v are happen to be unit vectors with the nonzero component being the i th and j th entry respectively, $u = e_i, v = e_j$, so that $u v^T$ is a matrix with the (i, j) th element in the matrix being 1 and others zero. The Sherman-Morrison formula (2.22) then allows us to write down the inverse of any matrix of the following form

$$A + \alpha_{(i,j)} u v^T = \begin{pmatrix} \lambda_1 & & & \\ & \lambda_2 & & \alpha_{(i,j)} \\ & & \ddots & \\ & & & \ddots & \\ & & & & \lambda_n \end{pmatrix} \quad (2.23)$$

for arbitrary values of $\lambda_1, \lambda_2, \dots, \lambda_n$ and α . For a generic matrix, we iterate the above algorithm, adding nonzero entries one at a time. Namely we regard all the off-diagonal terms as perturbations and calculate the inverse using Sherman-Morrison formula (2.22) until all entries are included.

For a propagator matrix at one loop, we can do slightly better than the brute force method explained above. The 3-point propagator matrix written down in Appendix B is 2×2 , its inverse can then be readily written down using the formula exclusively for 2×2 matrices. However note that the 3-point propagator matrix M_3 can be written as a perturbation to a matrix $M_{3,0}$ that resembles the tree propagator matrix (1.3).

$$M_3 = M_{3,0} + \begin{pmatrix} \alpha_1 & \alpha_2 \\ -\alpha_1 & -\alpha_2 \end{pmatrix}, \quad (2.24)$$

where

$$M_{3,0} = \frac{1}{D_\ell D_{\ell 1}} \begin{pmatrix} \frac{1}{D_{\ell 12}} + \frac{1}{s_{23}} & -\frac{1}{s_{23}} \\ -\frac{1}{s_{23}} & \frac{1}{D_{\ell 13}} + \frac{1}{s_{23}} \end{pmatrix} \quad (2.25)$$

and the parameters α_1, α_2 are given by

$$\begin{aligned} \alpha_1 &= \frac{1}{D_\ell D_{\ell 12}} \left(\frac{1}{s_{12}} + \frac{1}{s_{13}} \right), \\ \alpha_2 &= \frac{1}{D_\ell D_{\ell 13}} \left(\frac{1}{s_{12}} + \frac{1}{s_{13}} \right), \end{aligned} \quad (2.26)$$

respectively.

The fact that the 3-point propagator matrix M_3 can be written as such a perturbation is not a coincidence. The extra pieces α_1, α_2 are due to shifting, which is the feature that distinguishes the tree and one loop level propagators. From this viewpoint the one loop level propagator matrix can be understood as a tree propagator matrix perturbed by the shifting terms.

The tree level-like piece $M_{3,0}$ has an inverse that we learned from the analytic formula for momentum kernel.

$$\begin{aligned} S_{3,0} = M_{3,0}^{-1} &= \frac{D_\ell D_{\ell 1}}{D_{\ell 12} + D_{\ell 13} + s_{23}} \\ &\times \begin{pmatrix} D_{\ell 12}(D_{\ell 13} + s_{23}) & D_{\ell 12} D_{\ell 13} \\ D_{\ell 12} D_{\ell 13} & D_{\ell 13}(D_{\ell 12} + s_{23}) \end{pmatrix} \end{aligned} \quad (2.27)$$

In viewing the Sherman-Morrison formula, we write the 3-point propagator matrix as the following two-step

perturbations,

$$M_3 = M_{3,0} + \alpha_1 u v_1^T + \alpha_2 u v_2^T, \quad (2.28)$$

where the vectors u, v_1 , and v_2 are given by

$$u = \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \quad v_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad v_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad (2.29)$$

respectively. We find the feature illustrate through the 3-point example here also resides in the higher-point case, even though the complexity involved in applying the Sherman-Morrison formula increases rapidly.

III. CONDITIONS REQUIRED BY IDENTIFYING n -GONS WITH WELDED TREES

In this section we discuss a few problems relating to loop and tree structures. In particular, under what condition can the welded tree numerators be used directly as one loop numerators. Recall that we explained in (ii) in the introduction that the BCJ formula of integrand (1.2) can be regarded as a sum over polygons attached with various subtrees, so that if we use the partial fraction identity (1.11) to decompose the loop dependent propagators of the polygons and regroup, the original BCJ integrand formula can be reexpressed as a sum over forward limit amplitudes $A_{\text{BCJ}}^{\text{tree}}$. At 2- and 3-points these are given by (1.12) and (1.13) respectively, and generically we have¹¹

$$\begin{aligned} \mathcal{I}_n(\ell, k_1, k_2, \dots, k_n) &= \frac{1}{\ell^2} A_{\text{BCJ}}^{\text{tree}}(\ell, 1, 2, 3, \dots, n, -\ell) + \frac{1}{(\ell + k_1)^2} A_{\text{BCJ}}^{\text{tree}}(\ell + k_1, 2, 3, \dots, n, 1, -(\ell + k_1)) \\ &+ \frac{1}{(\ell + k_1 + k_2)^2} A_{\text{BCJ}}^{\text{tree}}(\ell + k_1 + k_2, 3, \dots, n, 1, 2, -(\ell + k_1 + k_2)) + \dots \end{aligned} \quad (3.1)$$

where by $A_{\text{BCJ}}^{\text{tree}}$ we mean the BCJ tree formula (1.1) with the two parallel legs of every numerator welded, and then swapped by the corresponding polygon numerator at one loop. We mentioned there that $A_{\text{BCJ}}^{\text{tree}}$ formally resembles welded forward limit tree amplitudes, therefore motivates the question about whether we may simply identify the value obtained from Feynman rules, $A_{\text{Feyn}}^{\text{tree}}$, with these amplitudes.

$$\mathcal{I}_2(\ell, k_1, k_2) = \ell \left(\text{diagram 1} \right) + \left(\text{diagram 2} \right) \ell + k_1$$

FIG. 1. 2-point color-ordered integrand of a hypothetical theory that only has 4-vertex.

This resemblance actually goes further. The above forward limit decomposition (3.1) is actually not limited to cubic structure. The fact that it generalizes can be seen by considering a hypothetical theory that contains only a 4-vertex. The resulting integrand in this theory at n -point will also be a sum over polygons, and with vertices lying on the loop, from which subtrees are attached. (The polygon structure is illustrated in Fig. 1. Terms in this figure are all Feynman graphs, not numerators.) Following the same argument to replace loop propagators by partial fractions and then regroup, we see a similar decomposition to (3.1). Further including more types of vertices to the theory and

¹¹From Eq. (3.1) one sees that the tadpole numerators do not contribute to the (integrated) amplitude at one loop level, regardless of the actual analytic behavior of the numerator solutions. See Appendix C for discussion.

repeat, we see that integrands defined by general color-ordered Feynman rules also satisfy a similar forward limit decomposition.

$$\begin{aligned} \mathcal{I}_n(\ell, k_1, k_2, \dots, k_n) &= \sum_h \frac{1}{\ell^2} A_{\text{Feyn}}^{\text{tree}}(\ell^h, 1, 2, 3, \dots, n, -\ell^h) + \frac{1}{(\ell + k_1)^2} A_{\text{Feyn}}^{\text{tree}}((\ell + k_1)^h, 2, 3, \dots, n, 1, -(\ell + k_1)^h) \\ &\quad + \frac{1}{(\ell + k_1 + k_2)^2} A_{\text{Feyn}}^{\text{tree}}((\ell + k_1 + k_2)^h, 3, \dots, n, 1, 2, -(\ell + k_1 + k_2)^h) + \dots \end{aligned} \quad (3.2)$$

where in the above we have assumed the propagator of this theory can be “cut” by inserting complete states h , such as the Yang-Mills propagator in light-cone gauge $\eta^{\mu\nu}/\ell^2 = \sum_{\pm} \epsilon^{\pm, \mu} \epsilon^{\mp, \nu} / \ell^2$.

The remarkable resemblance between the two decompositions (3.1) and (3.2) again suggests that we identify the values of $A_{\text{BCJ}}^{\text{tree}}$ with $A_{\text{Feyn}}^{\text{tree}}$. Furthermore, from (3.1) and (3.2) we see that the numerator solutions obtained from identifying $A_{\text{BCJ}}^{\text{tree}}$ with $A_{\text{Feyn}}^{\text{tree}}$ is actually imposing a stronger condition than the method explained in Sec. II: In the following we discuss solutions obtained by identifying the two, so that the $A_{\text{BCJ}}^{\text{tree}}$ and $A_{\text{Feyn}}^{\text{tree}}$ appear in Eqs. (3.1) and (3.2) must be equal term-by-term, while in Sec. II the numerators were solved from linear equations between the whole integrands and numerators. Therefore the solutions discussed here, if exists, automatically satisfies the linear equations of Sec. II, but the reverse is not necessarily true.

To determine the numerators from $A_{\text{Feyn}}^{\text{tree}}$, recall that we argued in Sec. II C that the expansion coefficients for $A_{\text{BCJ}}^{\text{tree}}$ with respect to basis n -gons $N(\ell, \sigma(1), \sigma(2), \dots, \sigma(n), -\ell)$ are just the tree propagator matrix $m(\alpha|\beta)$, with forward

limit taken. Therefore the basis numerators can be solved from linear equations similar to (1.3), with the amplitudes and numerators appear in the equation identified as $A_{\text{Feyn}}^{\text{tree}}$ and $N(\ell, \sigma(1), \sigma(2), \dots, \sigma(n), -\ell)$ respectively.

Note however, during the partial fraction derivation that leads to (3.1), the propagator of one n -gon is decomposed into several terms, and regrouped into several separate $A_{\text{BCJ}}^{\text{tree}}$. So that the n -gon $N(\ell, 1, 2, 3, \dots, n, -\ell)$ appear in $A_{\text{BCJ}}^{\text{tree}}(\ell, 1, 2, 3, \dots, n, -\ell)$ needs to be the same n -gon appear in $A_{\text{BCJ}}^{\text{tree}}(\ell + k_1, 2, 3, \dots, n, 1, -(\ell + k_1))$, equivalently denoted as $N(\ell, 1, 2, 3, \dots, n, -\ell)$ or as $N(\ell + k_1, 2, 3, \dots, n, 1, -(\ell + k_1))$ according to the nomenclature. If we were to identify $A_{\text{BCJ}}^{\text{tree}}$ with $A_{\text{Feyn}}^{\text{tree}}$, this requires that the numerator solved from the first terms $A_{\text{Feyn}}^{\text{tree}}(\ell^h, 1, 2, 3, \dots, n, -\ell^h)$ in the forward limit decomposition (3.2) needs to have the same value with those solved from the second terms $A_{\text{Feyn}}^{\text{tree}}((\ell + k_1)^h, 2, 3, \dots, n, 1, -(\ell + k_1)^h)$ and so on. These appear as separate matrix equations when solving the numerators using the method just described. Explicitly, we need the following extra condition.

$$\sum_h N^{\text{tree}}(\ell^h, \sigma(1), \sigma(2), \dots, \sigma(n), -\ell^h) = \sum_h N^{\text{tree}}((\ell + k_{\sigma(1)})^h, \sigma(2), \dots, \sigma(n), \sigma(1), -(\ell + k_{\sigma(1)})^h) \quad (3.3)$$

Namely, suppose if we would like to identify an n -gon with the tree numerators solved from $A_{\text{Feyn}}^{\text{tree}}$, then the identifications corresponding to all possible incision locations of the n -gon need to be all equal. Generically, tree numerators solved from different $A_{\text{Feyn}}^{\text{tree}}$ ’s can take different generalized gauge. For example, the extra condition may read

$$\begin{aligned} &\frac{1}{\ell^2} \sum_{\rho \in S_n} \sum_h \mathcal{S}[\sigma(1), \sigma(2), \dots, \sigma(n)|\rho]_{\ell} A_{\text{Feyn}}^{\text{tree}}(\ell^h, \rho(1), \rho(2), \dots, \rho(n), -\ell^h) \\ &= \frac{1}{(\ell + k_{\sigma(1)})^2} \sum_{\rho \in S_n} \sum_h \mathcal{S}[\sigma(2), \dots, \sigma(n), \sigma(1)|\rho]_{\ell + k_{\sigma(1)}} A_{\text{Feyn}}^{\text{tree}}((\ell + k_{\sigma(1)})^h, \rho(1), \rho(2), \dots, \rho(n), -(\ell + k_{\sigma(1)})^h) \end{aligned} \quad (3.4)$$

or some numerators may come from $(n-3)$ -basis $((n-3)!$ -basis) and so on.

Additionally note that it was discovered by [13] that the rank of the propagator matrix becomes further reduced compared with tree level ones when forward limit is taken. In view of (1.3), the reduced rank suggests more identities

must be satisfied by the forward limit amplitude $A_{\text{Feyn}}^{\text{tree}}$ in order to yield numerator solutions. Here we assumed these conditions are also met and the numerators can be solved by inverting the propagator matrix.

Addressing (ii): When forward limit amplitudes $A_{\text{Feyn}}^{\text{tree}}$ calculated from Feynman rules satisfy the conditions due to

reduced rank just mentioned, and that the welded tree numerators solved by inverting the propagator matrix are compatible with the loop numerator nomenclature (2.16), which is explicitly given by (3.4), we have a consistent set of basis numerators (the n -gons). Other numerators are generated by this set through the same manipulations as in Sec. II. Such a set is indeed a solution can be seen from that when multiplied with propagators, they yield $A_{\text{Feyn}}^{\text{tree}}$, so that the whole integrand is correctly reconstructed term-by-term through (3.2). When the extra conditions are violated, the numerators obtained conflicts with the nomenclature. Also those supposedly be the same n -gons appear in $A_{\text{Feyn}}^{\text{tree}}(\ell^h, 1, 2, 3, \dots, n, -\ell^h)$ and $A_{\text{Feyn}}^{\text{tree}}((\ell + k_1)^h, 2, 3, \dots, n, 1, -(\ell + k_1)^h)$ disagree with each other, so that we cannot identify the welded tree numerators as the solutions of the one loop numerators.

From the discussion at the beginning of this section one also sees that in the extreme case, where we have a Jacobi satisfying cubic theory, and additionally when there is a natural operation that welds tree numerator to give exactly what is supposed to be the loop numerator, then Eqs. (3.1) and (3.2) are identical graph-by-graph, instead of just amplitude-by-amplitude. The welded tree numerator therefore naturally is the loop numerator. Such condition is apparently satisfied by the self-dual Yang-Mills numerators, as they are given by products of structure constants of diffeomorphism algebras, contracted to form a loop, $N_{\text{SDYM}}^{\text{tree}}(\ell^h, \sigma(1), \sigma(2), \dots, \sigma(n), -\ell^h) = \sum_{\pm} f^{\ell^{\pm}, \sigma(1)}_{*} f^{*, \sigma(2)}_{*} \dots f^{*, \sigma(n)}_{\ell^{\mp}}$. The same can be said for NLSM numerators, which we demonstrate in Appendix A. Note that unlike the bypassing method mentioned in (i) in the introduction and explained in Sec. II, not all theories satisfy the stronger condition discussed in this section. A quick way to see this is by considering a counter example where we have a hypothetical theory that has only a 4-vertex in its Feynman rules. For concreteness we may choose the vertex to be a polynomial $V(1, 2, 3, 4) = c + c_{\mu}^{(i)} k_i^{\mu} + c_{\mu, \nu}^{(i, j)} k_i^{\mu} k_j^{\nu} + \dots$, assuming only KK and BCJ relations for tree amplitudes, which leave undetermined parameters that may be adjusted to violate the condition (3.4). The fact that both NLSM and SDYM satisfy

this extra condition seems to suggest that this is the more physically interesting scenario that we should consider.

