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Recursive construction for expansions of tree Yang–Mills amplitudes from soft theorem

Chang Hu[1,2,a], **Kang Zhou**[3,b]

[1] School of Fundamental Physics and Mathematical Sciences, Hangzhou Institute for Advanced Study, UCAS, Hangzhou 310024, China
[2] University of Chinese Academy of Sciences, Beijing 100049, China
[3] Center for Gravitation and Cosmology, College of Physical Science and Technology, Yangzhou University, Yangzhou 225009, China

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Abstract In this paper, we introduce a fundamentally different approach, based on a bottom-up methodology, for expanding tree-level Yang–Mills (YM) amplitudes into Yang–Mills-scalar (YMS) amplitudes and bi-adjoint-scalar (BAS) amplitudes. Our method relies solely on the intrinsic soft behavior of external gluons, eliminating the need for external aids such as Feynman rules or CHY rules. The recursive procedure consistently preserves explicit gauge invariance at every step, ultimately resulting in a manifest gauge-invariant outcome when the initial expression is already framed in a gauge-invariant manner. The resulting expansion can be directly analogized to the expansions of gravitational (GR) amplitudes using the double copy structure. When combined with the expansions of Einstein–Yang–Mills amplitudes obtained using the covariant color-kinematic duality method from existing literature, the expansions presented in this note yield gauge-invariant Bern–Carrasco–Johansson (BCJ) numerators.

1 Introduction

In recent decades, significant progress has been made in understanding scattering amplitudes, revealing hidden mathematical structures that go beyond traditional Feynman rules. These advancements have uncovered interconnections between amplitudes from various theories. For instance, gravitational (GR) and Yang–Mills (YM) amplitudes at the tree level are linked through the Kawai–Lewellen–Tye (KLT) relation [1] and the Bern–Carrasco–Johansson (BCJ) color-kinematic duality [2–5]. In the well-known CHY formalism [6–10], tree amplitudes for the a large variety of theories can be generated from the tree GR amplitudes through the compactification, squeezing and the generalized dimensional reduction procedures [6–10]. Similar unifying relations have emerged, allowing tree amplitudes from one theory to be expressed in terms of those from others [11–20].

The expansions of tree-level gravitational (GR) amplitudes into Yang–Mills (YM) amplitudes have garnered significant attention due to their role in constructing BCJ numerators [14,21]. These expansions involve recursive techniques, breaking down GR amplitudes into linear combinations of tree-level Einstein–Yang–Mills (EYM) amplitudes where some gravitons become gluons. They also expand tree-level EYM amplitudes into versions with fewer gravitons and more gluons [14,15,18]. By iteratively applying these recursions, one can derive the desired GR to YM expansions.

The coefficients or BCJ numerators obtained through the aforementioned process are local, without any spurious poles in the expansions. However, establishing gauge invariance is challenging. Recent developments in scattering amplitude research have shown that amplitudes manifesting gauge invariance at the expense of locality often lead to innovative insights and unexpected mathematical structures. For instance, the Britto–Cachazo–Feng–Witten (BCFW) on-shell recursion relations [22,23], inspiring novel amplitude constructions like the Grassmannian representation and the Amplituhedron [24–26]. Thus, exploring expansion techniques that explicitly showcase gauge invariance is valuable.

To achieve these new expansions, a natural approach is to modify existing recursive expansions. Fortunately, we have alternative recursive expansions for tree Einstein–Yang–Mills (EYM) amplitudes that explicitly exhibit gauge invariance for each polarization carried by external particles. These new expansions, discovered by Cheung and Mangan using the covariant color-kinematic duality [27], can also be derived using a technique based on soft theorems, similar to

[a] e-mail: isiahalbert@126.com
[b] e-mail: zhoukang@yzu.edu.cn (corresponding author)

the one presented in this paper [28]. Another challenge is to discover new expansions that manifest gauge invariance while expanding tree GR amplitudes into EYM ones. This can be achieved by altering the old GR expansions through the addition of new terms that vanish due to the gauge invariance of the expanded GR amplitudes, as outlined in subsection IV A. Ensuring that the original expansions describe gauge-invariant amplitudes is essential, making it logical to derive the old expansions from a gauge-invariant foundational framework, such as the traditional Lagrangian or CHY formalism. In other words, modifying the old expansions is a top-down construction.

The central aim of the modern S-matrix program is to construct amplitudes from a bottom-up approach, free from reliance on Lagrangian techniques. One prominent example involves bootstrapping three-point amplitudes within the spinor-helicity formalism and subsequently generating higher-point amplitudes through the application of the BCFW recursive method [22,23]. The primary objective of this paper is to provide a concise bottom-up approach for constructing expansions of tree-level gravitational (GR) amplitudes into tree-level Einstein-Yang-Mills (EYM) amplitudes. This approach ensures the explicit manifestation of gauge invariance for the polarization of each external particle.

The method presented in this paper is based on the sub-leading soft behavior for external gluons. Initially, soft theorems at the tree level were derived using Feynman rules for photons and gravitons [29,30]. In 2014, new soft theorems were discovered for gravity (GR) and Yang–Mills (YM) theory at the tree level by applying BCFW recursion relations [31,32]. In GR, the soft theorem was extended beyond the leading order to sub-leading and sub-sub-leading levels, while in YM theory, it was identified at the leading and sub-leading orders. These new soft theorems were subsequently generalized to arbitrary spacetime dimensions [33,34] using CHY formulas [6–10]. These soft theorems have been instrumental in constructing tree amplitudes, such as through the inverse soft theorem program, and by utilizing another type of soft behavior known as the Adler zero to construct amplitudes for various effective theories [35–41]. In this paper, we build upon the idea of constructing tree amplitudes from soft theorems, but our approach differs significantly from the techniques found in existing literature.

Instead of expanding GR (gravity) amplitudes to EYM (Einstein–Yang–Mills) ones, this paper focuses on the expansions of color-ordered single-trace tree YM (Yang–Mills) amplitudes [3,42] into tree Yang–Mills-scalar (YMS) amplitudes, which describe gluons and bi-adjoint scalars (BAS). This choice is motivated by several factors. Firstly, both expansions share the same coefficients due to the double copy structure [1–5,8]. Secondly, the pure BAS amplitudes only contain propagators without numerators [8]. The approach starts by bootstrapping the lowest three-point tree YM amplitudes, while assuming that higher-point tree amplitudes are uniquely determined by the soft behaviors of gluons. The advantage lies in the sub-leading soft factor of gluons, which inserts the soft external leg in a manifestly gauge-invariant manner. Consequently, if the original three-point amplitude is expressed in a manifestly gauge-invariant formula, this gauge invariance is preserved throughout the process. As demonstrated, relying on the assumption that soft behaviors fully determine amplitudes, gauge invariance is established for the old expansions without necessitating a top-down derivation.