Remark: The fact that numerator solution always exist when solving from integrands $\mathcal{I}_n(\ell, \sigma(1), \dots, \sigma(n))$ (using the method explained in Sec. II) but not from forward limit tree amplitudes $A_{\text{Feyn}}^{\text{tree}}(\ell, \sigma(1), \dots, \sigma(n), -\ell)$ might appear puzzling at first sight. Roughly speaking, the distinct feature that affects the solution is that $A_{\text{Feyn}}^{\text{tree}}$ is not in general invariant under the symmetry transformation (2.16) (cyclic permutation together with a shifting in the loop momentum ℓ) while integrand can be made so with proper loop momentum assignment. This is because integrand constructed from Feynman rules is cyclic, and that it is possible to choose a loop momentum convention to make it compatible with this symmetry. On the other hand, forward limit tree amplitudes $A_{\text{Feyn}}^{\text{tree}}(\ell, \sigma(1), \dots, \sigma(n), -\ell)$ constructed from the same Feynman rules has a distinctive “cut.” 4-vertices and higher cannot be placed across this cut. It is only when cyclically summed (3.2) that the symmetry is restored.

A. Relation between tree and loop numerators

In the event when the extra conditions are not satisfied, as we have just argued in Sec. III, $A_{\text{BCJ}}^{\text{tree}}$ and $A_{\text{Feyn}}^{\text{tree}}$ cannot be identified, and that the one loop numerators are not simply the welded tree numerators. In this scenario the one loop numerators, which can still be determined using the shifting method explained in Sec. II, and the welded tree numerators, by which we mean the solutions to linear equations such as (1.3) determined by $A_{\text{Feyn}}^{\text{tree}}$, are still related, as the two must give the same color-ordered integrand.

We use the 2-point case to illustrate the relation, even though generalization to n -point should be straightforward. At 2-point we have only one independent color-ordered integrand $\mathcal{I}_2(\ell, k_1, k_2)$, and its decomposition (3.2) contains only two terms, $\frac{1}{\ell^2} A_{\text{Feyn}}^{\text{tree}}(\ell, 1, 2, -\ell)$ and $\frac{1}{(\ell + k_1)^2} A_{\text{Feyn}}^{\text{tree}}(\ell + k_1, 2, 1, -(\ell + k_1))$. [This is not to be confused with (3.1).] The first term has the following relation with forward limit tree numerators.

$$\frac{1}{\ell^2} \sum_h A_{\text{Feyn}}^{\text{tree}}(\ell^h, 1, 2, -\ell^h) \quad (3.5)$$

$$= \sum_h \frac{1}{\ell^2} m(\ell, 1, 2, -\ell | \ell, 1, 2, -\ell) N^{\text{tree}}(\ell^h, 1, 2, -\ell^h) + \frac{1}{\ell^2} m(\ell, 1, 2, -\ell | \ell, 2, 1, -\ell) N^{\text{tree}}(\ell^h, 2, 1, -\ell^h) \quad (3.6)$$

$$\sim \sum_h \frac{1}{\ell^2} m(\ell, 1, 2, -\ell | \ell, 1, 2, -\ell) N^{\text{tree}}(\ell^h, 1, 2, -\ell^h) + \frac{1}{(\ell + k_1)^2} m(\ell + k_1, 1, 2, -(\ell + k_1) | \ell + k_1, 2, 1, -(\ell + k_1)) N^{\text{tree}}((\ell + k_1)^h, 2, 1, -(\ell + k_1)^h) \quad (3.7)$$

where we have used the fact that $\frac{1}{\ell^2} A_{\text{Feyn}}^{\text{tree}}(\ell, 1, 2, -\ell)$ is a term in the integrand so that adding difference terms related by a constant shift does not alter the integral result. Similar relation can be written down for term $\frac{1}{(\ell+k_1)^2} A_{\text{Feyn}}^{\text{tree}}(\ell+k_1, 2, 1, -(\ell+k_1))$. Note for tree numerators, now we are not assuming $N^{\text{tree}}(\ell^h, 1, 2, -\ell^h) = N^{\text{tree}}((\ell+k_1)^h, 2, 1, -(\ell+k_1)^h)$, so that these two terms do not combine.

On the other hand the same integrand is assumed to be expressible as (3.1). For the 2-point case this is (1.12), or more explicitly given by (1.8). We have argued in great length that this equals $\frac{1}{\ell^2(\ell+k_1)^2} N(\ell, 1, 2, -\ell)$ in Sec. II A. This time using $N(\ell, 1, 2, -\ell) = N(\ell+k_1, 2, 1, -(\ell+k_1))$, because both refer to the same bubble numerator.

The two expressions above must be equal, as they should both give the same integrand that is given by the color-ordered Feynman rules, therefore we have

$$N(\ell, 1, 2, -\ell) = \ell^2(\ell+k_1)^2 \times \left(\sum_h \frac{1}{\ell^2} m(\ell, 1, 2, -\ell | \ell, 1, 2, -\ell) N^{\text{tree}}(\ell^h, 1, 2, -\ell^h) + \frac{1}{(\ell+k_1)^2} m(\ell+k_1, 1, 2, -(\ell+k_1) | \ell+k_1, 2, 1, -(\ell+k_1)) N^{\text{tree}}((\ell+k_1)^h, 2, 1, -(\ell+k_1)^h) + \dots \right) \quad (3.8)$$

where the ... refers to the similar terms that come from $\frac{1}{(\ell+k_1)^2} A_{\text{Feyn}}^{\text{tree}}(\ell+k_1, 2, 1, -(\ell+k_1))$. At higher-point, the above becomes a matrix equation.

IV. KLT AND DOUBLE COPY FORMULATION AT ONE LOOP

Recall that at tree level, the KLT [3–5], the Del Duca-Dixon-Maltoni (DDM) [64,65], and the double-copy formulation [2] are all known to be equivalent [65]. Starting from double copies, the other two formulations can be readily obtained by expanding with respect to half-ladder basis and using the fact that the momentum kernel is the inverse of the propagator matrix.

$$A_{GR}^{\text{tree}}(123\dots n) = \sum_{\text{all cubic graphs } \Gamma} \frac{N_{\Gamma} \bar{N}_{\Gamma}}{\prod_i \Gamma_i D_i} \quad (4.1)$$

$$= \sum_{\sigma \in S_{n-2}} N(1\sigma n) \bar{A}_{YM}(1\sigma n) \quad (4.2)$$

$$= \frac{1}{k_n^2} \sum_{\alpha, \beta \in S_{n-2}} A_{YM}(1\alpha n) S[\alpha^T | \beta] \bar{A}_{YM}(1\beta n) \quad (4.3)$$

The relation between their generalizations at one loop level following the reasoning explained in Sec. II, however, is less straightforward. Generically one finds a relative shift between the loop momentum dependence of each component. In this section we illustrate this issue through a 2-point example, even though the same issue also resides in the 3-point amplitudes.

We start from a double-copy gravity integrand $\mathcal{I}_{GR}$ with the assumption that it can be defined by biadjoint ϕ^3 -like structure, with the loop momentum dependence of the two sets of kinematic numerators aligned.

$$\mathcal{I}_{GR}(\ell, 1, 2) = \frac{1}{\ell^2(\ell+k_1)^2} \times \frac{1}{\ell^2} \times \frac{1}{s_{12}} \times \frac{1}{\ell^2} \times \frac{1}{s_{12}} \times \text{diagrams} \quad (4.4)$$

We leave the first term as it is. For the second term, we expand one manually chosen copy (the unbarred numerators represented by numerator graphs shown in black) in the following with respect to the corresponding basis. This requires using Jacobi identities and then shift ℓ by the appropriate amount to allow the unbarred numerator be traded by the consistency condition (1.6), creating a difference term in the process.

$$\frac{(N(\ell, 12, -\ell) - N(\ell, 21, -\ell))(\bar{N}(\ell, 12, -\ell) - \bar{N}(\ell, 21, -\ell))}{D_{\ell} s_{12}} \quad (4.5)$$

$$= \frac{N(\ell, 12, -\ell)}{D_{\ell} s_{12}} (\bar{N}(\ell, 12, -\ell) - \bar{N}(\ell, 21, -\ell)) - \frac{N(\ell, 12, -\ell)}{D_{\ell} s_{12}} (\bar{N}(\ell+k_1, 12, -(\ell+k_1)) - \bar{N}(\ell+k_1, 21, -(\ell+k_1))) + \text{difference terms} \quad (4.6)$$

Collecting terms with respect to the unbarred basis, we see there are now two (barred/blue) tadpoles appearing as its coefficients, as required by color-ordered integrand.

$$\begin{aligned}
 & \tilde{\mathcal{I}}_{GR}(\ell, 12) \\
 &= \left(\frac{1}{D_\ell D_{\ell,1}} \times \text{tadpole}(\ell, \ell+k_1) \times \text{tadpole}(\ell, \ell+k_1) \right. \\
 & \quad \left. + \frac{1}{D_\ell s_{12}} \times \text{tadpole}(\ell, \ell+k_1) \times \text{tadpole}(\ell, 12) + \frac{1}{D_{\ell,1} s_{12}} \times \text{tadpole}(\ell, \ell+k_1) \times \text{tadpole}(\ell, 12) \right) \\
 &= N(\ell, 12, -\ell) \times \tilde{\mathcal{I}}_{YM}(\ell, 12).
 \end{aligned} \tag{4.7}$$

Note the barred integrand has not acquired any shifting in this derivation.

To obtain the analog of KLT expression (4.3) we need to further translate the unbarred numerator into integrand. However recall the manipulation explained in Sec. II A requires shifting the integrand to allow identification using the consistency condition (1.6), otherwise one faces the infinite matrix problem. Therefore the reasoning we use in this paper relates the 2-point numerator with shifted integrand instead of the original one, where loop momentum ℓ follows the convention inherited from string integrand [17].

$$\begin{aligned}
 N(\ell, 12, -\ell) &= (D_\ell D_{\ell,1}) \tilde{\mathcal{I}}_{YM}(\ell, 12) \\
 &= (D_\ell D_{\ell,1}) (\mathcal{I}_{YM}(\ell, 12) + \Delta_\ell)
 \end{aligned} \tag{4.8}$$

Plugging the above back into (4.7) and we see that one either choose manually an unequal-footing expression in the KLT formula, where one of the integrand acquires an extra difference term, or we start with a double copy formulation that has loop momentum dependence that violates the convention of [17].

$$\tilde{\mathcal{I}}_{GR}(\ell, 12) = (\mathcal{I}_{YM}(\ell, 12) + \Delta_\ell) S[1|1]_\ell \tilde{\mathcal{I}}_{YM}(\ell, 12). \tag{4.9}$$

Here the difference term $\Delta_\ell = f(\ell) - f(\ell + c)$ acts as a factor in the integrand so that it generically has non-vanishing contribution to the loop integral. We find the same issue exists also at 3-point.

Note that this issue was identified early in the development of the color-kinematics duality by [66–68] and various research groups. We revisit them here for the sake of conceptual completeness and to adapt the discussion to the specific assumptions and settings used in this paper.

While this paper was being completed, we became aware of Ref. [34], which also discusses one-loop KLT-type relations. In that reference, the resulting expression for

the gravitational integrand appears manifestly symmetric between the two YM copies. This difference can be traced back to the distinct starting assumptions adopted in the two approaches. In [34], the symmetry arises from assuming a one-loop generalized DDM relation from the outset, together with the use of a shifted color-ordered YM integrand $\tilde{\mathcal{I}}$ (see Eq. (9) of [34]). The subsequent integrand $\mathcal{I}(1, \alpha)$ is then obtained by collecting terms related by symmetry. By contrast, in the present work we assume the validity of a symmetric double-copy formula (4.4) and show that this assumption is equivalent to a one-loop generalized DDM representation formulated in terms of the unshifted YM integrand (4.7), which in turn is equivalent to a nonsymmetric KLT relation. In terms of the conventions used in this paper, the two YM integrands appearing in [34] are therefore both shifted, and is equivalent to a non-symmetric double copy formula.

V. A TWO-STEP EXPANSION STRATEGY FOR ONE-LOOP YANG-MILLS NUMERATORS

In previous sections, we addressed the question of whether BCJ-compatible numerators exist for a given one-loop integrand, and, if so, whether they are unique. By exploring the consistency conditions of the nomenclature of the numerators and integrands, we established a full-rank linear transformation between the two, showing that for a properly shifted integrand, the numerators satisfying Jacobi identities are uniquely determined.

Although this establishes the conceptual existence and uniqueness of one-loop numerators, the explicit inversion of the associated transformation matrix becomes rapidly intractable beyond three points. To circumvent this difficulty, we develop in this and the next few sections a constructive, algebraically motivated approach that yields explicit numerator expressions without resorting to matrix inversion.

Our key idea is to express the Yang–Mills integrand as its unique linear expansion of propagator matrix elements, allowing us to directly read off the numerators as the corresponding expansion coefficients. In fact, writing the Yang–Mills integrand in the form of the propagator-matrix expression (2.18) is precisely equivalent to expanding it as a linear combination of BS integrands. This two-step procedure proceeds as follows:

- (i) In the first step, the Yang–Mills integrand is expanded in terms of scalar-loop integrands in the so-called YMS (Yang–Mills-scalar) theory, where external legs are gluons and scalars while the loop contains only scalar propagators.
- (ii) In the second step, each YMS integrand is recursively expanded in terms of biadjoint scalar (BS) integrands, resulting in an overall factorization of the original Yang–Mills integrand in terms of known BS integrands.

To make this expansion precise, we introduce a consistent notation system to describe the Yang–Mills integrands, the YMS integrands (with scalar internal lines), and the BS integrands. We then formulate the expansion in terms of these structures, and extract the kinematic coefficients (which we later identify as the color-stripped numerators) in such a way that they manifestly satisfy the one-loop consistency conditions upon shifting and relabeling.

A. Notation for scalar-loop YMS integrands

We begin by introducing a convenient notation to describe one-loop integrands where the internal loop consists purely of scalars, and external particles can be scalars and gluons. We will be referring such integrand as the scalar-loop Yang–Mills-scalar (YMS) integrand, which is actually only part of the YMS integrand, as the full YMS integrand defined by Feynman rules should include gluon loops (more detail can be found in [31]). The absence of gluon self-interactions in the loop allows for a simpler

structure of integrands, making them suitable intermediate bases for constructing Yang–Mills numerators.

We denote such YMS integrand by $\mathcal{I}^{\text{YMS}}(\mathbf{j}||\mathbf{g}|\boldsymbol{\rho})$, where the arguments are defined as follows (This is the notation used by [62,69])

- (i) $\boldsymbol{\rho}$ denotes the global cyclic ordering of all external particles (i.e., both scalars and gluons), which determines the arrangement of propagators in the full loop integrand.
- (ii) $\mathbf{j} = \{j_1, \dots, j_m\}$ denotes the cyclically ordered external scalars. These scalars determine the second color-order index. We use both $\boldsymbol{\rho}$ and $\mathbf{j}$ to label the integrand $\mathcal{I}^{\text{YMS}}$. Both color factors corresponding to $\boldsymbol{\rho}$ and $\mathbf{j}$ are stripped.
- (iii) $\mathbf{g} = \{g_1, \dots, g_{n-m}\}$ denotes the set of external gluons.

Each integrand $\mathcal{I}^{\text{YMS}}(\mathbf{j}||\mathbf{g}|\boldsymbol{\rho})$ represents a sum over Feynman graphs, in which tree level currents with gluons and/or scalars are attached to the scalar loop, via three-point scalar vertex, two-scalar-one-gluon vertex or two-scalar-two-gluon vertex, as demonstrated by [62].

This notation cleanly separates the contributions from different loop insertion patterns and will prove instrumental in formulating the Yang–Mills integrand as a linear combination of YMS building blocks in the next subsection.