The method presented in this paper represents a significant advancement and improvement compared to the one used in [43]. The new version constructs general expansions starting from the lowest-point amplitudes, which can be determined through bootstrapping. As pointed out in [43], the soft theorem for gluons can be uniquely fixed by assuming the universality of soft behaviors. More explicitly, one can find the expansion of tree YMS amplitudes with one external gluon by imposing the universality of the soft behaviors of BAS scalars, and then derive the soft theorem for gluons from the resulted expansion of such YMS amplitudes. On the other hand, since the pure BAS amplitudes only contain propagators, the soft behaviors of BAS scalars are obvious. Thus, in the whole story, the expansions of YM amplitudes to YMS ones indeed arise from the assumptions of universality of soft behaviors.

The remainder of this note is organized as follows. In Sect. 2, we introduce necessary background including the expansions of tree amplitudes to the Kleiss–Kuijf (KK) BAS basis, the recursive expansions of tree YMS (EYM) amplitudes, as well as the soft theorems for external BAS scalars and gluons at tree level. In Sect. 3, we introduce our recursive method, and construct the old expansions of tree YM amplitudes to YMS ones, from the three-point amplitudes fixed by bootstrapping. In Sect. 4, we derive the new expansions which manifest the gauge invariance by applying both the direct construction and the recursive technique. Finally, we end with a brief summary in Sect. 5.

2 Background

For readers' convenience, in this section we give a brief review of necessary background. In Sect. 2.1, we introduce the concept of tree level amplitudes of bi-adjoint scalar (BAS) theory and Yang–Mills scalar (YMS) theory. Meanwhile, we draw the conclusion that any theory consisting solely of massless particles can be expanded onto the KK BAS basis. In Sect. 2.2, we briefly list the previously established soft theorems for scalars and gluons in various theories. In Sect. 2.3, we provide a concise introduction on how to recursively expand YMS tree-level amplitudes into the KK basis.

2.1 Expanding tree level amplitudes to BAS basis

The double color-ordered tree amplitudes in BA) theory exclusively feature propagators for massless scalars. Each amplitude exhibits simultaneous planarity with respect to two color orderings. We take the five-point amplitude $\mathcal{A}_{\mathrm{BAS}}(1,2,3,4,5|1,4,2,3,5)$ as an example. In Fig. 1, both $(a1)$ and $(a2)$ correspond to the same tree diagram. Specifically, a1 is associated with color ordering $(1,2,3,4,5)$, while $(a2)$ corresponds to color ordering $(1,4,2,3,5)$. However, in Fig. 1, the tree diagram represented by figure b can only conform to color ordering $(1,2,3,4,5)$ and does not satisfy color ordering $(1,4,2,3,5)$. Similarly, one can draw additional tree diagrams that satisfy color ordering $(1,2,3,4,5)$, but it will be observed that none of them conforms to color ordering $(1,4,2,3,5)$. Then the tree BAS amplitude $\mathcal{A}_{\mathrm{BAS}}(1,2,3,4,5|1,4,2,3,5)$ can be computed as

$$\mathcal{A}_{\mathrm{BAS}}(1,2,3,4,5|1,4,2,3,5)=(-1)^{n_{\mathrm{flip}}}\frac{1}{s_{23}}\frac{1}{s_{51}}. \tag{1}$$

The Mandelstam variable $s_{i\cdots j}$ is defined as

$$s_{i\cdots j}\equiv k_{i\cdots j}^2, \quad k_{i\cdots j}\equiv\sum_{a=i}^{j}k_a, \tag{2}$$

where k_a is the momentum carried by the external leg a.

Each double color-ordered BAS amplitude carries an overall sign $(-1)^{n_{\mathrm{flip}}}$, where n_{flip} is determined by these two color orderings. Readers should be aware that in this paper, when these two color orderings are identical, n_{flip} equals zero, implying that the overall sign is $+$. The systematic method for determining n_{flip} and evaluating double color-ordered partial amplitudes can be referenced in [8], and as it is not pertinent to the current paper, it will not be further elaborated upon here.[1]

The Yang–Mills-scalar (YMS) amplitudes pertain to scalars that are coupled with gluons. In this context, we are specifically concerned with a subset of YMS amplitudes known as single-trace YMS amplitudes. The single-trace YMS amplitude, denoted as $\mathcal{A}_{\mathrm{YMS}}(1,\ldots,n;\{p_1,\ldots,p_m\}|\sigma_{n+m})$, comprises n external scalars represented by $\{1,\ldots,n\}$ and m external gluons labeled as $\{p_1,\ldots,p_m\}$. The ordering σ_{n+m} on the right-hand side of $|$ encompasses all external legs within $\{1,\ldots,n\}\cup\{p_1,\ldots,p_m\}$. On the left-hand side of $|$, $(1,\ldots,n)$ signifies an alternative overall ordering of external scalars, which is also the reason it is referred to as 'single-trace', while $\{p_1,\ldots,p_m\}$ constitutes an unordered set. In simpler terms, the external scalars are BAS scalars, which have a dual ordering, whereas the external gluons belong to a single ordering, σ_{n+m}.

Tree level amplitudes for any theory, as long as they contain only massless particles and cubic vertices, can be expanded to double color-ordered BAS amplitudes, due to the observation that each Feynman diagram for pure propagators is included in at least one BAS amplitude. In addition, tree diagrams involving higher point vertices can be decomposed into BAS amplitudes with solely cubic vertices by multiplying both the numerator and denominator by the propagator D. An example is shown in Fig. 2. Since each Feynman diagram contributes propagators that can be mapped to BAS amplitudes, along with a numerator, we can conclude that each tree-level amplitude can be expanded into double color-ordered BAS amplitudes. These expanded amplitudes have coefficients that are polynomials depending on Lorentz invariants created by external kinematic variables.

In reality, not all BAS amplitudes are independent; therefore, such an expansion requires the selection of appropriate basis. Such a basis can be determined by the well-known Kleiss–Kuijf (KK) relation [44]

$$\mathcal{A}_{\mathrm{BAS}}(1,\vec{\boldsymbol{\alpha}},n,\vec{\boldsymbol{\beta}}|\sigma_n)=(-)^{|\vec{\boldsymbol{\beta}}|}\,\mathcal{A}_{\mathrm{BAS}}(1,\vec{\boldsymbol{\alpha}}\shuffle\vec{\boldsymbol{\beta}}^T,n|\sigma_n), \tag{3}$$

where $\vec{\boldsymbol{\alpha}}$ and $\vec{\boldsymbol{\beta}}$ are two ordered subsets of external scalars, and $\vec{\boldsymbol{\beta}}^T$ stands for the ordered set generated from $\vec{\boldsymbol{\beta}}$ by reversing the original ordering. The $|\vec{\boldsymbol{\beta}}|$ on overall sign represents the number of elements in subset $\vec{\boldsymbol{\beta}}$. The symbol $\shuffle$ means summing over all possible shuffles of two ordered sets $\vec{\boldsymbol{\beta}}_1$ and $\vec{\boldsymbol{\beta}}_2$, i.e., all permutations in the set $\vec{\boldsymbol{\beta}}_1\cup\vec{\boldsymbol{\beta}}_2$ while preserving the orderings of $\vec{\boldsymbol{\beta}}_1$ and $\vec{\boldsymbol{\beta}}_2$. For instance, suppose $\vec{\boldsymbol{\beta}}_1=\{1,2\}$ and $\vec{\boldsymbol{\beta}}_2=\{3,4\}$; then

$$\begin{aligned}\vec{\boldsymbol{\beta}}_1\shuffle\vec{\boldsymbol{\beta}}_2=&(1,2,3,4)+(1,3,2,4)+(1,3,4,2)\\&+(3,1,2,4)+(3,1,4,2)+(3,4,1,2).\end{aligned} \tag{4}$$

One should note that the n-point BAS amplitude $\mathcal{A}_{\mathrm{BAS}}(1,\vec{\boldsymbol{\alpha}},n,\vec{\boldsymbol{\beta}}|\sigma_n)$ at the l.h.s of (3) carries two color orderings. We can also have an analogous KK relation for the second color ordering σ_n. Therefore, the KK relation implies that the basis can be chosen as BAS amplitudes $\mathcal{A}_{\mathrm{BAS}}(1,\sigma_1,n|1,\sigma_2,n)$, where 1 and n are fixed at two ends in each ordering. Such a basis is called the KK BAS basis. Based on the discussion above, any amplitude which includes only massless particles can be expanded to this basis.[2] In the

[1] In fact, in reference A, the overall sign is defined as $(-1)^{n-3+n_{\mathrm{flip}}}$, where n is the number or external legs. However, for the convenience of our subsequent work in this paper, we adopt the notation $(-1)^{n_{\mathrm{flip}}}$. The advantage of the new convention stems from the fact that when we remove a soft external scalar from an n-point amplitude, it changes the number of external legs to $n-1$. Therefore, we desire that this overall sign contains information solely about the relative ordering between the two color orderings of the origin n-point amplitude, excluding the influence of changes in the number of external legs on this sign.

[2] The well-known Bern–Carrasco–Johansson (BCJ) relation [2–5] links BAS amplitudes in the KK basis together, and the independent BAS amplitudes can be obtained by fixing three legs at three particular positions in the color orderings. However, in the BCJ relation, coefficients of BAS amplitudes depend on Mandelstam variables; this

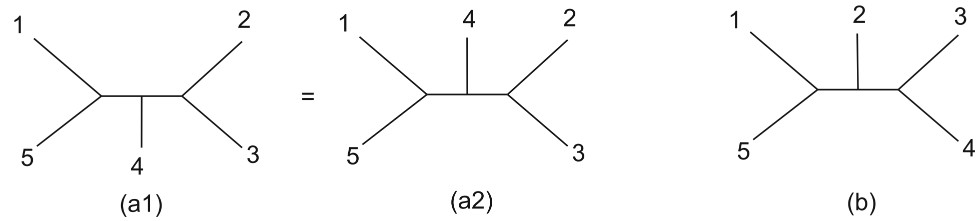

Fig. 1 Two five-point diagrams. Figures (**a1**) and (**a2**) are the same tree diagram, while (**a1**) represents the color ordering 12345 and (**a2**) represents the color ordering 14235

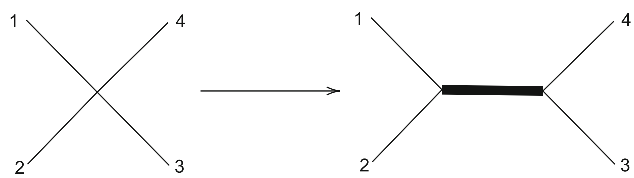

Fig. 2 Turn the four-point vertex to three-point ones. The bold line corresponds to the inserted propagator $1/s_{12}$. This manipulation turns the original numerator N to $s_{12}N$, and splits the original coupling constant g into two $\sqrt{g}$ for two cubic vertices

expansion, the KK basis supplies the propagators, while the coefficients in the expansions provide the numerators.

In this paper, we will concentrate on the expansion of pure YM amplitudes. The n-point YM amplitude $\mathcal{A}_{\text{YM}}(\sigma_n)$ with color ordering σ_n can be expanded to KK BAS basis as

$$\mathcal{A}_{\text{YM}}(\sigma_n) = \sum_{\alpha_{n-2}} \mathcal{C}(\alpha_{n-2}, \epsilon_i, k_i)\, \mathcal{A}_{\text{BAS}}(1, \alpha_{n-2}, n|\sigma_n), \quad (5)$$

where α_{n-2} denotes color orderings among external legs of $\{2, \cdots, n-1\}$. The double copy structure [1–5] indicates that the coefficient $\mathcal{C}(\alpha_{n-2}, \epsilon_i, k_i)$ depends on polarization vectors ϵ_i and momenta k_i of external gluons, as well as the ordering α_{n-2}, but remains independent of ordering σ_n.[3] Therefore, within this expansion, the investigation of the structure of YM amplitudes is transformed into the study of the structure of the coefficients $\mathcal{C}(\alpha_{n-2}, \epsilon_i, k_i)$. These coefficients are known as BCJ numerators [14,21].

2.2 Soft theorems for external scalars and gluons

In this subsection, we provide a brief overview of the soft scattering theorems for external scalars and gluons, which are crucial for the discussions in the subsequent sections.