B. Decomposition of Yang–Mills integrands into YMS building blocks

Having introduced the notation for scalar-loop YMS integrands, we now present a decomposition of the one-loop Yang–Mills integrand $\mathcal{I}^{\text{YM}}(\boldsymbol{\rho})$ into a sum over YMS integrands of the form $\mathcal{I}^{\text{YMS}}(\mathbf{j}||\mathbf{G}\backslash\mathbf{j}|\boldsymbol{\rho})$. This expansion separates out contributions according to the number and ordering of gluons inserted on the scalar loop and reflects the algebraic structure of color-dressed integrands.

The decomposition reads [29,31,61,62]

$$\mathcal{I}^{\text{YM}}(\boldsymbol{\rho}) = (D-2)\mathcal{I}^{\text{YMS}}(\emptyset||\mathbf{G}|\boldsymbol{\rho}) + \sum_{l=2}^n (-1)^l \sum_{\substack{\mathbf{j} \subset \mathbf{G} \\ |\mathbf{j}|=l}} \text{Tr}(F_{j_1} \cdots F_{j_l}) \mathcal{I}^{\text{YMS}}(j_1, \dots, j_l||\mathbf{G}\backslash\{j_1, \dots, j_l\}|\boldsymbol{\rho}). \quad (5.1)$$

In this expression

- (i) $\mathbf{G} = \{1, 2, \dots, n\}$ denotes the full set of external gluon labels;
- (ii) the sum runs over all subsets of fixed length l , $\mathbf{j} \subset \mathbf{G}$ of size l , modulo cyclic permutations;
- (iii) $\text{Tr}(F_{j_1} \cdots F_{j_l})$ denotes the color-ordered trace of field-strength tensors; and
- (iv) each $\mathcal{I}^{\text{YMS}}(\mathbf{j}||\mathbf{G}\backslash\mathbf{j}|\boldsymbol{\rho})$ is the one loop integrand defined by the YMS color-ordered Feynman rules, with $\mathbf{j}$ scalars and $\mathbf{G}\backslash\mathbf{j}$ gluons inserted on the scalar loop.

This decomposition formula sets the stage for directly reading off numerators as expansion coefficients once the YMS integrands are further expressed in terms of biadjoint scalar integrands.

By rewriting the Yang–Mills integrand as a sum over trace-labeled YMS building blocks, we effectively translate the problem of constructing BCJ-compatible numerators into a more tractable task: determining the expansion of each YMS integrand in terms of BS integrands. We will carry out this step in the following section.

VI. EXPANDING SCALAR-LOOP INTEGRANDS INTO BIADJOINT SCALAR INTEGRANDS

Having expressed the Yang-Mills integrand as a sum over scalar-loop YMS integrands, our next task is to expand each YMS integrand into a linear combination of biadjoint scalar (BS) integrands. This second step is grounded in a direct comparison of the Feynman rules of the two theories: the scalar-loop YMS theory, which includes scalar, gluon, and mixed vertices, and the purely scalar BS theory. By matching loop graphs and their associated kinematic factors, we systematically determine the expansion coefficients. In doing so, we complete the two-stage reduction

of the original problem of constructing one-loop BCJ numerators into the determination of kinematic coefficients appearing in a well-structured expansion.

As discussed earlier in our analysis of color-ordered one-loop integrands, scalar-loop integrands in the YMS theory naturally admit a representation in terms of the propagator matrix structure (2.18). Furthermore, each YMS integrand $\mathcal{I}^{\text{YMS}}$ can be further stripped of its scalar-loop color factor, yielding a doubly color stripped integrand $\mathcal{I}_{\text{DCS}}^{\text{YMS}}(l; 1, \sigma | \mathbf{G} | \rho)$. With the second set of color factors stripped from (2.18), this object can be written as the following expansion.

$$\mathcal{I}_{\text{DCS}}^{\text{YMS}}(\ell; 1, \sigma | \mathbf{G} | \rho) = \sum_{\gamma \in \text{Perms}(\mathbf{G}), \alpha \in \gamma \sqcup \sigma} N_{\text{DCS}}(\ell; 1, \alpha | \rho) I^{\text{BS}}(\ell; 1, \alpha | \rho), \quad (6.1)$$

By comparing the Feynman-graph expansions of the YMS and BS integrands, we find that the coefficient $N_{\text{DCS}}(\ell; 1, \alpha | \rho)$ depends only on the ordering α . We therefore denote it by $C(\ell; 1, \alpha)$ and rewrite (6.1) as

$$\mathcal{I}_{\text{DCS}}^{\text{YMS}}(\ell; 1, \sigma | \mathbf{G} | \rho) = \sum_{\gamma \in \text{Perms}(\mathbf{G}), \alpha \in \gamma \sqcup \sigma} C(\ell; 1, \alpha) I^{\text{BS}}(\ell; 1, \alpha | \rho), \quad (6.2)$$

where:

- (i) The symbol $\sqcup$ denotes the shuffle between the scalar index σ and the gluons γ , preserving the scalar orderings while summing over all gluon orderings;
- (ii) $\mathcal{I}_{\text{DCS}}^{\text{BS}}(\ell; 1, \alpha | \rho)$ denotes the doubly color ordered biadjoint scalar integrand with color ordering $1, \alpha$ and ρ , constructed from cubic graphs with quadratic propagators; and
- (iii) $C(\ell; 1, \alpha)$ are the expansion coefficients (loop-momentum-dependent in general) associated with the ordering $1, \alpha$ around the loop. The coefficients $C(\ell; 1, \alpha)$ are purely kinematic and will be determined in the next subsection.

This expansion inherits a crucial property from the YMS integrands: all coefficients $C(\ell; 1, \alpha)$ are independent of loop momentum routing ambiguities and can be chosen to satisfy a one-loop version of the kinematic consistency conditions. In particular, they obey

$$\begin{aligned} C(\ell; 1, \alpha_1, \dots, \alpha_r) &= C(\ell + k_1; \alpha_1, \dots, \alpha_r, 1) = \dots \\ &= C\left(\ell + \sum_{i=1}^r k_{\alpha_i}; \alpha_r, 1, \alpha_1, \dots, \alpha_{r-1}\right), \end{aligned} \quad (6.3)$$

ensuring compatibility with the cyclic invariance and shift identities of the loop integrand.

As a result, combining the YMS decomposition of the YM integrand in Eq. (5.1) with the expansion Eq. (6.2) of each YMS integrand into BS building blocks leads directly

to the desired propagator-matrix representation

$$\mathcal{I}^{\text{YM}}(\rho) = \sum_{\sigma \in S_{n-1}} N(l; 1, \sigma) \mathcal{I}^{\text{BS}}(\ell; 1, \sigma | \rho), \quad (6.4)$$

with the coefficients $N(l; 1, \sigma)$ being linear combinations of the field-strength traces $\text{Tr}(F_{j_1} \cdots F_{j_l})$ weighted by the expansion coefficients $C(\ell; 1, \alpha)$.

A key observation is that the field-strength traces $\text{Tr}(F_{j_1} \cdots F_{j_l})$ are independent of the loop momentum, so that cyclic symmetry, which is apparently satisfied by traces, in this special case becomes identical to the consistency condition of the nomenclature (2.5). On the other hand, we require the factors $C(\ell; 1, \alpha)$ satisfy the same condition (6.3) separately, therefore the weighted sum $N(\ell; 1, \sigma)$ automatically satisfy the loop-shift consistency conditions

$$\begin{aligned} N(\ell; 1, \sigma_1, \dots, \sigma_{n-1}) &= N(\ell + k_{\sigma_1}; \sigma_1, \dots, \sigma_{n-1}, 1) = \dots \\ &= N\left(\ell + \sum_{i=1}^{n-1} k_{\sigma_i}; \sigma_{n-1}, 1, \sigma_1, \dots, \sigma_{n-2}\right), \end{aligned} \quad (6.5)$$

making them suitable as BCJ numerators for use in the double-copy construction at one loop. We write the i th element $\sigma(i)$ of the ordered set σ as σ_i for short.

In the next subsection, we will provide an explicit construction of the coefficients $C(\ell; 1, \alpha)$ in Eq. (6.2) from a diagrammatic algorithm based on scalar loop topologies

and insertion rules. Final formulas for the 2- and 3-point YM numerators $N(l; 1, \sigma)$ calculated using the two-step method explained above is shown in Eq. (7.46).

VII. CONSTRUCTIVE PRESCRIPTION FOR THE YMS EXPANSION COEFFICIENTS

To construct the coefficients in (6.2) that satisfy the constraint (6.3), we note that the YMS integrand $\mathcal{I}_{\text{DCS}}^{\text{YMS}}(\ell; 1, \sigma || \mathbf{G} | \rho)$ can be arranged as a sum over Feynman graphs, each of which is expressed by attaching tree level currents to the loop as demonstrated in [62]. Each tree level current is further expanded in terms of BS currents with proper kinematic coefficients. The YMS integrand is therefore expressed by a combination of Feynman graphs with proper kinematic coefficients. After this manipulation, one can collect all contributions of such graphs with respect to a given cyclic ordering $1, \alpha$. We denote such terms by $\mathcal{I}^{\text{YMS}}(l; 1, \alpha | \rho)$, the YMS integrand is then expressed as a sum over such terms with varying α , where α runs over all shuffles of the fixed scalar sequence σ with all permutations of the gluon set $\mathbf{G}$.

$$\mathcal{I}_{\text{DCS}}^{\text{YMS}}(\ell; 1, \sigma || \mathbf{G} | \rho) = \sum_{\alpha \in \sigma \sqcup \text{perms } \mathbf{G}} \mathcal{I}^{\text{YMS}}(\ell; 1, \alpha | \rho). \quad (7.1)$$

Thus, we can formally define the coefficient for a given permutation $\alpha \in \gamma \sqcup \sigma$ (where $\gamma \in \text{perms } \mathbf{G}$ are permutations of gluons) as follows.

$$C(\ell; 1, \alpha) \equiv \frac{\mathcal{I}^{\text{YMS}}(\ell; 1, \alpha | \rho)}{\mathcal{I}^{\text{BS}}(\ell; 1, \alpha | \rho)}. \quad (7.2)$$

Apparently, these coefficients can be considered as the expansion coefficients in (6.2) and produce the correct YMS integrand. *Although the coefficient itself does not satisfy the consistency condition (6.3), we will show that they can induce compact expressions of coefficients satisfying the consistency condition (6.3).*

In the following, we answer the questions: What are the expressions of $\mathcal{I}^{\text{BS/YMS}}(\ell; 1, \alpha | \rho)$? How to induce the coefficients satisfying the consistency condition equation (6.3), starting from Eq. (7.2)? Recall that both $\mathcal{I}^{\text{BS}}$ and $\mathcal{I}^{\text{YMS}}$ are defined as sums over one-loop Feynman graphs, which in these scalar-loop theories take the form of polygons built from scalar propagators. External particles are attached to the loop via tree-level currents emanating from the vertices of the polygon. A natural way to systematically enumerate such Feynman graphs is as follows:

- (i) First, enumerate all possible cyclic divisions $\mathcal{D}$ of the external ordering $1, \alpha$. (A cyclic division of $1, \alpha$ is defined as follows. Consider $1, \alpha$ as cyclic order and divide this cyclic order into ordered subsets.); and
- (ii) Then, for each ordered subset in $\mathcal{D}$, enumerate all possible structures that are expressed by attaching currents to the loop via possible vertices.

We group together all such Feynman graphs that correspond to a fixed cyclic division $\mathcal{D}$, and denote their sum as $\mathcal{I}_{\mathcal{D}}^{\text{YMS}}(l; 1, \alpha | \rho)$. The full integrand $\mathcal{I}^{\text{YMS}}(l; 1, \alpha | \rho)$ is then the sum over all such division-based contributions.

$$\mathcal{I}^{\text{YMS/BS}}(\ell; 1, \alpha | \rho) = \sum_{\mathcal{D} \in \text{CycDiv}\{1, \alpha\}} \mathcal{I}_{\mathcal{D}}^{\text{YMS/BS}}(\ell; 1, \alpha | \rho). \quad (7.3)$$

We now turn to the detailed construction of $\mathcal{I}_{\mathcal{D}}^{\text{YMS/BS}}(\ell; 1, \alpha | \rho)$ associated with a given cyclic partition $\mathcal{D}$.

(i) For *BS integrand*, recall that $\mathcal{I}_{\mathcal{D}}^{\text{BS}}(\ell; 1, \alpha | \rho)$ denotes the sum of BS Feynman graphs associated with a fixed cyclic division $\mathcal{D}$ of the ordering $1, \alpha$. More explicitly, if the division takes the form $\{1, \alpha\} \rightarrow \alpha_1 = \alpha_{1L} 1 \alpha_{1R}, \alpha_2, \dots, \alpha_I$, then $\mathcal{I}_{\mathcal{D}}^{\text{BS}}(\ell; 1, \alpha | \rho)$ is obtained by summing all BS Feynman graphs whose loop topology matches the cyclic polygon defined by the parts $\alpha_1, \dots, \alpha_I$, with each part attached to a tree corresponding to the double ordering $(\alpha_i | \rho_i)$.¹²

$$\begin{aligned} \mathcal{I}_{\mathcal{D}}^{\text{BS}}(\ell; 1, \alpha | \rho) &= \sum_{\substack{\text{CycDiv } \rho \\ |\alpha_i| = |\rho_i|}} \text{Diagram} \\ &\equiv \sum_{\substack{\text{CycDiv } \rho \\ |\alpha_i| = |\rho_i|}} \frac{1}{(\ell - k_{\alpha_{1L}})^2} \phi_{\alpha_{1L} 1 \alpha_{1R} | \rho_1} \frac{1}{(\ell + k_1 + k_{\alpha_{1R}})^2} \phi_{\alpha_2 | \rho_2} \\ &\quad \times \dots \times \frac{1}{(\ell + k_1 + k_{\alpha_{1R}} + k_{\alpha_2} + \dots + k_{\alpha_I})^2} \phi_{\alpha_I | \rho_I}, \end{aligned} \quad (7.4)$$

¹²Graphs in this section represent Feynman graphs. In addition, the direction of loop momentum ℓ is supposed to be reflected. These adjustments are introduced in order to agree with the conventions in [62].

in which, we summed over all cyclic divisions of ρ such that each ordered subset ρ_i has the same number of elements with the corresponding α_i . The right permutations in the graph on the first line have been hidden for

convenience, while each $\phi_{\alpha_i|\rho_i}$ ($i = 1, \dots, I$) on the second line denotes a tree-level Berends-Giele current of BS (see Appendix D).

(ii) The *YMS integrand* $\mathcal{I}_D^{\text{YMS}}(\ell; 1, \alpha|\rho)$ can be given by

$$\begin{aligned} \mathcal{I}_D^{\text{YMS}}(\ell; 1, \alpha|\rho) &= C(\alpha_{1L}1\alpha_{1R})C(\alpha_2)\dots C(\alpha_I) \times \sum_{\substack{\text{CycDiv } \rho \\ |\alpha_i|=|\rho_i|}} \text{Diagram} \\ &\equiv \sum_{\substack{\text{CycDiv } \rho \\ |\alpha_i|=|\rho_i|}} C(\alpha_{1L}1\alpha_{1R})C(\alpha_2)\dots C(\alpha_I) \frac{1}{(\ell - k_{\alpha_{1L}})^2} \phi_{\alpha_{1L}1\alpha_{1R}|\rho_1} \\ &\quad \times \frac{1}{(\ell + k_1 + k_{\alpha_{1R}})^2} \phi_{\alpha_2|\rho_2} \dots \frac{1}{(\ell + k_1 + k_{\alpha_{1R}} + k_{\alpha_2} + \dots + k_{\alpha_I})^2} \phi_{\alpha_I|\rho_I}. \end{aligned} \quad (7.5)$$

The above expression originates from the local expression of YMS integrand derived in [62]. In particular, we express the full YMS integrand according to the formula given in [62], expand the subcurrents attached to the loop in terms of BS ones and collect all contributions (i.e., all cyclic divisions) for a given ordering $\{1, \alpha\}$. For a given cyclic division $\{1, \alpha\} \rightarrow \alpha_1 = \alpha_{1L}1\alpha_{1R}, \alpha_2, \dots, \alpha_I$, the coefficient

$$C(\alpha_{1L}1\alpha_{1R})C(\alpha_2)\dots C(\alpha_I) \quad (7.6)$$

is just the product of kinematic factors coming from the corresponding subcurrents. If there is a four-point vertex structure for a given subset α_i ($|\alpha_i| \geq 2$, α_i only contains gluons) in the division, the coefficient $C(\alpha_i)$ must be given by Lorentz contraction of two coefficients corresponding to the two subcurrents attached to this four-point vertex structure. More detail can be found in Appendix E.

In the following subsections, we evaluate (7.2) and simplify it into a more compact form without loop-momentum denominators, focusing on integrands with up to three gluons.

A. YMS integrand with one gluon

We first investigate the simplest case of the expansion formula Eq. (6.2) with coefficients (7.2), i.e., the YMS integrand with only one gluon. Without loss of generality, we take the integrand with three scalars 1, 2, 3 and one gluon p as an example. According to (7.2), the coefficient reads

$$C(\ell; 1, \alpha) = \frac{\mathcal{I}_D^{\text{YMS}}(\ell; 1, \alpha|\rho)}{\mathcal{I}_D^{\text{BS}}(\ell; 1, \alpha|\rho)}, \quad \alpha \in \{p\} \sqcup \{2, 3\} \quad (7.7)$$

To show the explicit expressions of $\mathcal{I}_D^{\text{YMS}}$ and $\mathcal{I}_D^{\text{BS}}$, we take the permutation $\{1, \alpha\} = \{1, p, 2, 3\} \in \{1, \{p\} \sqcup \{2, 3\}\}$ as an example. All possible cyclic partitions of this ordering are

$$\begin{aligned} &\{1, p, 2, 3\}, \quad \{3, 1, p, 2\}, \quad \{2, 3, 1, p\}, \quad \underline{\{p, 2, 3, 1\}}, \quad \underline{\{1\}\{p, 2, 3\}}, \quad \{1, p, 2\}\{3\}, \\ &\{2, 3, 1\}\{p\}, \quad \{3, 1, p\}\{2\}, \quad \{1, p\}\{2, 3\}, \quad \underline{\{3, 1\}\{p, 2\}}, \quad \{1\}\{p\}\{2, 3\}, \quad \{1, p\}\{2\}\{3\}, \\ &\underline{\{1\}\{p, 2\}\{3\}}, \quad \{3, 1\}\{p\}\{2\}, \quad \{1\}\{p\}\{2\}\{3\}, \end{aligned} \quad (7.8)$$

where the divisions with underlines are those exist only in $\mathcal{I}_D^{\text{BS}}$ but not in $\mathcal{I}_D^{\text{YMS}}$ (note that in the definition of YMS current with both scalars and gluons, the first element in the permutation must be scalar, see Appendix E). Let us write down explicit expressions for specific divisions as illustrative examples, according to Appendix E. For division $\mathcal{D} \rightarrow \{1, p\}\{2\}\{3\}$, the $\mathcal{I}_D^{\text{BS}}$ and $\mathcal{I}_D^{\text{YMS}}$ are respectively given by

$$\mathcal{I}_D^{\text{BS}}(\ell; 1, p, 2, 3|\rho) = \text{Diagram 1}, \quad \mathcal{I}_D^{\text{YMS}}(\ell; 1, p, 2, 3|\rho) = \epsilon_p \cdot k_1 \times \text{Diagram 2}. \quad (7.9)$$

For division $\mathcal{D} \rightarrow \{3, 1\}\{p\}\{2\}$, the explicit expressions of $\mathcal{I}_{\mathcal{D}}^{\text{BS}}$ and $\mathcal{I}_{\mathcal{D}}^{\text{YMS}}$ are displayed as

$$\mathcal{I}_{\mathcal{D}}^{\text{BS}}(\ell; 1, p, 2, 3 | \rho) = \text{diagram}, \quad \mathcal{I}_{\mathcal{D}}^{\text{YMS}}(\ell; 1, p, 2, 3 | \rho) = \epsilon_p \cdot (\ell + k_1) \times \text{diagram}. \quad (7.10)$$

Following a similar way, the $\mathcal{I}_{\mathcal{D}}^{\text{BS/YMS}}$ with other divisions can also be provided explicitly.

The coefficient (7.7) itself does not obey the consistency condition (6.3). In addition, there is loop momentum in the denominator of each coefficient (7.7). In the following, we try to reduce the expansion coefficient (7.7) into an appropriate form such that they obey the condition (7.7) and the loop momentum is only involved in the numerator. To achieve this, we classify the cyclic divisions into the following two types.

- (i) Gluon p is a single-particle subcurrent attached to the loop, e.g., the division $\mathcal{D} \rightarrow \{3, 1\}\{p\}\{2\}$.
- (ii) Gluon p is involved in a subcurrent with at least one scalar, e.g., the division $\mathcal{D} \rightarrow \{1, p\}\{2\}\{3\}$.

For a *type (i) division*, e.g., $\mathcal{D} \rightarrow \{3, 1\}\{p\}\{2\}$, the kinematic coefficient is presented as

$$C(3, 1)C(p)C(2) = \epsilon_p \cdot (\ell + k_1), \quad (7.11)$$

where the fact that the coefficient associating to a *pure scalar subcurrent* is 1 has been applied. This coefficient can be generalized to the pattern

$$\epsilon_p \cdot X_p(\ell; 1, \alpha), \quad (7.12)$$

where $X_p(\ell; 1, \alpha)$ is defined by the sum of loop momentum ℓ^μ and the total momentum of elements between ℓ^μ and

the gluon p

$$X_p^\mu(\ell; \alpha) = \ell^\mu + \sum_{i < p} k_i^\mu, \quad (7.13)$$

in which, the notation $i < p$ means the position of i is less than the position of p , when 1 is considered as the first element in the permutation $\{1, \alpha\}$. For instance, if the permutation is $\{1, \alpha\} = \{1, p, 2, 3\}$, the X_p^μ is $X_p^\mu = \ell^\mu + k_1^\mu$, while if the permutation is $\{1, \alpha\} = \{1, 2, p, 3\}$, we have $X_p^\mu = \ell^\mu + k_1^\mu + k_2^\mu$.

The *type (ii) divisions*, e.g., the division $\mathcal{D} \rightarrow \{1, p\}\{2\}\{3\}$, would contribute to $\mathcal{I}^{\text{YMS}}(\ell; 1, \alpha | \rho)$ with different orderings α : The kinematic coefficient from the subtree current is given by

$$C(1, p) = \epsilon_p \cdot k_1. \quad (7.14)$$

With the $U(1)$ -decoupling identity

$$\text{diagram} + \text{diagram} = 0, \quad (7.15)$$

the expression for $\mathcal{I}_{\{\{1, p\}, \{2\}, \{3\}\}}^{\text{YMS}}(\ell; 1, p, 2, 3 | \rho)$ can be equivalently written as

$$(\epsilon_p \cdot k_1) \times \text{diagram} \cong \epsilon_p \cdot (\ell + k_1) \times \text{diagram} + \epsilon_p \cdot \ell \times \text{diagram} \quad (7.16)$$

The first term can combine with $\epsilon_p \cdot (\ell + k_1) \times \mathcal{I}_{\{\{1\}, \{p\}, \{2\}, \{3\}\}}^{\text{BS}}(\ell; 1, p, 2, 3 | \rho)$ and other partitions in the ordering $\{1, p, 2, 3\}$ to get $\mathcal{I}^{\text{YMS}}(\ell; 1, p, 2, 3 | \rho) = \epsilon_p \cdot (\ell + k_1) \times \mathcal{I}^{\text{BS}}(\ell; 1, p, 2, 3 | \rho)$ and the second term in (7.16) will combine with other terms in the ordering $\{1, 2, 3, p\}$ to get $\mathcal{I}^{\text{YMS}}(\ell; 1, 2, 3, p | \rho) = \epsilon_p \cdot (\ell + k_1 + k_2 + k_3) \times \mathcal{I}^{\text{BS}}(\ell; 1, 2, 3, p | \rho)$.

With this manipulation, the contribution from partitions of type (ii) also agrees with the general pattern (7.12). When the above discussions are applied to all permutations α and all possible cyclic divisions, the $\mathcal{I}^{\text{YMS}}(\ell; 1, \alpha)$, $\forall \alpha \in \{p\} \sqcup \{2, 3\}$ turns into a multiple of $\mathcal{I}^{\text{BS}}(\ell; 1, \alpha)$, with coefficient $\epsilon_p \cdot X_p(\ell; 1, \alpha)$. Therefore, we can redefine the coefficient (7.7) as

$$C(\ell; 1, \alpha) \cong \epsilon_p \cdot X_p(\ell; 1, \alpha) \frac{\mathcal{I}^{\text{BS}}(\ell; 1, \alpha)}{\mathcal{I}^{\text{BS}}(\ell; 1, \alpha)} = \epsilon_p \cdot X(\ell; 1, \alpha). \quad \forall \alpha \in \{p\} \sqcup \{2, 3\} \quad (7.17)$$

The above example is straightforwardly generalized to YMS integrands with one gluon and an arbitrary number of scalars

$$C(\ell; 1, \alpha) \cong \epsilon_p \cdot X_p(\ell; 1, \alpha). \quad (7.18)$$

Apparently, this coefficient satisfies the consistency condition (6.3) and it is a polynomial function of the loop momentum. Another important feature of (7.18) is that $C(\ell; 1, \alpha)$ is independent of the choice of the right permutation ρ .

B. YMS integrand with two gluons

For integrands with two gluons, we use the example with two scalars 1, 2 and two gluons p, q to demonstrate the general construction of expansion coefficients. The

coefficient (7.2) is now explicitly given by

$$C(\ell; 1, \alpha) = \frac{\mathcal{I}^{\text{YMS}}(\ell; 1, \alpha | \rho)}{\mathcal{I}^{\text{BS}}(\ell; 1, \alpha | \rho)}, \quad \alpha \in \{p\} \sqcup \{q\} \sqcup \{2\}. \quad (7.19)$$

The concrete expression of (7.19) for a given α can be obtained by expressing the YMS and BS integrands by summations over cyclic divisions, as we have done in the case of only one gluon. Particularly, the denominator $\mathcal{I}^{\text{BS}}(\ell; 1, \alpha | \rho)$ in (7.19) for a given $\alpha \in \{p\} \sqcup \{q\} \sqcup \{2\}$, is just given by summing all possible BS Feynman graphs corresponding to the cyclic divisions for $\{1, \alpha\}$. For example, all cyclic divisions contributing to $\mathcal{I}^{\text{BS}}(\ell; 1, \alpha | \rho)$ are following

$$\begin{aligned} &\{1, p, q, 2\}, \quad \{2, 1, p, q\}, \quad \{q, 2, 1, p\}, \quad \{p, q, 2, 1\}, \quad \{1, p, q\}\{2\}, \quad \{2, 1, p\}\{q\}, \\ &\{q, 2, 1\}\{p\}, \quad \{1, p\}\{q, 2\}, \quad \{2, 1\}\{p, q\}, \quad \{1, p\}\{q\}\{2\}, \quad \{2, 1\}\{p\}\{q\}, \quad \{1\}\{p, q\}\{2\}, \\ &\{1\}\{p\}\{q, 2\}, \quad \{1\}\{p\}, \{q\}, \{2\}. \end{aligned} \quad (7.20)$$

Thus the denominator is given by summing all possible BS diagrams (with cubic vertices) corresponding to these cyclic divisions

$$\mathcal{I}^{\text{BS}}(\ell; 1, p, q, 2 | \rho) = \text{diagram 1} + \text{diagram 2} + \text{diagram 3} + \text{diagram 4} + \text{diagram 5} + \text{diagram 6} + \dots, \quad (7.21)$$

The numerator $\mathcal{I}^{\text{YMS}}(\ell; 1, \alpha | \rho)$ can also be provided by summing over all cyclic divisions with correct kinematic coefficients according to Appendix E.

In the following, we classify the coefficients $C(\ell; 1, \alpha)$ according to different powers of $\epsilon_p \cdot \epsilon_q$ in the numerator, and then reduce each coefficient into a proper form that satisfies the condition (6.3) and does not involve loop momentum in the denominator.

1. The part with $(\epsilon_p \cdot \epsilon_q)^0$

Now let us investigate the terms in $C(\ell; 1, \alpha)$ without powers of $(\epsilon_p \cdot \epsilon_q)$. According to (7.5), the numerator

of (7.19), i.e., $\mathcal{I}^{\text{YMS}}$ in this part, for a given permutation $\{1, \alpha\} \in \{1, \{p\} \sqcup \{q\} \sqcup \{2\}\}$ is obtained by summing over all Feynman graphs (or equivalently all cyclic divisions) that are constructed by attaching subcurrents (with proper kinematic coefficients) to the scalar loop. Each diagram is characterized by a cyclic division of this permutation. For example, for the doubly color-ordered integrand $\mathcal{I}^{\text{YMS}}(\ell; 1, \alpha | \rho)$, if $\alpha = \{p, q, 2\}$, the cyclic divisions $\mathcal{D}$ of $\{1, \alpha\}$ with terms containing $(\epsilon_p \cdot \epsilon_q)^0$ factor are

$$\begin{aligned} &\{1, p, q, 2\}, \quad \{2, 1, p, q\}, \quad \{1, p, q\}\{2\}, \quad \{2, 1, p\}\{q\}, \quad \{2, 1\}\{p, q\}, \quad \{1, p\}\{q\}\{2\}, \\ &\{2, 1\}\{p\}\{q\}, \quad \{1\}\{p, q\}\{2\}, \quad \{1\}\{p\}, \{q\}, \{2\}. \end{aligned} \quad (7.22)$$

Comparing to (7.20), we have just deleted those divisions with parts satisfying the following two conditions: (i) it contains both gluons and scalars, (ii) the first element is a gluon.

$$\begin{aligned}
\mathcal{I}^{\text{YMS}}(\ell; 1, p, q, 2 | \rho) = (\epsilon_p \cdot \epsilon_q) \Bigg\{ & (-k_p \cdot k_1) \times \text{Diagram 1} + [-k_p \cdot (k_1 + k_2)] \times \text{Diagram 2} \\
& + (-k_p \cdot k_1) \times \text{Diagram 3} + [-k_p \cdot (k_1 + \ell)] \times \text{Diagram 4} \\
& + \left(-\frac{1}{2}\right) \times \text{Diagram 5} + [-k_p \cdot (k_1 + \ell)] \times \text{Diagram 6} \\
& + \left(-\frac{1}{2}\right) \times \text{Diagram 7} \Bigg\}.
\end{aligned} \tag{7.29}$$

Thus the coefficient $C(\ell; 1, p, q, 2)$ is obtained by substituting this expression into (7.19). Coefficients for other permutations can be obtained analogously.

Now we transform the coefficients (7.19) into equivalent ones which do not contain loop momentum in the denominator. The crucial point of this is to add terms which integrate to zero to the YMS integrand $\mathcal{I}^{\text{YMS}}$, so that (i) Each new $\mathcal{I}^{\text{YMS}}(\ell; 1, \alpha | \rho)$ is proportional to $\mathcal{I}^{\text{BS}}(\ell; 1, \alpha | \rho)$, and the proportionality factor (in other words the new defined kinematic coefficient) is a rational function of Lorentz contractions of external polarizations, momenta and the loop momentum. (ii) The new coefficient does not involve loop momentum ℓ^μ in the denominators. We now derive such coefficients by the following steps.