For the double color-ordered BAS amplitude $\mathcal{A}_{\text{BAS}}(1, \ldots, n|\sigma_n)$, we rescale k_i as $k_i \to \tau k_i$, and expand the amplitude with respect to τ,

$$\mathcal{A}_{\text{BAS}}(1, \ldots, n|\sigma_n) = \mathcal{A}^{(0)_i}_{\text{BAS}}(1, \ldots, n|\sigma_n) + \mathcal{A}^{(1)_i}_{\text{BAS}}(1, \ldots, n|\sigma_n) + \mathcal{O}(\tau). \quad (6)$$

The leading-order contribution $\mathcal{A}^{(0)_i}_{\text{BAS}}(1, \ldots, n|\sigma_n)$ arises explicitly from the two-point channels $1/s_{1(i+1)}$ and $1/s_{(i-1)i}$, which are at the $1/\tau$ order. In other words,

$$\begin{aligned}\mathcal{A}^{(0)_i}_{\text{BAS}}(1, \ldots, n|\sigma_n) &= \frac{1}{\tau}\left(\frac{\delta_{i(i+1)}}{s_{i(i+1)}} + \frac{\delta_{(i-1)i}}{s_{(i-1)i}}\right) \mathcal{A}_{\text{BAS}}(1, \ldots, i-1, \ni, i+1, \ldots, n|\sigma_n\backslash i)\\ &= S_s^{(0)_i}\, \mathcal{A}_{\text{BAS}}(1, \ldots, i-1, \ni, i+1, \ldots, n|\sigma_n \setminus i),\end{aligned} \quad (7)$$

where $\ni$ stands for removing the leg i, $\sigma_n\backslash i$ means the color ordering generated from σ_n by eliminating i. In Eq. (7), δ_{ab} is not the well-known Kronecker symbol. Its value is determined by the second color ordering σ_n. When a, b in σ_n are not adjacent, δ_{ab} takes the value of 0. When a, b in σ_n are adjacent and maintain the same order as in the first color ordering $(1, \ldots, n)$, δ_{ab} takes the value of 1. When a, b in σ_n are adjacent but have the reverse order compared to their order in the first color ordering $(1, \ldots, n)$, it takes the value of -1. The leading soft operator $S_s^{(0)}(i)$ for the scalar i is observed as

$$S_s^{(0)_i} \equiv \frac{1}{\tau}\left(\frac{\delta_{i(i+1)}}{s_{i(i+1)}} + \frac{\delta_{(i-1)i}}{s_{(i-1)i}}\right). \quad (8)$$

For example, for four-point amplitude $\mathcal{A}_{BAS}(1234|1234)$, we rescale k_4 as $k_4 \to \tau k_4$; then by our notation, we have

$$\begin{aligned}&\mathcal{A}^{(0)}_{\text{BAS}}(1234|1234) = \frac{1}{\tau}(\frac{1}{s_{41}} + \frac{1}{s_{34}})\\ &\mathcal{A}_{\text{BAS}}(123|123) = +1.\end{aligned} \quad (9)$$

According to our definition of δ_{ab}, we know that $\delta_{34} = \delta_{41} = 1$ since 3, 4, 1 remains the same in both color orderings. So we verified

$$\mathcal{A}^{(0)_4}_{\text{BAS}}(1234|1234) = \frac{1}{\tau}\left(\frac{\delta_{41}}{s_{41}} + \frac{\delta_{34}}{s_{34}}\right) \mathcal{A}_{\text{BAS}}(123|123). \quad (10)$$

Footnote 2 continued
character leads to poles in coefficients when expanding to BCJ basis. On the other hand, when expanding to the KK basis, one can find the expanded formula in which the coefficients contain no poles. In this paper, we opt for the KK basis, as we aim to ensure that all poles of tree amplitudes are encompassed within the basis, with coefficients solely serving as numerators.

[3] Originally, the concept of the double copy implied that the general relativity (GR) amplitude could be factorized as $\mathcal{A}_{\text{G}} = \mathcal{A}_{\text{YM}} \times \mathcal{S} \times \mathcal{A}_{\text{YM}}$, where the kernel $\mathcal{S}$ is derived by inverting BAS amplitudes. Our assumption that the coefficients depend on only one color ordering is consistent with the original version, as discussed in [43].

For four-point amplitude $\mathcal{A}_{\text{BAS}}(1234|1243)$, we also rescale k_4 as $k_4 \to \tau k_4$; then by our notation, we have

$$\mathcal{A}^{(0)}_{\text{BAS}}(1234|1243) = \frac{1}{\tau}\left(-\frac{1}{s_{34}}\right)$$
$$\mathcal{A}_{\text{BAS}}(123|123) = +1. \tag{11}$$

Because 3 and 4 have opposite orders in the two color orderings 1234 and 1243, we have $\delta_{34} = -1$. And since 4 and 1 are not adjacent in the second color ordering 1243, we have $\delta_{41} = 0$. So we verified

$$\mathcal{A}^{(0)_4}_{\text{BAS}}(1234|1243) = \frac{1}{\tau}\left(\frac{\delta_{41}}{s_{41}} + \frac{\delta_{34}}{s_{34}}\right)\mathcal{A}_{\text{BAS}}(123|123). \tag{12}$$

In our previous work, we introduced an assumption that the soft operator form should be universal across different theories. For example, in the YMS theory, scalar particles, and in the BAS theory, scalar particles, both share the same form for their respective soft operators. Then the leading contribution of YMS amplitude is

$$\mathcal{A}^{(0)_i}_{\text{YMS}}(1,\ldots,n;\,p_1,\ldots,p_m|\sigma_{n+m}) = S^{(0)_i}_s$$
$$\mathcal{A}_{\text{YMS}}(1,\ldots,i-1,\ni,i+1,\ldots,n;\,p_1,\ldots,p_m|\sigma_{n+m}\setminus i). \tag{13}$$

Based on (8), it can be observed that this soft operator $S^{(0)_i}_s$ does not act on external gluons.

The soft theorems for external gluons at leading and sub-leading orders can be obtained via various approaches [32–34,43]. Such soft theorems are given as

$$\mathcal{A}^{(0)_{p_i}}_{\text{YMS}}(1,\ldots,n;\,p_1,\ldots,p_m|\sigma_{n+m})$$
$$= S^{(0)_{p_i}}_g\,\mathcal{A}_{\text{YMS}}(1,\ldots,n;\,p_1,\ldots,\not{p}_i,\ldots,$$
$$p_m|\sigma_{n+m}\setminus p_i), \tag{14}$$

and

$$\mathcal{A}^{(1)_{p_i}}_{\text{YMS}}(1,\ldots,n;\,p_1,\ldots,p_m|\sigma_{n+m}) = S^{(1)_{p_i}}_g$$
$$\mathcal{A}_{\text{YMS}}(1,\ldots,n;\,p_1,\ldots,\not{p}_i,\ldots,p_m|\sigma_{n+m}\setminus p_i), \tag{15}$$

where the external momentum k_{p_i} is rescaled as $k_{p_i} \to \tau k_{p_i}$. The soft factors at leading and sub-leading orders are given by

$$S^{(0)_{p_i}}_g = \frac{1}{\tau}\sum_{a\in\sigma}\frac{\delta_{ap_i}\,(\epsilon_{p_i}\cdot k_a)}{s_{ap_i}}, \tag{16}$$

and

$$S^{(1)_{p_i}}_g = \sum_{a\in\sigma}\frac{\delta_{ap_i}\,\left(\epsilon_{p_i}\cdot J_a\cdot k_{p_i}\right)}{s_{ap_i}}, \tag{17}$$

respectively [32,33]. Here, δ_{ab} is solely determined by the second color ordering σ_{n+m}. When a, b are adjacent in σ_{n+m} (in a cyclically symmetric sense), δ_{ab} takes the value of 1 if a precedes b, and -1 if a follows b. When a, b are not adjacent in σ_{n+m}, δ_{ab} takes the value of 0. $J^{\mu\nu}_a$ is the angular momentum operator. In (16) and (17), one should sum over all external legs a, i.e., these soft operators for external gluon act on both external scalars and gluons.

The sub-leading soft operator (17) for external gluons plays a central role in the subsequent sections. Here, we present some valuable results regarding the operation of this operator. The angular momentum operator $J^{\mu\nu}_a$ acts on the Lorentz vector k^ρ_a with the orbital component of the generator and on ϵ^ρ_a with the spin component of the generator in the vector representation

$$J^{\mu\nu}_a\,k^\rho_a = k^{[\mu}_a\frac{\partial k^\rho_a}{\partial k_{a,\nu]}}, \quad J^{\mu\nu}_a\,\epsilon^\rho_a = \left(\eta^{\nu\rho}\,\delta^\mu_\sigma - \eta^{\mu\rho}\,\delta^\nu_\sigma\right)\epsilon^\sigma_a. \tag{18}$$

Then the action of $S^{(1)_p}_g$ can be re-expressed as

$$S^{(1)_p}_g = -\sum_{V_a}\frac{\delta_{ap}}{s_{ap}}\,V_a\cdot f_p\cdot\frac{\partial}{\partial V_a}, \tag{19}$$

due to the observation that the amplitude is linear in each polarization vector. We observe that in (19), the summation over V_a includes all Lorentz vectors, encompassing both momenta and polarizations. The operator (19) is a differential operator that adheres to Leibniz's rule. Employing (19), we promptly obtain

$$\left(S^{(1)_p}_g\,k_a\right)\cdot V = -\frac{\delta_{ap}}{s_{ap}}\,(k_a\cdot f_p\cdot V), \quad \left(S^{(1)_p}_g\,\epsilon_a\right)\cdot$$
$$V = -\frac{\delta_{ap}}{s_{ap}}\,(\epsilon_a\cdot f_p\cdot V), \tag{20}$$

where V is an arbitrary Lorentz vector, and

$$V_1\cdot\left(S^{(1)_p}_g\,f_a\right)\cdot V_2 = \frac{\delta_{ap}}{s_{ap}}\,V_1\cdot(f_p\cdot f_a - f_a\cdot f_p)\cdot V_2, \tag{21}$$

for two arbitrary Lorentz vectors V_1 and V_2, where the anti-symmetric tensor f_i is defined as $f^{\mu\nu}_i \equiv k^\mu_i\epsilon^\nu_i - \epsilon^\mu_i k^\nu_i$, as introduced previously.

2.3 Recursive expansion of single-trace YMS amplitudes

The discussion for the expansion of tree level amplitudes in the previous Sect. 2.1 indicates that the YMS amplitudes can also be expanded to the KK BAS basis. This expansion can be achieved by applying the following recursive expansion iteratively:

$$\mathcal{A}_{\text{YMS}}(1,\ldots,n;\{p_1,\ldots,p_m\}|\sigma_{n+m})$$
$$= \sum_{\vec{\boldsymbol{\alpha}}}\left(\epsilon_p\cdot F_{\vec{\boldsymbol{\alpha}}}\cdot Y_{\vec{\boldsymbol{\alpha}}}\right)\mathcal{A}_{\text{YMS}}(1,\{2,\ldots,n-1\}\sqcup\{\vec{\boldsymbol{\alpha}},p\},$$
$$n;\{p_1,\ldots,p_m\}\setminus\{p\cup\boldsymbol{\alpha}\}|\sigma_{n+m}), \tag{22}$$

where p is the fiducial gluon which can be chosen as any element in $\{p_1,\ldots,p_m\}$, and $\boldsymbol{\alpha}$ are subsets of $\{p_1,\ldots,p_m\}\setminus p$

which is allowed to be empty. When $\boldsymbol{\alpha} = \{p_1, \ldots, p_m\}\backslash p$, the YMS amplitudes in the second line of (22) are reduced to BAS ones. The ordered set $\vec{\boldsymbol{\alpha}}$ is generated from $\boldsymbol{\alpha}$ by endowing an order among elements in $\boldsymbol{\alpha}$. The tensor $F^{\mu\nu}_{\vec{\boldsymbol{\alpha}}}$ is defined as

$$F^{\mu\nu}_{\vec{\boldsymbol{\alpha}}} \equiv \left(f_{\alpha_k} \cdot f_{\alpha_{k-1}} \cdots f_{\alpha_2} \cdot f_{\alpha_1}\right)^{\mu\nu}, \tag{23}$$

for $\vec{\boldsymbol{\alpha}} = \{\alpha_1, \ldots \alpha_k\}$. The combined momentum $Y_{\vec{\boldsymbol{\alpha}}}$ is the summation of momenta carried by external gluons at the l.h.s of α_1 in the color ordering $\{2, \ldots, n-1\} \shuffle \vec{\boldsymbol{\alpha}}$. The summation in (38) is over all nonequivalent ordered sets $\vec{\boldsymbol{\alpha}}$. The recursive expansion (22) is found via various methods [32–34,43]. It should be noted that this recurrence relation can be independently derived through the recursive construction based on soft behaviors. For detailed information, please refer to reference [43]. In the recursive expansion (22), the YMS amplitude undergoes expansion, resulting in YMS amplitudes with fewer gluons and more scalars. By iteratively applying this expansion, it becomes possible to expand any YMS amplitude into pure BAS amplitudes.