Step 1 Reversing the localization process in ([62]) to transform the local YMS integrand

$$\mathcal{I}^{\text{YMS}}(\ell; 1, 2 | \{p, q\} | 1, \rho) \tag{7.30}$$

as a proper combination of BS Feynman graphs with *nonlocal coefficients* (i.e. Lorentz contraction separated by loop propagators). There are three key techniques for this step:

- (i) *First*, the generalized $U(1)$ -decoupling identity of a BS subcurrent (7.23), helps one to introduce a factor $(-k_p \cdot \ell_i)$ into a subcurrent by adding the following zeros to the full integrand

$$\begin{aligned}
& (\epsilon_p \cdot \epsilon_q)(-k_p \cdot \ell_i) \times \sum_{\sqcup} \text{Diagram 1}, & (\epsilon_p \cdot \epsilon_q)(-k_p \cdot \ell_i) \times \sum_{\sqcup} \text{Diagram 2}, \\
& (\epsilon_p \cdot \epsilon_q)(-k_p \cdot \ell_i) \times \sum_{\sqcup} \text{Diagram 3}, & \\
& \sum_{\sqcup_1} (\epsilon_p \cdot \epsilon_q)(-k_p \cdot (\ell_i + X_p(\ell; \sqcup_1))) \times \sum_{\sqcup_2} \text{Diagram 4}, &
\end{aligned} \tag{7.31}$$

where A, B are ordered scalar subsets, ℓ_i denotes the momentum of the loop propagator that is connected to the corresponding subcurrent from left (as shown in the Feynman graphs).

- (ii) *Second*, if there are subcurrents $\phi_{A|\tilde{A}}$, $\phi_{p|p}$ and $\phi_{B|\tilde{B}}$ attached to the loop in turn, where $\{x_1, A\}$, $\{y_1, B\}$ refer to ordered scalar subsets, the elements of $\{x_1, A\}$ ($\{y_1, B\}$) are identical to those of $\tilde{A}$ ($\tilde{B}$)

so that these subcurrent do not vanish, we have the following identity related to such structure

$$0 = \sum_{\sqcup} (-k_p \cdot X_p(\ell; \sqcup)) \times \text{Diagram 1} + (-k_p \cdot \ell_i) \times \text{Diagram 2} + \sum_{\sqcup} (-k_p \cdot X_p(\ell; \sqcup)) \times \text{Diagram 3}, \quad (7.32)$$

where the right permutation of the subcurrent in the first and the last terms are respectively $\{x_1, A, p\}$ and $\{p, y_1, B\}$.

(iii) *Third*, the following relation, by which a four-point vertex structure is transformed into BS Feynman graphs (with only three-point vertices), as

$$\text{Diagram 4} = \sum_{\sqcup} (-k_p \cdot X_p(\ell; \sqcup)) \times \text{Diagram 5} + (-k_p \cdot \ell_i) \times \text{Diagram 6} \quad (7.33)$$

where A is an ordered set of scalars, $X_p(\ell; \sqcup)$ in the first term denotes the total momentum of the particles to the left of p in the permutation $\{x_1, A \sqcup \{p\}\}$, ℓ_i in the second term denotes the momentum of the propagator attached to p from left.

After this step, the full integrand $\mathcal{I}^{\text{YMS}}(\ell; 1, 2 || \{p, q\} | \rho)$ is transformed into a proper combination of BS Feynman graphs

$$\begin{aligned} \mathcal{I}^{\text{YMS}}(\ell; 1, 2 || \{p, q\} | \rho) &\cong (\epsilon_p \cdot \epsilon_q) \left[\sum_{\alpha} (-k_p \cdot X_p(\ell; 1, \alpha)) \mathcal{I}_1^{\text{BS}}(\ell; 1, \alpha \in \{2\} \sqcup \{p, q\} | \rho) \right. \\ &\quad \left. + \sum_{\beta \text{ s.t. } \beta_1 \neq 1} (-k_p \cdot X_p(\ell'; \beta)) \mathcal{I}_2^{\text{BS}}(\ell'; \beta \in \text{cyc}\{1, 2\} \sqcup \{p, q\} | \rho) \right]. \end{aligned} \quad (7.34)$$

In the above expression, $\mathcal{I}_1^{\text{YMS}}(\ell; 1, \alpha | \rho)$ and $\mathcal{I}_2^{\text{YMS}}(\ell'; \beta | \rho)$ respectively refer to the sum of all possible diagrams (in other words all cyclic divisions) of permutations $\{1, \alpha\}$ and β , where the first element in the subcurrent containing the scalar 1 is 1 (for $\mathcal{I}_1^{\text{YMS}}$) and $\beta_1 (\neq 1)$ (for $\mathcal{I}_2^{\text{YMS}}$). In $\mathcal{I}_1^{\text{YMS}}$, the momentum of the loop propagator, which is attached to the subcurrent containing 1, is ℓ , while in $\mathcal{I}_2^{\text{YMS}}$, this loop momentum is $\ell' = \ell - k_{\beta_L}$ (β_L denotes the elements between ℓ' and 1 in the permutation $\beta \equiv \{\beta_L, 1, \beta_R\}$). The X_p always denotes the sum of ℓ (or ℓ') and the total external momenta between ℓ (or ℓ'), p . To clarify terms in (7.34), we write down the coefficients associating with the following diagrams (which come from $\mathcal{I}_1^{\text{YMS}}(\ell; 1, p, q, 2 | \rho)$ and $\mathcal{I}_2^{\text{YMS}}(\ell'; 2, p, 1, q | \rho)$)

$$\begin{aligned} \mathcal{I}_1^{\text{YMS}}(\ell; 1, p, q, 2 | \rho) : & \text{Diagram 7} \rightarrow (\epsilon_p \cdot \epsilon_q) [-k_p \cdot (\ell + k_1)], \\ \mathcal{I}_2^{\text{YMS}}(\ell'; 2, p, 1, q | \rho) : & \text{Diagram 8} \rightarrow (\epsilon_p \cdot \epsilon_q) [-k_p \cdot (\ell' + k_2)] = (\epsilon_p \cdot \epsilon_q) [-k_p \cdot (\ell - k_p)], \\ \mathcal{I}_2^{\text{YMS}}(\ell'; p, 2, 1, q | \rho) : & \text{Diagram 9} \rightarrow (\epsilon_p \cdot \epsilon_q) (-k_p \cdot \ell') = (\epsilon_p \cdot \epsilon_q) [-k_p \cdot (\ell - k_p - k_2)]. \end{aligned} \quad (7.35)$$

An important fact we emphasize here is the expression (7.34) now is nonlocal (i.e., there are contractions between polarizations and momenta living in distinct subcurrents that are separated by loop propagators) and does not satisfy the consistency condition (6.3). To remedy the consistency and to construct expressions proportional to the $\mathcal{I}_1^{\text{BS}}$ in the denominator of (7.19), we need a further step.

Step 2 Adding to the full integrand (7.34) of YMS the following *vanishing term*:

$$0 = \frac{\epsilon_p \cdot \epsilon_q}{k_p \cdot k_q} \left[\sum_{\alpha} (k_q \cdot Y_q(\ell; 1, \alpha)) (-k_p \cdot X_p(\ell; 1, \alpha)) \mathcal{I}_1^{\text{BS}}(\ell; 1, \alpha \in \{2\} \sqcup \{p\} \sqcup \{q\} | \rho) \right. \\ \left. + \sum_{\beta} (k_q \cdot Y_q(\ell'; \beta)) (-k_p \cdot X_p(\ell'; \beta)) \mathcal{I}_2^{\text{BS}}(\ell'; \beta \in \text{cyc}\{2, 1\} \sqcup \{p\} \sqcup \{q\} | \rho) \right], \quad (7.36)$$

where $Y_q(\alpha)$ ($Y_q(\beta)$) denotes the sum of ℓ (ℓ') and the total momenta of *scalars* (i.e., the gluons p, q are excluded) between ℓ (ℓ') and q . In fact, each term of the identity (7.36) has to vanish. This is a consequence of the fundamental BCJ relation [16,18] for gluon q when the position of p is fixed. Such BCJ relation can be verified via expressing the $\mathcal{I}_1^{\text{BS}}$ or $\mathcal{I}_2^{\text{BS}}$ in terms of Feynman graphs and then grouping graphs with the substructures in (7.32), or with generalized $U(1)$ -decoupling identity (7.23) together.

Now we sum (7.34) and (7.36) together, we get a newly defined $\mathcal{I}^{\text{YMS}}$

$$\mathcal{I}^{\text{YMS}} \cong \frac{\epsilon_p \cdot \epsilon_q}{k_p \cdot k_q} \left[\sum_{\alpha} (k_q \cdot X_q(\ell; 1, \alpha)) (-k_p \cdot X_p(\ell; 1, \alpha)) \mathcal{I}_1^{\text{BS}}(\ell; 1, \alpha \in \{2\} \sqcup \{p\} \sqcup \{q\} | \rho) \right. \\ \left. + \sum_{\beta} (k_q \cdot X_q(\ell'; \beta)) (-k_p \cdot X_p(\ell'; \beta)) \mathcal{I}_2^{\text{BS}}(\ell'; \beta \in \{2, 1\} \sqcup \{p\} \sqcup \{q\} | \rho) \right], \quad (7.37)$$

noting that in a permutation if $p < q$, $X_q^\mu = Y_q^\mu + k_p^\mu$, if $q < p$, $X_q^\mu = Y_q^\mu$.

A further observation is that the $X_p(\ell'; \beta)$ ($X_q(\ell'; \beta)$) of the second term in fact is equivalent to those defined by the sum of ℓ (instead of ℓ') and the total external momentum between ℓ and p (q). For example, for $\mathcal{I}_2^{\text{BS}}(\ell'; p, 2, 1, q | \rho)$, we have

$$X_p^\mu = \ell'^\mu = \ell^\mu - k_p^\mu - k_2^\mu = \ell^\mu + k_1^\mu + k_q^\mu, \\ X_q^\mu = \ell'^\mu + k_p^\mu + k_2^\mu + k_1^\mu = (\ell^\mu - k_p^\mu - k_2^\mu) + k_p^\mu + k_2^\mu + k_1^\mu = \ell^\mu + k_1^\mu. \quad (7.38)$$

Therefore, the $\mathcal{I}^{\text{YMS}}$ in (7.37) is finally converted into

$$\mathcal{I}^{\text{YMS}} \cong \sum_{\alpha} \left(-\frac{\epsilon_p \cdot \epsilon_q}{k_p \cdot k_q} \right) (k_p \cdot X_p(\ell; 1, \alpha)) (k_q \cdot X_q(\ell; 1, \alpha)) \mathcal{I}^{\text{BS}}(\ell; 1, \alpha \in \{2\} \sqcup \{p\} \sqcup \{q\} | \rho), \quad (7.39)$$

where $\mathcal{I}^{\text{BS}}(\ell; 1, \alpha \in \{2\} \sqcup \{p\} \sqcup \{q\} | \rho)$ is the full integrand when the scalar 1 is fixed as the first element. It is now clear that the $(\epsilon_p \cdot \epsilon_q)^1$ part of coefficient can be defined by

$$C^{(1)}(\ell; 1, \alpha) = \left(-\frac{\epsilon_p \cdot \epsilon_q}{k_p \cdot k_q} \right) (k_p \cdot X_p(\ell; 1, \alpha)) (k_q \cdot X_q(\ell; 1, \alpha)), \quad (7.40)$$

which naturally satisfies the consistency condition (6.3) and is apparently independent of the choice of the right permutation ρ .

3. The final result of the kinematic coefficients

Now we generalize the calculations of the above example to integrand with two gluons p, q and an arbitrary number of scalars $1, \dots, r$. The YMS integrand $\mathcal{I}^{\text{YMS}}(\ell; 1, \dots, r | \{p, q\} | \rho)$ can be expanded in terms of BS ones as

$$\mathcal{I}^{\text{YMS}}(\ell; 1, \dots, r | \{p, q\} | \rho) = \sum_{\alpha \in \{p\} \sqcup \{q\}} C(\ell; 1, \alpha) \mathcal{I}^{\text{BS}}(\ell; 1, \alpha | \{p, q\} | \rho), \quad (7.41)$$

in which, the kinematic coefficient $C(l; 1, \alpha)$ for any given α can be defined by the following compact expression

$$C(\ell; 1, \alpha) \cong \left[(\epsilon_p)_\mu (\epsilon_q)_\nu - \frac{\epsilon_p \cdot \epsilon_q}{k_p \cdot k_q} (k_p)_\mu (k_q)_\nu \right] X_p^\mu(\ell; 1, \alpha) X_q^\nu(\ell; 1, \alpha), \quad (7.42)$$

which satisfies the consistency condition (6.3), is independent of the choice of the right permutation, and does not contain loop momentum in the denominator. With these coefficients, one can write down the expansion of single-trace EYM integrand

$$\mathcal{I}^{\text{EYM}}(\ell; 1, \dots, r || \{p, q\}) = \sum_{\alpha \in \{p\} \sqcup \{q\}} C(\ell; 1, \alpha) \mathcal{I}^{\text{EYM}}(\ell; 1, \alpha || \{p, q\}), \quad (7.43)$$

where $1, \dots, r$ now denote gluons with fixed color ordering, while p, q are gravitons.

C. YMS integrand with three gluons

The discussions on YMS integrands with one and two gluons can further be extended to YMS integrands with three gluons. This can be derived following similar

discussions on the one and two gluon cases, but the vanishing terms that are added to the original YMS integrand have a more complicated form. We just present the main result without providing the details of the calculation. The integrand $\mathcal{I}^{\text{YMS}}(\ell; 1, \dots, r || \{p, q, s\} | \rho)$ with scalars $1, \dots, r$ and three gluons p, q, s can be expressed as

$$\mathcal{I}^{\text{YMS}}(\ell; 1, \dots, r || \{p, q, s\} | \rho) = \sum_{\alpha \in \{p\} \sqcup \{q\} \sqcup \{s\}} C(\ell; 1, \alpha) \mathcal{I}^{\text{BS}}(\ell; 1, \alpha || \{p, q, s\} | \rho), \quad (7.44)$$

in which, the coefficients are defined by

$$C(\ell; 1, \alpha) = \left[(\epsilon_p)_\mu (\epsilon_q)_\nu (\epsilon_s)_\tau - \frac{\epsilon_p \cdot \epsilon_q}{k_p \cdot k_q} (k_p)_\mu (k_q)_\nu (\epsilon_s)_\tau - \frac{\epsilon_p \cdot \epsilon_s}{k_p \cdot k_s} (k_p)_\mu (\epsilon_q)_\nu (k_s)_\tau - \frac{\epsilon_q \cdot \epsilon_s}{k_q \cdot k_s} (\epsilon_p)_\mu (k_q)_\nu (k_s)_\tau \right] X_p^\mu(\ell; 1, \alpha) X_q^\mu(\ell; 1, \alpha) X_s^\tau(\ell; 1, \alpha) \quad (7.45)$$

This coefficient $C(\ell; 1, \alpha)$ has a symmetric form under the exchanging of p, q, s . Moreover, They naturally satisfy the consistency condition (6.3) and do not contain loop momentum in the numerators. As the results with one and two gluons (7.26), these coefficients are independent of the right permutations. One can verify the expansion formula of YMS integrand with the coefficients defined by (7.18), (7.42), and (7.45) by combining unitary cut and the tree level relations which will be presented in the next section.