Furthermore, we can also observe that in the recursive expansion (22), the gauge invariance for each gluon in $\{P_1, \ldots, p_m\} \setminus p$ is manifest, since the tensor $f^{\mu\nu}$ vanishes automatically under the replacement $\epsilon_i \to k_i$, due to the definition. However, the gauge invariance for the fiducial gluon p has not been manifested. When applying (22) iteratively, fiducial gluons will be chosen at every step. Consequently, in the resulting expansion to pure BAS amplitudes, the gauge invariance for each gluon will be compromised. To achieve a manifestly gauge-invariant expansion, an alternative recursive expansion should be employed:

$$\begin{aligned}&\mathcal{A}_{\mathrm{YMS}}(1, \ldots, n; \{p_1, \ldots, p_m\}|\sigma_{n+m})\\ &\quad= \sum_{\vec{\boldsymbol{\alpha}}} \frac{k_r \cdot F_{\vec{\boldsymbol{\alpha}}} \cdot Y_{\vec{\boldsymbol{\alpha}}}}{k_r \cdot k_{p_1 \ldots p_m}} \mathcal{A}_{\mathrm{YMS}}(1, \{2, \ldots, n-1\} \shuffle \vec{\boldsymbol{\alpha}}, n;\\ &\qquad \{p_1, \ldots, p_m\}\backslash\boldsymbol{\alpha}|\sigma_{n+m}),\end{aligned} \tag{24}$$

where k_r is a reference massless momentum. In this context, the notations align with those in (22), and $\boldsymbol{\alpha}$ represents subsets of $p_1, \ldots, p_m$. The formula (24) was originally discovered by Clifford Cheung and James Mangan within the framework of the covariant color-kinematic duality. It was also independently derived by applying the recursive construction based on soft theorems [43]. Notably, the expansion of (24) does not necessitate the use of a fiducial gluon, and it inherently exhibits gauge invariance for all polarizations. Through iterative application of (22), one eventually arrives at the manifestly gauge-invariant expansion of YMS amplitudes into the KK BAS basis.

3 Expand YM amplitudes to YMS ones

In this section, we derive the color-ordered Yang–Mills (YM) amplitudes as part of the formula for expanding YM amplitudes into Yang–Mills-scalar (YMS) amplitudes. The technique employed in this section is based on the analysis of the sub-leading-order soft behavior. It represents an improvement over the method utilized in [43]. In comparison with the previous method from [43], the new approach allows us to construct the expanded formula recursively, starting from the lowest three-point amplitudes that can be uniquely determined through bootstrapping. This is achieved without the need to rely on other frameworks, such as Feynman rules or CHY formalism. However, it should be noted that the resulting expansion in this section does not exhibit gauge invariance for all polarizations. The manifestation of gauge invariance is the objective of the next section.

3.1 Three-point amplitudes

To ensure our construction is self-contained, without relying on Feynman rules or the CHY formula, we fix the three-point color-ordered Yang–Mills (YM) amplitudes using a bootstrapping method. Our construction is primarily based on the following ansatz:

1. The amplitude $\mathcal{A}_{\mathrm{YM}}(1, 2, 3)$ with the color ordering $(1, 2, 3)$ has a mass dimension of 1, and due to the absence of factorization channels for the lowest-point amplitudes, it does not contain any pole structures.
2. This amplitude is linearly dependent on polarization vectors ϵ_1, ϵ_2 and ϵ_3.
3. Due to cyclic symmetry, $\mathcal{A}_{\mathrm{YM}}(1, 2, 3)$ remains invariant under permutation transformations $(1 \to 2, 2 \to 3, 3 \to 1)$.

In this manner, we establish the foundational elements for our self-contained construction as

$$\begin{aligned}\mathcal{A}_{\mathrm{YM}}(1, 2, 3) = (k_1 \cdot \epsilon_2)\,(\epsilon_3 \cdot \epsilon_1) + (k_2 \cdot \epsilon_3)\,(\epsilon_1 \cdot \epsilon_2)\\ +(k_3 \cdot \epsilon_1)\,(\epsilon_2 \cdot \epsilon_3).\end{aligned} \tag{25}$$

It's worth noting that replacing $k_1 \cdot \epsilon_2$, $k_2 \cdot \epsilon_3$, and $k_3 \cdot \epsilon_1$ with $k_3 \cdot \epsilon_2$, $k_1 \cdot \epsilon_3$, and $k_2 \cdot \epsilon_1$, respectively, results in an overall sign change. This occurs due to both momentum conservation and the on-shell condition $k_i \cdot \epsilon_i = 0$.

We can expand $\mathcal{A}_{\mathrm{YM}}(1, 2, 3)$ onto YMS amplitudes and BAS amplitudes in the manner of Eq. (22), by $\mathcal{A}_{\mathrm{YMS}}(1, 3; 2 |1, 2, 3) = (\epsilon_2 \cdot k_1)\, \mathcal{A}_{\mathrm{BAS}}(1, 2, 3|1, 2, 3)$ and $\mathcal{A}_{\mathrm{BAS}}(1, 2, 3| 1, 2, 3) = 1$, we have

$$\begin{aligned}\mathcal{A}_{\mathrm{YM}}(1, 2, 3) = \left(\epsilon_3 \cdot \epsilon_1\right) \mathcal{A}_{\mathrm{YMS}}(1, 3; 2|1, 2, 3)\\ +\left(\epsilon_3 \cdot f_2 \cdot \epsilon_1\right) \mathcal{A}_{\mathrm{BAS}}(1, 2, 3|1, 2, 3).\end{aligned} \tag{26}$$

Then the double copy structure indicates the expansion for general three-point color ordered YM amplitude

$$\mathcal{A}_{\text{YM}}(\sigma_3) = \big(\epsilon_3 \cdot \epsilon_1\big)\, \mathcal{A}_{\text{YMS}}(1,3;2|\sigma_3) + \big(\epsilon_3 \cdot f_2 \cdot \epsilon_1\big)\, \mathcal{A}_{\text{BAS}}(1,2,3|\sigma_3), \tag{27}$$

where σ_3 is an arbitrary ordering among legs in $\{1, 2, 3\}$. Equation (27) serves as the initial step for the recursive construction in this section.

3.2 Recursive construction for four-point amplitudes

In this subsection, we derive the expansion of four-point Yang–Mills (YM) amplitudes based on the previously expanded formula for three-point amplitudes in Eq. (27). This is accomplished by examining the sub-leading-order soft behavior of the four-point amplitude. We label the external legs of the four-point amplitude $\mathcal{A}_{\text{YM}}(\sigma_4)$ as $\sigma_4 = \{1, 2, 3, s\}$ and choose the KK basis such that legs 1 and 3 are fixed at two ends in the left color ordering. We focus on the soft behavior of the external particle s by rescaling k_s as $k_s \to \tau k_s$ and expanding $\mathcal{A}_{\text{YM}}(\sigma_4)$ with respect to τ. This process of constructing four-point amplitudes from three-point amplitudes provides valuable insights for addressing more general cases in our subsequent discussions.