Comments on the results with coefficients (7.18), (7.42), and (7.45):

- (i) Although the first element in the above discussion is always fixed as a scalar, say 1, one can also generalize these results to expressions with a gluon fixed as the

first element instead, following a similar discussion. For example, if we fix gluon p as the one next to the loop momentum ℓ , we simply replace $X_i(\ell; 1, \alpha)$ ($i = p, q, r$) by $X_i(\ell; p, \alpha)$ in (7.18), (7.42) or (7.45), without changing the definition of X .

- (ii) For YMS integrands involving two or three gluons but no external scalar, momentum conservation and the on-shell condition result in a vanishing denominator in the $\epsilon \cdot \epsilon$ terms of (7.42) or (7.45). However, this singularity is divided out when we consider the full integrand, and the final result is nonsingular.

Taking into account the subtleties discussed above, and plugging the results of Secs. VII A, VII B, and VII C back, we see that the pure YM numerators at 2- and 3-point are given by

$$\begin{aligned} N^{\text{YM}}(\ell; 1, 2) &= (D-2) \left[(\epsilon_1)_\mu (\epsilon_2)_\nu - \frac{\epsilon_1 \cdot \epsilon_2}{k_1 \cdot k_2} (k_1)_\mu (k_2)_\nu \right] \ell^\mu (\ell + k_1)^\nu + \text{Tr}[F_1 \cdot F_2], \\ N^{\text{YM}}(\ell; 1, 2, 3) &= (D-2) \left[(\epsilon_1)_\mu (\epsilon_2)_\nu (\epsilon_3)_\tau - \frac{\epsilon_1 \cdot \epsilon_2}{k_1 \cdot k_2} (k_1)_\mu (k_2)_\nu (\epsilon_3)_\tau - \frac{\epsilon_1 \cdot \epsilon_3}{k_1 \cdot k_3} (k_1)_\mu (\epsilon_2)_\nu (k_3)_\tau - \frac{\epsilon_2 \cdot \epsilon_3}{k_2 \cdot k_3} (\epsilon_1)_\mu (k_2)_\nu (k_3)_\tau \right] \\ &\quad \times \ell^\mu (\ell + k_1)^\nu (\ell + k_1 + k_2)^\tau + \text{Tr}[F_2 \cdot F_3] \epsilon_1 \cdot \ell + \text{Tr}[F_1 \cdot F_3] \epsilon_2 \cdot (\ell + k_1) \\ &\quad + \text{Tr}[F_1 \cdot F_2] \epsilon_3 \cdot (\ell + k_1 + k_2) - \text{Tr}[F_1 \cdot F_2 \cdot F_3] \epsilon_1 \cdot \ell \epsilon_2 \cdot (\ell + k_1) \epsilon_3 \cdot (\ell + k_1 + k_2). \end{aligned} \quad (7.46)$$

VIII. WELDING YMS FORWARD LIMIT TREE NUMERATORS

Having seen that the YMS numerators at one loop can be calculated directly using the method explained in the previous section, the next natural question then is whether this result is identical to the welded forward limit tree numerators. Namely, suppose if we instead use tree level techniques to solve for half-ladder numerators from YMS tree amplitudes, then take the forward limit on these half-ladders, would the n -gon basis numerators calculated in the previous section be identical to the forward limit half-ladder with both sides welded?

Note especially that the numerator solutions are known to be nonunique at tree level, so that even when given a theory such as NLSM or self-dual Yang-Mills with built-in kinematic algebra structure and therefore inherited a natural numerator solution expressible as products of structure constants, one can still write down other equivalent

numerator solutions by deliberately applying generalized gauge shifts. The resulting sets of kinematic numerator yield exactly the same tree amplitudes and are therefore also legitimate numerator solutions. On the other hand, we saw in the derivation in Sec. II that the propagator matrix at one loop level are generically full-rank, so that given an integrand, the numerator the solution at one loop is unique. Additionally, we argued in Sec. III that the forward limit tree numerator solution, when both sides are welded, gives exactly this unique numerator solution at one loop if they satisfy the consistency conditions that arise from the nomenclature (3.3). For the YMS case actually one sees readily that the numerator solution at tree level based on graphical rules of [38] indeed satisfy these conditions, and therefore corresponds to this unique numerator solution at one loop.

Recall at tree level, the YMS amplitude and the propagator matrix (equivalently, the doubly color-ordered biadjoint scalar amplitudes) are related by the following.

$$A_{\text{tree}}^{\text{YMS}}(1, \dots, r || \mathbf{G} | \rho) = \sum_{\alpha \in \{2, \dots, r-1\} \sqcup \text{perms } \mathbf{G}} C(1, \alpha) A_{\text{tree}}^{\text{BS}}(1, \alpha, r | \rho), \quad (8.1)$$

where $1, \dots, r$ and $\mathbf{G}$ denote the scalar and gluon legs, respectively. The expansion coefficients, for the one, two, and three gluon cases are given by

$$\begin{aligned} C(1, \alpha) &\equiv \epsilon_p \cdot X_p(1, \alpha), & \text{if } \mathbf{G} = \{p\} \\ C(1, \alpha) &\equiv \left[(\epsilon_p)_\mu (\epsilon_q)_\nu - \frac{\epsilon_p \cdot \epsilon_q}{k_p \cdot k_q} (k_p)_\mu (k_q)_\nu \right] X_p^\mu(1, \alpha) X_q^\nu(1, \alpha), & \text{if } \mathbf{G} = \{p, q\} \\ C(1, \alpha) &\equiv \left[(\epsilon_p)_\mu (\epsilon_q)_\nu (\epsilon_s)_\tau - \frac{\epsilon_p \cdot \epsilon_q}{k_p \cdot k_q} (k_p)_\mu (k_q)_\nu (\epsilon_s)_\tau - \frac{\epsilon_p \cdot \epsilon_s}{k_p \cdot k_s} (k_p)_\mu (\epsilon_q)_\nu (k_s)_\tau \right. \\ &\quad \left. - \frac{\epsilon_q \cdot \epsilon_s}{k_q \cdot k_s} (\epsilon_p)_\mu (k_q)_\nu (k_s)_\tau \right] X_p^\mu(1, \alpha) X_q^\nu(1, \alpha) X_s^\tau(1, \alpha), & \text{if } \mathbf{G} = \{p, q, s\}. \end{aligned} \quad (8.2)$$

Take the two-scalar-one-gluon scattering event as an example, and let k_1, k_2 be the momenta carried by the scalar and k_3 by the gluon respectively. In view of (3.2), the color-ordered integrand $\mathcal{I}_2(\ell, k_1^s, k_2^s, k_3^g)$ is given by

$$\begin{aligned} \mathcal{I}_2(\ell, k_1^s, k_2^s) &= \frac{1}{\ell^2} A_{\text{Feyn}}^{\text{tree}}(\ell, 1^s, 2^s, 3^g, -\ell) + \frac{1}{(\ell + k_1)^2} A_{\text{Feyn}}^{\text{tree}}(\ell + k_1, 2^s, 3^g, 1^s, -(\ell + k_1)) \\ &\quad + \frac{1}{(\ell + k_1 + k_2)^2} A_{\text{Feyn}}^{\text{tree}}(\ell + k_1 + k_2, 3^g, 1^s, 2^s, -(\ell + k_1 + k_2)) \end{aligned} \quad (8.3)$$

Restoring the color factor carried by the scalars on both sides of the Eq. (8.1), and we read off the forward limit tree numerators. For $A_{\text{Feyn}}^{\text{tree}}(\ell, 1^s, 2^s, 3^g, -\ell)$, we have the following half-ladder.

$$N^{\text{tree}}(\ell, 1^s, 2^s, 3^g, -\ell) = \sum_{e_1, e_2} C(1, \alpha) f^{e_1, 1, e_2} f^{e_2, 2, e_1} \quad (8.4)$$

$$= \epsilon_3 \cdot (\ell + k_1 + k_2) \sum_{e_1, e_2} f^{e_1, 1, e_2} f^{e_2, 2, e_1} \quad (8.5)$$

The kinematic part of the numerator $C(1, \alpha) = \epsilon_3 \cdot X$ contains a sum over momenta lying on one side of the gluon line, which in this case includes the loop scalar ℓ , and two external scalar lines k_1, k_2 . On the other hand, for $A_{\text{Feyn}}^{\text{tree}}(\ell + k_1, 2^s, 3^g, 1^s, -(\ell + k_1))$ we have

$$N^{\text{tree}}(\ell + k_1, 2^s, 3^g, 1^s, -(\ell + k_1)) = \epsilon_3 \cdot ((\ell + k_1) + k_2) \sum_{e_1, e_2} f^{e_1, 1, e_2} f^{e_2, 2, e_1} \quad (8.6)$$

The kinematic part of the numerator this time includes only two lines: The loop scalar, now carrying momenta $\ell + k_1$, and a scalar, carrying k_2 . The momentum sum is identical to that in (8.5), and we see that

$$N^{\text{tree}}(\ell, 1^s, 2^s, 3^g, -\ell) = N^{\text{tree}}(\ell + k_1, 2^s, 3^g, 1^s, -(\ell + k_1)) \quad (8.7)$$

as required. Similarly for the numerator $N^{\text{tree}}(\ell + k_1 + k_2, 3^g, 1^s, 2^s, -(\ell + k_1 + k_2))$, and others related by permutations of the external legs.

It is straightforward to see the above example generalizes to cases with a single gluon and an arbitrary number of scalars. At n -point the basis numerators are n -gons, with the color part of the numerator given by a product of $(n - 1)$ structure constants $f^{*\sigma(1)*} f^{*\sigma(2)*} \dots f^{*\sigma(n)*}$ which depends only on the cyclic ordering of the scalar legs, so that the welded tree numerators $N^{\text{tree}}(\ell, \sigma(1), \sigma(2), \dots, \sigma(n), -\ell)$, $N^{\text{tree}}(\ell + k_{\sigma(1)}, \sigma(2), \dots, \sigma(n), \sigma(1), -(\ell + k_{\sigma(1)}))$, $\dots$, $N^{\text{tree}}(\ell + k_{\sigma(1)} + \dots + k_{\sigma(n-1)}, \sigma(n), \sigma(1), \dots, \sigma(n-1), -(\ell k_{\sigma(1)} + \dots + k_{\sigma(n-1)}))$ all carry this common (loop independent) factor. The kinematic part of the tree numerator $\epsilon_g \cdot X_g := \epsilon_g \cdot \sum_{\text{all momenta on the left}} k_i$ is given by a sum of all momenta lying on one side of the gluon. Tree numerators $N^{\text{tree}}(\ell, \sigma(1), \sigma(2), \dots, \sigma(n), -\ell)$, $N^{\text{tree}}(\ell + k_{\sigma(1)}, \sigma(2), \dots, \sigma(n), \sigma(1), -(\ell + k_{\sigma(1)}))$, $\dots$, $N^{\text{tree}}(\ell + k_{\sigma(1)} + \dots + k_{\sigma(n-1)}, \sigma(n), \sigma(1), \dots, \sigma(n-1), -(\ell k_{\sigma(1)} + \dots + k_{\sigma(n-1)}))$ have different set of scalar legs lying on the left of the gluon line, however the ℓ appears in each tree numerator is shifted accordingly to compensate

the missing scalar leg momenta, so that the sums all yield the same result, and the welded tree numerators therefore all agree with each other, fulfilling the consistency requirement (3.3). For cases involving two or three gluons and arbitrary number of scalars, one sees that the welded forward limit tree numerators also satisfy the consistency requirement (3.3) and are therefore identical to the unique numerator solution at one loop. The verification follows more or less the same calculations, as they also expressible in terms of the factor $X_g := \sum_{\text{all momenta on the left of } g} k_i$. Equivalently, one can also check the welded tree numerators are in these cases identical to the n -gon numerator formulas (7.26), (7.42), and (7.45) calculated in the previous section.

IX. A BRIEF REMARK ON GRAVITY AND EYM NUMERATORS AT ONE LOOP

In this section we briefly remark on the gravity and Einstein-Yang-Mills (EYM) numerators. A first observation is that tree level EYM amplitudes satisfy the same expansion formula with the YMS ones.

$$A_{\text{tree}}^{\text{EYM}}(1, \dots, r || \mathbf{H}) = \sum_{\alpha \in \{2, \dots, r-1\} \sqcup \text{perms } \mathbf{H}} C(1, \alpha) A_{\text{tree}}^{\text{YM}}(1, \alpha, r), \quad (9.1)$$

where the $1, \dots, r$ denotes gluons, while $\mathbf{H}$ is the graviton set. The coefficients $C(1, \alpha)$ have the same form with those in (8.2) but the polarizations therein are now half gravitons. This can be straightforwardly proved using either BCJ relations or CHY formula.

When combining the tree-level expansion formula (9.1) with the forward limit expressed one loop EYM integrand, as stated by the world sheet approach ([24, 27, 29, 31]), we get

$$\begin{aligned} \mathcal{I}^{\text{EYM}}(\ell; 1, \dots, r || \mathbf{H}) &= \sum_{\rho \in \text{perms}(\{1, \dots, r\} \cup \mathbf{H})} \sum_{\sigma \in \{1, \dots, r\} \sqcup \text{perms } \mathbf{H}} \frac{1}{(\ell - k_{\sigma_L})^2} C(+, \sigma, -) \times A^{\text{YM}}(+, \sigma, -) + \text{cyc}(1, \dots, r) \\ &= \sum_{\rho \in \text{perms}(\{1, \dots, r\} \cup \mathbf{H})} \sum_{\sigma \in \{1, \dots, r\} \sqcup \text{perms } \mathbf{H}} \frac{1}{(\ell - k_{\sigma_L})^2} C(+, \sigma, -) \\ &\quad \times A^{\text{BS}}(+, \sigma, - | +, \rho, -) \tilde{N}(+, \rho, -) + \text{cyc}(1, \dots, r), \end{aligned} \quad (9.2)$$

where the YM tree amplitudes with forward limit is further expanded in terms of BS ones, by using the numerators $\tilde{N}(+, \boldsymbol{\rho}, -)$ satisfying the consistency condition. A technical treatment [62,69] is the following. When expanding the $A^{\text{BS}}(+, \boldsymbol{\sigma}, -|+, \boldsymbol{\rho}, -)$ in terms of Feynman graphs which have the form that tree level BS currents are planted at the loop propagator line between $\pm$, one can always find other related terms in the summations over $\boldsymbol{\rho}$, $\boldsymbol{\sigma}$ and the cyclic orderings of external gluons, so that these terms are

related to each other by a cyclic permutation of the BS currents. When all these terms are collected together and the consistency conditions of both $C(+, \boldsymbol{\sigma}, -)$ and $\tilde{N}(+, \boldsymbol{\rho}, -)$ are taken into account, the Feynman graphs related by cyclic permutations of BS currents produce one loop Feynman graphs of BS integrand, with quadratic propagators and coefficients $C(+, \boldsymbol{\sigma}, -)$ and $\tilde{N}(+, \boldsymbol{\rho}, -)$. Therefore, we arrive at the expansion formula of EYM integrand

$$\begin{aligned} \mathcal{I}^{\text{EYM}}(\ell; 1, \dots, r || \mathbf{H}) &= \sum_{\sigma \in \{1, \dots, r\} \sqcup \text{perms } \mathbf{H}} C(\ell; 1, \boldsymbol{\sigma}) \left[\frac{1}{(\ell - k_{\sigma_L})^2} \sum_{\rho \in \text{perms}(\{1, \dots, r\} \cup \mathbf{H})} \mathcal{I}^{\text{BS}}(\ell; 1, \boldsymbol{\sigma} | \boldsymbol{\rho}) \tilde{N}(\ell'; 1, \boldsymbol{\rho}) \right] \\ &= \sum_{\sigma \in \{1, \dots, r\} \sqcup \text{perms } \mathbf{H}} C(\ell; 1, \boldsymbol{\sigma}) \mathcal{I}^{\text{YM}}(\ell; 1, \boldsymbol{\sigma}), \end{aligned} \quad (9.3)$$

where the coefficients $C(\ell; 1, \boldsymbol{\sigma})$ were given by (7.18), (7.42), and (7.45) corresponding to the 1, 2, and 3 graviton cases. The loop momentum ℓ' in the right numerator $\tilde{N}(\ell'; 1, \boldsymbol{\rho})$ is understood as follows. If the subcurrent containing scalar 1 in a diagram of $\mathcal{I}^{\text{BS}}$ have the form $\phi_{\sigma_A 1 \sigma_B | \rho_A 1 \rho_B}$, $\ell' \equiv l - k_{\rho_A} + k_{\rho_B}$. More detail can be

found in the paper [71] by two of the authors of the current work.