According to the soft theorem in (15) and (17), the sub-leading contribution is given as

$$\begin{aligned}\mathcal{A}^{(1)_s}_{\text{YM}}(\sigma_4) &= S^{(1)_s}_g\, \mathcal{A}_{\text{YM}}(\sigma_4\backslash s)\\ &= S^{(1)_s}_g \Big[\big(\epsilon_3 \cdot \epsilon_1\big)\, \mathcal{A}_{\text{YMS}}(1,3;2|\sigma_4\backslash s)\\ &\quad + \big(\epsilon_3 \cdot f_2 \cdot \epsilon_1\big)\, \mathcal{A}_{\text{BAS}}(1,2,3|\sigma_4\backslash s)\Big]\\ &= P_1 + P_2.\end{aligned} \tag{28}$$

The second line is derived by substituting the expansion (27) into the first line. The sub-leading contribution is then split into two parts, denoted as P_1 and P_2:

$$\begin{aligned}P_1 &= (\epsilon_3 \cdot \epsilon_1)\Big[S^{(1)_s}_g \mathcal{A}_{\text{YMS}}(1,3;2|\sigma_4\backslash s)\Big]\\ &\quad + (\epsilon_3 \cdot f_2 \cdot \epsilon_1)\Big[S^{(1)_s}_g \mathcal{A}_{\text{BAS}}(1,2,3|\sigma_4\backslash s)\Big],\\ P_2 &= \Big[S^{(1)_s}_g\, (\epsilon_3 \cdot \epsilon_1)\Big] \mathcal{A}_{\text{YMS}}(1,3;2|\sigma_4\backslash s)\\ &\quad + \Big[S^{(1)_s}_g\, (\epsilon_3 \cdot f_2 \cdot \epsilon_1)\Big] \mathcal{A}_{\text{BAS}}(1,2,3|\sigma_4\backslash s).\end{aligned} \tag{29}$$

Here, P_1 is obtained by applying the sub-leading soft operator $S^{(1)_s}_g$ to YMS or BAS amplitudes, and P_2 is obtained by acting $S^{(1)_s}_g$ on coefficients.

Our objective is to deduce the expanded formula of $\mathcal{A}_{\text{YM}}(\sigma_4)$ from the soft behavior of $\mathcal{A}^{(1)s}_{\text{YM}}(\sigma_4)$. Hence, it becomes imperative to construe $\mathcal{A}^{(1)s}_{\text{YM}}(\sigma_4)$ as a synthesis of the soft behaviors inherent in the constituent components of the expansion. Here, by "components," we refer to the individual constituents akin to $\mathcal{A}^{(1)_s}_{\text{YMS}}$ and $\mathcal{A}^{(0)_s}_{\text{BAS}}$ within the expansion. For the P_1 part, the soft theorem suggests

$$P_1 = \big(\epsilon_3 \cdot \epsilon_1\big)\, \mathcal{A}^{(1)_s}_{\text{YMS}}(1,3;s,2|\sigma_4) + \big(\epsilon_3 \cdot f_2 \cdot \epsilon_1\big)\, \mathcal{A}^{(1)_s}_{\text{YMS}}(1,2,3;s|\sigma_4). \tag{30}$$

The second part P_2 can be evaluated by applying relations (20) and (21),

$$\begin{aligned}P_2 &= \big(\epsilon_3 \cdot f_s \cdot \epsilon_1\big)\left(\frac{\delta_{1s}}{s_{1s}} + \frac{\delta_{s3}}{s_{s3}}\right) \mathcal{A}_{\text{YMS}}(1,3;2|\sigma_4\backslash s)\\ &\quad + \big(\epsilon_3 \cdot f_2 \cdot f_s \cdot \epsilon_1\big)\left(\frac{\delta_{1s}}{s_{1s}} + \frac{\delta_{s2}}{s_{s2}}\right) \mathcal{A}_{\text{BAS}}(1,2,3|\sigma_4\backslash s)\\ &\quad + \big(\epsilon_3 \cdot f_s \cdot f_2 \cdot \epsilon_1\big)\left(\frac{\delta_{2s}}{s_{2s}} + \frac{\delta_{s3}}{s_{s3}}\right) \mathcal{A}_{\text{BAS}}(1,2,3|\sigma_4\backslash s).\end{aligned} \tag{31}$$

Since the symbol δ_{ab} will not appear in the expansion of $\mathcal{A}_{\text{YM}}(\sigma_4)$, it should be absorbed into the soft behaviors of YMS amplitudes. By applying the soft theorem (7) and (8) for the BAS scalars, we can recognize that

$$\begin{aligned}\left(\frac{\delta_{1s}}{s_{1s}} + \frac{\delta_{s2}}{s_{s2}}\right) \mathcal{A}_{\text{BAS}}(1,2,3|\sigma_4\backslash s) &= \tau\, \mathcal{A}^{(0)_s}_{\text{BAS}}(1,s,2,3|\sigma_4),\\ \left(\frac{\delta_{2s}}{s_{2s}} + \frac{\delta_{s3}}{s_{s3}}\right) \mathcal{A}_{\text{BAS}}(1,2,3|\sigma_4\backslash s) &= \tau\, \mathcal{A}^{(0)_s}_{\text{BAS}}(1,2,s,3|\sigma_4).\end{aligned} \tag{32}$$

This observation eliminates δ_{ab} in second and third lines in (31). Then we turn to the first line in (31). Expanding $\mathcal{A}_{\text{YMS}}(1,3;2|\sigma_4 \setminus s)$ as in (22), we get

$$\begin{aligned}&\left(\frac{\delta_{1s}}{s_{1s}} + \frac{\delta_{s3}}{s_{s3}}\right) \mathcal{A}_{\text{YMS}}(1,3;2|\sigma_4\backslash s)\\ &= (\epsilon_2 \cdot k_1)\left(\frac{\delta_{1s}}{s_{1s}} + \frac{\delta_{s3}}{s_{s3}}\right) \mathcal{A}_{\text{BAS}}(1,2,3|\sigma_4\backslash s)\\ &= (\epsilon_2 \cdot k_1)\left(\frac{\delta_{1s}}{s_{1s}} + \frac{\delta_{s2}}{s_{s2}} + \frac{\delta_{2s}}{s_{2s}} + \frac{\delta_{s3}}{s_{s3}}\right) \mathcal{A}_{\text{BAS}}(1,2,3|\sigma_4\backslash s)\\ &= \tau\, (\epsilon_2 \cdot k_1)\, \mathcal{A}^{(0)_s}_{\text{BAS}}(1, 2 \sqcup s, 3|\sigma_4).\end{aligned} \tag{33}$$