For gravity integrand¹³ there is an analog to the expansion formula (5.1) that expands the gravity integrand in terms of EYM integrands with fewer graviton external lines ([24,27,29,31,34,69]),

$$\mathcal{I}^{\text{GR}} \cong (D-2) \mathcal{I}^{\text{EYM}}(\emptyset || \mathbf{H}) + \sum_{l=2}^n (-1)^l \sum_{(j_1 \dots j_l) \in S_i \setminus Z_i} \text{Tr}[F_{j_1} \cdot \dots \cdot F_{j_l}] \mathcal{I}^{\text{EYM}}(j_1, \dots, j_l || \mathbf{H} \setminus \{j_1, \dots, j_l\}). \quad (9.4)$$

This relation, together with the formula (9.3) will result in an expansion formula for GR integrands

$$\mathcal{I}^{\text{GR}} = \sum_{\sigma \in S_{n-1}} n_{\ell; 1, \boldsymbol{\sigma}} \mathcal{I}^{\text{YM}}(\ell; 1, \boldsymbol{\sigma}). \quad (9.5)$$

We emphasize that the discussions in this section are based on Eq. (9.2), which is derived from the world sheet approach. Establishing Eq. (9.2) purely within a field-theoretic framework, in particular by starting directly from the EYM and YM Feynman rules, appears to be highly nontrivial. Indeed, experience from the scattering amplitude literature indicates that demonstrating double copy relations directly at the level of Feynman integrands is often technically challenging.¹⁴

Alternatively, the reasoning presented here can be understood in the following conditional sense. Assuming the field theory double copy relation between EYM and YM observed at tree level [35,56] generalizes to one loop (for

example at 2-point we have Eq. (4.4) and similarly at higher points), the argument of Sec. IV allows one to write the EYM integrand in the form of the one-loop generalized DDM representation (4.7). This representation can then be recast into Eq. (9.2) by applying the partial-fraction decomposition described in Sec. III, see Eq. (3.2). The calculation presented in this section then proceeds from Eq. (9.2).

X. CONCLUSION

In this work we have analyzed the algebraic consistency conditions underlying the construction of one-loop kinematic numerators, clarified their relation to welded forward-limit tree numerators, and provided explicit solutions for Yang-Mills-scalar theory up to three gluons. Our findings highlight several conceptual features of color-kinematics duality at one loop that are absent at tree level.

At tree level, BCJ numerators are defined only up to the kernel of propagator matrices. Consequently, many inequivalent sets of half-ladder numerators lead to the same physical amplitude. At one loop, however, the situation is markedly different: the nomenclature consistency conditions identify all n -gon representations of the same loop graph—that is, all expressions related by cyclic

¹³By gravity here we mean the Einstein-Hilbert gravity coupled to B fields and dilaton.

¹⁴One possible way to do this is to adapt the argument used in [72–74] to the EYM case.

relabeling of external legs and corresponding loop-momentum shifts—as describing a single physical object. The resulting quotient removes the redundancy associated with different “pictures” of the same polygon diagram, and the effective propagator matrix derived from this quotient is generically of full rank. As a result, a color-ordered integrand fixes a *unique* numerator assignment (up to integrand-level shift symmetries). This gives a natural projection map from any set of tree-level numerators—with their usual gauge freedom—onto the unique one-loop solution compatible with the nomenclature consistency condition. Our analysis of welded forward-limit numerators confirms that, whenever the physical conditions discussed in Sec. III are satisfied, this projection coincides with welding the tree numerators and identifying the two parallel legs. The same analysis can be extended to Einstein–Yang–Mills theory, whose mixed gluon-graviton integrands follow the same algebraic pattern once the loop-momentum dependence of both sectors is taken into account.

The situation is more subtle for gravitylike theories such as Einstein–Yang–Mills and gravity. The discussion in Sec. IX suggests that, once both copies of the integrand carry loop-momentum dependence, consistent double-copy constructions may require *additional* physical conditions. In particular, the naive expectation that the KLT kernel provides a loop-level inverse to the propagator matrix is obstructed: ordering the gravity integrand via the forward-limit decomposition necessarily introduces either misaligned loop momenta between the two Yang–Mills copies or a difference term of the form $\Delta_\ell = f(\ell) - f(\ell + c)$. This misalignment indicates that the standard KLT and double-copy prescriptions cannot both be simultaneously realized in a loop-momentum-local form, and the resolution may again lie in additional physical constraints on the loop integrands.

Beyond these structural observations, our explicit results for YMS and EYM theories demonstrate that the simple tree-level building blocks, organized by generalized momentum-sum symbols X^μ , extend naturally to one loop. The n -gon decomposition

$$\mathcal{I}_n^{\text{YMS}}(\ell, 1, \dots, n) = \sum_{\sigma \in S_{n-1}} N(\ell; 1, \sigma) \tilde{M}(1\sigma|12 \dots n),$$

together with the quotient over cyclic relabelings and

loop-momentum shifts, provides a constructive framework from which numerators can be extracted directly without requiring inversion of large propagator matrices. Our one-, two-, and three-gluon results confirm that the one-loop kinematic coefficients follow the same algebraic pattern as at tree level, once the appropriate generalized X^μ are used. This strongly suggests that the higher-point YMS numerators admit similarly compact and symmetry-transparent expressions.

Looking forward, several interesting directions remain open. It would be valuable to extend the explicit YMS numerator formulas to higher points, and to explore whether the same organizational principles extend further to gravity amplitudes and to higher loops. Clarifying the precise physical requirements for a fully consistent loop-level double copy—and resolving the apparent incompatibility between KLT relations and double-copy constructions—would shed further light on the analytic structure of gravity integrands. We expect that the structural perspective developed in this work, based on nomenclature consistency and forward-limit factorization, will provide a useful foundation for these developments.

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DATA AVAILABILITY

No data were created or analyzed in this study.

APPENDIX A: NONLINEAR SIGMA MODEL NUMERATORS

In this appendix we perform a simple consistency check on the NLSM numerators. It was shown in [75] that the tree level numerators of NLSM can be efficiently expressed as momentum kernel $N_{\text{NLSM}}^{\text{tree}}(123 \dots n) = S_1[23 \dots n - 1|23 \dots n - 1]$. The corresponding forward limit numerator is therefore

$$\begin{aligned} N(\ell, 1, 2, 3, \dots, n, -\ell) &= S_\ell[123 \dots n|123 \dots n] \\ &= (\ell \cdot k_1)((\ell + k_1) \cdot k_2)((\ell + k_1 + k_2) \cdot k_3) \dots ((\ell + k_1 + k_2 \dots + k_{n-1}) \cdot k_n) \end{aligned} \quad (\text{A1})$$

At n -point, consistency requires that the above numerator should be invariant under the following symmetry transformation.

$$\begin{aligned}
 \ell &\rightarrow \ell + k_1 \\
 k_1 &\rightarrow k_2 \\
 &\vdots \\
 k_n &\rightarrow k_1
 \end{aligned} \tag{A2}$$

Equation (A1) is manifestly invariant because each factor becomes the next one under such relabeling.

$$\begin{aligned}
 \ell \cdot k_1 &\rightarrow (\ell + k_1) \cdot k_2 \\
 (\ell + k_1) \cdot k_2 &\rightarrow (\ell + k_1 + k_2) \cdot k_3 \\
 &\vdots \\
 (\ell + k_1 + k_2 \dots + k_{n-1}) \cdot k_n &\rightarrow \ell \cdot k_1
 \end{aligned} \tag{A3}$$

where the last line above is guaranteed by momentum conservation.

APPENDIX B: 3-POINT INTEGRAND NUMERATOR RELATION

At 3-point we have two independent numerators (2.7) and (2.8), and the integrand is assumed to have the following graphical decomposition.

$$\begin{aligned}
 \mathcal{I}_3(\ell, 1, 2, 3) &= \text{Diagram 1} + \text{Diagram 2} + \text{Diagram 3} + \text{Diagram 4} \\
 &= \frac{N(\ell, 123, -\ell)}{D_\ell D_{\ell 1} D_{\ell 12}} + \frac{N(\ell, 123, -\ell) - N(\ell, 132, -\ell)}{D_\ell D_{\ell 1} s_{23}} \\
 &\quad + \frac{N(\ell + k_1, 231, -(\ell + k_1)) - N(\ell + k_1, 213, -(\ell + k_1))}{D_{\ell 1} D_{\ell 12} s_{13}} \\
 &\quad + \frac{N(\ell, 123, -\ell) - N(\ell, 213, -\ell)}{D_\ell D_{\ell 12} s_{12}}
 \end{aligned} \tag{B1}$$

where we introduced the notation $D_{\ell,a,b,\dots,c} = (\ell + k_a + k_b + \dots + k_c)^2$ frequently employed in loop amplitude calculations to denote the propagator involving ℓ squared. Adding difference terms as in (2.2) effectively shifts loop momenta. In the current example this allows us to write

$$\begin{aligned}
 \tilde{\mathcal{I}}_3(\ell, 123) &= \left(\frac{1}{D_\ell D_{\ell 1} D_{\ell 12}} + \frac{1}{D_\ell D_{\ell 1} s_{23}} + \frac{1}{D_{\ell 1} D_{\ell 12} s_{13}} + \frac{1}{D_\ell D_{\ell 12} s_{12}} \right) N(\ell, 123, -\ell) \\
 &\quad + \left(\frac{-1}{D_\ell D_{\ell 1} s_{23}} + \frac{-1}{D_\ell D_{\ell 13} s_{13}} + \frac{-1}{D_{\ell 1} D_{\ell 13} s_{12}} \right) N(\ell, 132, -\ell),
 \end{aligned} \tag{B2}$$

where again we use $\tilde{\mathcal{I}}_3$ to indicate that it is an effective integrand, related to the original one by terms that vanish after the integration. Cyclic symmetry suggests that there are only two independent color-ordered integrands. The other integrand can be rewritten following the same reasoning, which together leads to a 2×2 matrix equation between the color-ordered integrands and the master numerators, now with their loop momentum aligned to ℓ .

$$\begin{bmatrix} \tilde{\mathcal{I}}_3(\ell, 123) \\ \tilde{\mathcal{I}}_3(\ell, 132) \end{bmatrix} = \begin{bmatrix} \tilde{M}(23|23) & \tilde{M}(23|32) \\ \tilde{M}(32|23) & \tilde{M}(32|32) \end{bmatrix} \begin{bmatrix} N(\ell, 123, -\ell) \\ N(\ell, 132, -\ell) \end{bmatrix}. \tag{B3}$$

The one loop generalization of the propagator matrix is given by the same formula obtained in the context of CHY in [76].

$$\tilde{M} = \begin{bmatrix} \frac{1}{D_\ell D_{\ell 1} D_{\ell 12}} + \frac{1}{D_\ell D_{\ell 1} s_{23}} + \frac{1}{D_{\ell 1} D_{\ell 12} s_{13}} + \frac{1}{D_\ell D_{\ell 12} s_{12}} & \frac{-1}{D_\ell D_{\ell 1} s_{23}} + \frac{-1}{D_\ell D_{\ell 13} s_{13}} + \frac{-1}{D_{\ell 1} D_{\ell 13} s_{12}} \\ \frac{-1}{D_\ell D_{\ell 1} s_{23}} + \frac{-1}{D_\ell D_{\ell 12} s_{12}} + \frac{-1}{D_{\ell 1} D_{\ell 12} s_{13}} & \frac{1}{D_\ell D_{\ell 1} D_{\ell 13}} + \frac{1}{D_\ell D_{\ell 1} s_{23}} + \frac{1}{D_{\ell 1} D_{\ell 13} s_{12}} + \frac{1}{D_\ell D_{\ell 13} s_{13}} \end{bmatrix}. \quad (\text{B4})$$

APPENDIX C: TADPOLE CANCELLATION

In this appendix we briefly show that tadpole numerators do not contribute to the one loop amplitude after integration. Similar arguments were presented in [24,63]. However, we would like to show that tadpoles also drop out specifically for the settings used in this paper. Note the tadpole term in the tree amplitude $A_{\text{BCJ}}^{\text{tree}}(\ell, 1, 2, 3, \dots, n, -\ell)$ is the following.

$$A_{\text{BCJ}}^{\text{tree}}(\ell, 1, 2, 3, \dots, n, -\ell) \sim \text{Diagram} \quad (\text{C1})$$

Therefore if we pick out only the tadpoles in (3.1), up to shiftings which do not contribute to the integral, this is

$$\mathcal{I}_n(\ell, 1, 2, \dots, n) \quad (\text{C2})$$

$$\begin{aligned} & \sim \frac{1}{\ell^2} \tilde{A}_{\text{BCJ}}^{\text{tree}}(\ell, 1, 2, 3, \dots, n, -\ell) + \frac{1}{\ell^2} A_{\text{BCJ}}^{\text{tree}}(\ell, 2, 3, \dots, n, 1, -\ell) + \dots \\ & + \frac{1}{\ell^2} A_{\text{BCJ}}^{\text{tree}}(\ell, n, 1, 2, \dots, n-1, -\ell) \\ & \sim \text{Diagram 1} + \text{Diagram 2} + \dots + \text{Diagram } n-1 \end{aligned} \quad (\text{C3})$$

We would like to emphasize the above is a sum of numerators, which are regarded as yet-determined variables whose analytic behavior are to a large extent unknown. However this sum still vanishes because $U(1)$ -decoupling identity requires only the knowledge of antisymmetry of the cubic structure, and this is an assumed property of the BCJ numerators.

APPENDIX D: BERENDS-GIELE CURRENTS OF BS

The Berends-Giele current $\phi_{A|\tilde{A}}$, where A and $\tilde{A}$ are ordered sets with the same number of elements, is defined as follows ([77]):

$$\phi_{A|\tilde{A}} = \frac{1}{s_A} \sum_{\substack{A \rightarrow A_L, A_R \\ \tilde{A} \rightarrow \tilde{A}_L, \tilde{A}_R}} \left[\phi_{A_L|\tilde{A}_L} \phi_{A_R|\tilde{A}_R} - \phi_{A_R|\tilde{A}_L} \phi_{A_L|\tilde{A}_R} \right], \quad (\text{D1})$$

where $s_A \equiv k_A^2$, k_A^μ denotes the total momentum of elements in A . We summed over divisions $A \rightarrow A_L, A_R$, $\tilde{A} \rightarrow \tilde{A}_L, \tilde{A}_R$ in (D1) so that in the first term $|A_L| = |\tilde{A}_L|$, $|A_R| = |\tilde{A}_R|$, or in the second term $|A_R| = |\tilde{A}_L|$, $|A_L| = |\tilde{A}_R|$. The starting point of this definition is $\phi_{a|a} = 1$, $\phi_{a|b} = 0$ ($a \neq b$). A significant property of the BS current (D1) is the generalized

$U(1)$ -decoupling identity (7.23). Another property is the off-shell BCJ relation, see [40,78–80]. The off-shell BCJ relation is the key technique for deriving (7.32) and (7.33), see [62,69].

APPENDIX E: THE KINEMATIC COEFFICIENT FOR A GIVEN SUBSET IN A CYCLIC DIVISION

As shown in [62], a YMS integrand $\mathcal{I}^{\text{YMS}}(l; 1, \sigma || \mathbf{G} | \rho)$ can be expressed as a summation over independent cyclic partitions of external particles (scalars and gluons) $\{1, \sigma \sqcup \text{perms } \mathbf{G}\} \rightarrow \{A_1, A_2, \dots, A_I\}$, so that the relative cyclic ordering of scalars $\{1, \sigma\}$ is preserved. The concrete expression relies on the so-called *reference order* of elements in the gluon set $\mathbf{G}$. Each subset A_i is associated with a substructure which involves effective currents attached to the loop via a proper vertex. When decomposed in terms of BS currents, an effective subcurrent is further

expressed as a summation over permutations of elements in A_i , each permutation is accompanied by a kinematic coefficient. According to different particle types in A_i , the possible permutations, the coefficients (with up to two gluons) and the corresponding BS subcurrents are presented as follows:

- (i) If A_i contains only scalars in order $\{x_1, \dots, x_j\}$, the coefficient, permutation and BS currents are respectively presented as

$$C(\alpha_i) = 1, \quad \alpha_i = \{x_1, \dots, x_j\}, \phi_{\alpha_i|\rho_i}, \quad (\text{E1})$$

where ρ_i denotes the right permutation for this subcurrent.

- (ii) If A_i contains both scalars in order $\{x_1, \dots, x_j\}$ and elements in the gluon set $\mathbf{G}_i$ ($\mathbf{G}_i = \{p\}, \{q\}$ or $\{p, q\}$), we have

$$\begin{aligned} \text{For } \mathbf{G}_i = \{p\}(\text{or } \{q\}), \quad C(\alpha_i) &= \epsilon_{p(\text{or } q)} \cdot X_{p(\text{or } q)}(\alpha_i), \quad \alpha_i \in \{x_1, \{x_2, \dots, x_j\} \sqcup \{p\}(\text{or } \{q\})\}, \quad \phi_{\alpha_i|\rho_i}, \\ \text{For } \mathbf{G}_i = \{p, q\}, \quad C^{(0)}(\alpha_i) &= \epsilon_p \cdot X_p(\alpha_i) \epsilon_q \cdot X_q(\alpha_i), \quad \alpha_i \in \{x_1, \{x_2, \dots, x_j\} \sqcup \{p\} \sqcup \{q\}\}, \quad \phi_{\alpha_i|\rho_i}, \\ C^{(1)}(\alpha_i) &= (\epsilon_p \cdot \epsilon_q)(-k_p \cdot X_p(\alpha_i)), \quad \alpha_i \in \{x_1, \{x_2, \dots, x_j\} \sqcup \{p, q\}\}, \quad \phi_{\alpha_i|\rho_i}, \end{aligned} \quad (\text{E2})$$

where $C^{(0)}$ and $C^{(1)}$ respectively denote the $(\epsilon_p \cdot \epsilon_q)^0$ and the $(\epsilon_p \cdot \epsilon_q)^1$ sectors.

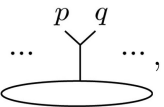
- (iii) If A_i contains one or two gluons but no scalar, the coefficients, permutations and corresponding BS subcurrents are given by

$$\text{For } \mathbf{G}_i = \{p\}(\text{or } \{q\}), \quad C(p(\text{or } q)) = \epsilon_{p(\text{or } q)} \cdot \ell_i, \quad \alpha_i = \{p\}(\text{or } \{q\}), \quad \phi_{\alpha_i|\rho_i} \quad (\text{E3})$$

$$\text{For } \mathbf{G}_i = \{p, q\}, \quad C^{(0)}(\alpha_i) = \begin{cases} \epsilon_p \cdot \ell_i \epsilon_q \cdot k_p, & \alpha_i = \{p, q\} \\ \epsilon_q \cdot \ell_i \epsilon_p \cdot k_q, & \alpha_i = \{q, p\} \end{cases}, \quad \phi_{\alpha_i|\rho_i} \quad (\text{E4})$$

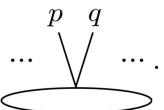
$$C^{(1)}(\alpha_i) = \begin{cases} (-k_p \cdot \ell_i)(\epsilon_p \cdot \epsilon_q), & \alpha_i = \{p, q\}, \quad \phi_{\alpha_i|\rho_i} \\ (-\frac{1}{2})\epsilon_p \cdot \epsilon_q, & \alpha_i = \{p - q\}, \quad \phi_{p|a} \phi_{q|b} \end{cases}, \quad (\text{E5})$$

In the case of $\mathbf{G}_i = \{p, q\}$, the $C^{(1)}$ has nonvanishing expression only when p appears to the left of q , due to our choice of reference order $p < q$. The total contribution of $(\epsilon_p \cdot \epsilon_q)^1$ is the sum of the $C^{(1)}(p, q)$ which reflects a substructure with a subcurrent $\phi_{\alpha_i|\rho_i}$ attached to the loop



$$(\text{E6})$$

and $C^{(1)}(p - q)$ which reflects the substructure with p, q , attached to the loop via a four-point vertex structure



$$(\text{E7})$$

APPENDIX F: UNDERSTANDING THE TREE-LEVEL EXPANSIONS FORMULAS (8.1)

According to the tree-level recursive expansion formula [36], when single-trace YMS (or EYM) amplitude with only one gluon (or graviton) p is expanded in terms of BS (or YM) amplitudes, the expansion coefficients have the form $\epsilon_p \cdot X_p$ which agree with (8.2).

For YMS (or EYM) amplitude with two gluons (or two gravitons) p, q , we apply the recursive expansion

relation [36] to express the full YMS (or EYM) amplitude in terms of BS or YM amplitudes with the reference order $p < q$. The resulted coefficients can be written as

$$C(1, \alpha) = C^{(0)}(1, \alpha) + C^{(1)}(1, \alpha), \quad (F1)$$

where the two terms corresponding to the $(\epsilon_p \cdot \epsilon_q)^0$ and $(\epsilon_p \cdot \epsilon_q)^1$ are given by

$$C^{(0)}(1, \alpha) = \epsilon_p \cdot X_p(1, \alpha) \epsilon_q \cdot X_q(1, \alpha)$$

$$C^{(1)}(1, \alpha) = \begin{cases} (-k_p \cdot X_p(1, \alpha))(\epsilon_p \cdot \epsilon_q), & \alpha \in \{2, \dots, r-1\} \sqcup \{p, q\} \\ 0, & \alpha \in \{2, \dots, r-1\} \sqcup \{q, p\} \end{cases}. \quad (F2)$$

To redefine the coefficients, we introduce the following combination of amplitudes

$$0 = \left(-\frac{\epsilon_p \cdot \epsilon_q}{k_p \cdot k_q} \right) \sum_{\alpha \in \{2, \dots, r-1\} \sqcup \{p\} \sqcup \{q\}} k_q \cdot Y_q(1, \alpha) k_p \cdot X_p(1, \alpha) A^{\text{BS}}(1, \alpha, r|\rho),$$

(or $A^{\text{BS}}(1, \alpha, r|\rho) \rightarrow A^{\text{YM}}(1, \alpha, r)$ for EYM).

(F3)

where $Y_q^\mu(1, \alpha)$ denotes the total momentum of scalars (or gluons) between 1 and q (including 1) for YMS (or EYM). The rhs vanishes due to the fundamental BCJ relation for p . When this vanishing term is added to the expansion relation (8.1) with coefficients (F1), (F2), the coefficient for a given permutation agrees with that in (8.2).

For tree-level YMS amplitude $A_{\text{tree}}^{\text{YMS}}(1, \dots, r|\mathbf{G}|\rho)$ with three gluons p, q, s , the expansion coefficients are given as

$$C(1, \alpha) = C^{(0)}(1, \alpha) + C_{\epsilon_p \cdot \epsilon_q}^{(1)}(1, \alpha) + C_{\epsilon_p \cdot \epsilon_s}^{(1)}(1, \alpha) + C_{\epsilon_q \cdot \epsilon_s}^{(1)}(1, \alpha), \quad (F4)$$

where $C^{(0)}(1, \alpha)$ denotes the coefficient with no $\epsilon \cdot \epsilon$, while $C_{\epsilon_p \cdot \epsilon_q}^{(1)}$, $C_{\epsilon_p \cdot \epsilon_s}^{(1)}$, $C_{\epsilon_q \cdot \epsilon_s}^{(1)}$ denote the coefficient with a factor $\epsilon_p \cdot \epsilon_q$, $\epsilon_p \cdot \epsilon_s$, $\epsilon_q \cdot \epsilon_s$, respectively. If we choose the reference order as $p < q < s$, these coefficients, according to [36] are displayed as follows:

$$C^{(0)}(1, \alpha) = \epsilon_p \cdot X_p(1, \alpha) \epsilon_q \cdot X_q(1, \alpha) \epsilon_s \cdot X_s(1, \alpha), \quad \alpha \in \{2, \dots, r-1\} \sqcup \{p\} \sqcup \{q\}$$

$$C_{\epsilon_p \cdot \epsilon_q}^{(1)}(1, \alpha) = \begin{cases} (-k_p \cdot X_p(1, \alpha))(\epsilon_p \cdot \epsilon_q)[\epsilon_s \cdot Y_s(1, \alpha) + \epsilon_s \cdot k_q], & \alpha \in \{2, \dots, r-1\} \sqcup \{p, q, s\} \\ (-k_p \cdot X_p(1, \alpha))(\epsilon_p \cdot \epsilon_q)(\epsilon_s \cdot k_p), & \alpha \in \{2, \dots, r-1\} \sqcup \{q, p, s\} \\ (-k_p \cdot X_p(1, \alpha))(\epsilon_p \cdot \epsilon_q)(\epsilon_s \cdot Y_s(1, \alpha)), & \alpha \in \{2, \dots, r-1\} \sqcup \{p, s, q\} \\ 0, & \alpha \in \{2, \dots, r-1\} \sqcup \{q, s, p\} \\ (-k_p \cdot X_p(1, \alpha))(\epsilon_p \cdot \epsilon_q)(\epsilon_s \cdot X_s(1, \alpha)), & \alpha \in \{2, \dots, r-1\} \sqcup \{s, p, q\} \\ 0, & \alpha \in \{2, \dots, r-1\} \sqcup \{s, q, p\} \end{cases}$$

$$C_{\epsilon_p \cdot \epsilon_s}^{(1)}(1, \alpha) = \begin{cases} (-k_p \cdot X_p(1, \alpha))(\epsilon_p \cdot \epsilon_s)(\epsilon_q \cdot X_q(1, \alpha)), & \alpha \in \{2, \dots, r-1\} \sqcup \{p, q, s\} \\ [(-k_p \cdot X_p(1, \alpha))(\epsilon_p \cdot \epsilon_s)(\epsilon_q \cdot X_q(1, \alpha)) \\ + (-k_q \cdot X_q(1, \alpha))(-\epsilon_q \cdot k_p)(\epsilon_p \cdot \epsilon_s)], & \alpha \in \{2, \dots, r-1\} \sqcup \{q, p, s\} \\ (-k_p \cdot X_p(1, \alpha))(\epsilon_p \cdot \epsilon_s)(\epsilon_q \cdot X_q(1, \alpha)), & \alpha \in \{2, \dots, r-1\} \sqcup \{p, s, q\} \\ 0, & \alpha \in \{2, \dots, r-1\} \sqcup \{q, s, p\} \\ 0, & \alpha \in \{2, \dots, r-1\} \sqcup \{s, p, q\} \\ 0, & \alpha \in \{2, \dots, r-1\} \sqcup \{s, q, p\} \end{cases}$$

$$C_{\epsilon_q \cdot \epsilon_s}^{(1)}(1, \alpha) = C_{\epsilon_p \cdot \epsilon_s}^{(1)}(1, \alpha)|_{p \leftrightarrow q}. \quad (F5)$$

The vanishing terms that are added to the full amplitude are presented by

$$\begin{aligned}
I &= I_{\epsilon_p \cdot \epsilon_q} + I_{\epsilon_p \cdot \epsilon_s} + I_{\epsilon_q \cdot \epsilon_s} \\
0 &= I_{\epsilon_p \cdot \epsilon_q} \equiv \left(-\frac{\epsilon_p \cdot \epsilon_q}{k_p \cdot k_q} \right) \left[\sum_{\alpha \in \{2, \dots, r-1\} \sqcup \{p\} \sqcup \{q, s\}} (k_q \cdot Y_q(1, \alpha)) (\epsilon_s \cdot k_q) (k_p \cdot X_p(1, \alpha)) A(1, \alpha, r | \rho) \right. \\
&\quad + \sum_{\alpha \in \{2, \dots, r-1\} \sqcup \{p\} \sqcup \{q\} \sqcup \{s\}} (k_q \cdot Y_q(1, \alpha)) (\epsilon_s \cdot Y_s(1, \alpha)) (k_p \cdot X_p(1, \alpha)) A(1, \alpha, r | \rho) \\
&\quad + \sum_{\alpha \in \{2, \dots, r-1\} \sqcup \{q\} \sqcup \{p, s\}} (k_p \cdot Y_p(1, \alpha)) (\epsilon_r \cdot k_p) (k_q \cdot X_q(1, \alpha)) A(1, \alpha, r | \rho) \\
&\quad \left. + \sum_{\alpha \in \{2, \dots, r-1\} \sqcup \{s, q\} \sqcup \{p\}} (\epsilon_r \cdot Y_r(1, \alpha)) (k_q \cdot k_r) (k_p \cdot X_p(1, \alpha)) A(1, \alpha, r | \rho) \right], \\
0 &= I_{\epsilon_p \cdot \epsilon_s} \equiv \left(-\frac{\epsilon_p \cdot \epsilon_s}{k_p \cdot k_s} \right) \left[\sum_{\alpha \in \{2, \dots, r-1\} \sqcup \{p\} \sqcup \{q\} \sqcup \{s\}} (\epsilon_q \cdot Y_q(1, \alpha)) (k_s \cdot Y_s(1, \alpha)) (k_p \cdot X_p(1, \alpha)) A(1, \alpha, r | \rho) \right. \\
&\quad + \sum_{\alpha \in \{2, \dots, r-1\} \sqcup \{p\} \sqcup \{s, q\}} (\epsilon_q \cdot k_s) (k_s \cdot Y_s(1, \alpha)) (k_p \cdot X_p(1, \alpha)) A(1, \alpha, r | \rho) \\
&\quad + \sum_{\alpha \in \{2, \dots, r-1\} \sqcup \{p\} \sqcup \{q, s\}} (\epsilon_q \cdot Y_q(1, \alpha)) (k_s \cdot k_q) (k_p \cdot X_p(1, \alpha)) A(1, \alpha, r | \rho) \\
&\quad \left. + \sum_{\alpha \in \{2, \dots, r-1\} \sqcup \{p, q\} \sqcup \{s\}} (k_p \cdot Y_p(1, \alpha)) (\epsilon_q \cdot k_p) (k_s \cdot X_s(1, \alpha)) A(1, \alpha, r | \rho) \right]. \\
0 &= I_{\epsilon_q \cdot \epsilon_s} = (I_{\epsilon_p \cdot \epsilon_s})|_{p \leftrightarrow q}.
\end{aligned} \tag{F6}$$

All the above terms vanish due to BCJ relations. When we add (F6) to the original expansion formula (8.1) of YMS amplitude with coefficients (F4), (F5), recollect the coefficient corresponding to each permutation, and apply the graphic BCJ relation [38] with three elements to the $\epsilon_p \cdot \epsilon_s$ and $\epsilon_q \cdot \epsilon_s$ parts, we get the expected symmetric coefficients (8.2) for the YMS amplitude with three gluons. The coefficients for EYM amplitude with three gravitons follow from the same construction.

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