The second equality relies on the property $\delta_{ab} = -\delta_{ba}$, while the third equality is predicated on the soft theorem as given in Eq. (7). Adding all of these terms together, we obtain

$$\begin{aligned}\mathcal{A}^{(1)_s}_{\text{YM}}(\sigma_4) &= \big(\epsilon_3 \cdot \epsilon_1\big)\, \mathcal{A}^{(1)_s}_{\text{YMS}}(1,3;s,2|\sigma_4)\\ &\quad + \big(\epsilon_3 \cdot f_2 \cdot \epsilon_1\big)\, \mathcal{A}^{(1)_s}_{\text{YMS}}(1,2,3;s|\sigma_4)\\ &\quad + \tau\Big[\big(\epsilon_3 \cdot f_s \cdot \epsilon_1\big)\big(\epsilon_2 \cdot k_1\big) \mathcal{A}^{(0)_s}_{\text{BAS}}(1, 2 \sqcup s, 3|\sigma_4)\\ &\quad + \big(\epsilon_3 \cdot f_2 \cdot f_s \cdot \epsilon_1\big)\, \mathcal{A}^{(0)_s}_{\text{BAS}}(1,s,2,3|\sigma_4)\\ &\quad + \big(\epsilon_3 \cdot f_s \cdot f_2 \cdot \epsilon_1\big)\, \mathcal{A}^{(0)_s}_{\text{BAS}}(1,2,s,3|\sigma_4)\Big].\end{aligned} \tag{34}$$

Some discussions are warranted regarding the expansion in (37). This expansion is derived by examining the soft behavior at the sub-leading order. The reason for selecting the sub-leading order rather than the leading one is that the leading-order contributions from the third, fourth, and fifth terms in (37) are of order τ^0, while $\mathcal{A}^{(0)_s}_{\text{YM}}(\sigma_4)$ is of order τ^{-1}. Consequently, these terms cannot be detected through the leading-order soft behavior of $\mathcal{A}^{(0)_s}_{\text{YM}}(\sigma_4)$. This leads to a natural question: does the full expansion include a term whose leading-order soft behavior is of order τ^1, making it undetectable when examining $\mathcal{A}^{(1)_s}_{\text{YM}}(\sigma_4)$?. We can rule out this possibility through the following argument. If such a term were to exist, it must involve a coefficient that is bilinear in k_s, since the leading-order soft behavior of each YMS amplitude is of order τ^{-1}. Consequently, the symmetry between legs s and 2 would imply the existence of another term featuring a coefficient that is bilinear in k_2. However, the new term with a coefficient bilinear in k_2 should be detectable when examining $\mathcal{A}^{(1)_s}_{\text{YM}}(\sigma_4)$ because mass dimension considerations prohibit the coefficient from being bilinear in both k_2 and k_s. Intriguingly, the associated contribution is conspicuously absent in (34). Consequently, we can confidently assert that the hypothesized undetectable term with leading-order behavior of τ^1 does not exist.

Next, we will go through each term step by step to demonstrate how to reconstruct the original amplitude $\mathcal{A}_{\text{YM}}(\sigma_4)$ from this soft behavior.

- $(\epsilon_3 \cdot \epsilon_1)\, \mathcal{A}^{(1)_s}_{\text{YMS}}(1, 3; s, 2|\sigma_4)$
  It is evident that this term arises from the expansion represented by $\big(\epsilon_3 \cdot \epsilon_1\big)\, \mathcal{A}_{\text{YMS}}(1, 3; s, 2|\sigma_4)$.
- $(\epsilon_3 \cdot f_2 \cdot \epsilon_1)\, \mathcal{A}^{(1)_s}_{\text{YMS}}(1, 2, 3; s|\sigma_4)$
  Due to the fact that k_s does not contribute to the leading-order terms, the coefficients resembling $(\epsilon_3 \cdot f_2' \cdot \epsilon_1)$ are all at leading order $\big(\epsilon_3 \cdot f_2 \cdot \epsilon_1\big)$. Where

$$(f_2')^{\mu\nu} \equiv (k_2^\mu + x k_s^\mu)\epsilon_2^\nu - \epsilon_2^\mu (k_2^\nu + y k_s^\nu), \tag{35}$$

  where x, y can take arbitrary constant values. Therefore, this term may originate from $(\epsilon_3 \cdot f_2' \cdot \epsilon_1)\mathcal{A}_{\text{YMS}}(1, 2, 3; s|\sigma_4)$ in the expansion. On the other hand, besides $\big(\epsilon_3 \cdot f_2 \cdot \epsilon_1\big)\, \mathcal{A}^{(1)_s}_{\text{YMS}}(1, 2, 3; s|\sigma_4)$, the sub-leading order of $(\epsilon_3 \cdot f_2' \cdot \epsilon_1)\mathcal{A}_{\text{YMS}}(1, 2, 3; s|\sigma_4)$ after rescale $k_s \to \tau k_s$ also contains

$$\tau\,\big(x(\epsilon_3 \cdot k_s)(\epsilon_2 \cdot \epsilon_1) - y(\epsilon_3 \cdot \epsilon_2)(k_s \cdot \epsilon_1)\big)\, \mathcal{A}^{(0)_s}_{\text{YMS}}(1, 2, 3; s|\sigma_4). \tag{36}$$

  Compared with (34), we observe that this kind of sub-leading soft behavior has not been detected, i,e, $x = y = 0$. In summary, the second term arises from $\big(\epsilon_3 \cdot f_2 \cdot \epsilon_1\big)\, \mathcal{A}_{\text{YMS}}(1, 2, 3; s|\sigma_4)$.
- $(\epsilon_3 \cdot f_s \cdot \epsilon_1)(\epsilon_2 \cdot k_1)\mathcal{A}^{(0)_s}_{\text{BAS}}(1, 2 \sqcup s, 3|\sigma_4)$
  The treatment of the third term, however, can be somewhat intricate. In addition, We anticipate that the expansion of $\mathcal{A}_{\text{YM}}(\sigma_4)$ should remain invariant under the interchange of 2 and s because both 2 and s represent on-shell massless particles that have not been fixed at any ends in the color orderings. Therefore, the appearance of $\big(\epsilon_3 \cdot f_2 \cdot \epsilon_1\big)\, \mathcal{A}_{\text{YMS}}(1, 2, 3; s|\sigma_4)$ in the expansion of $\mathcal{A}_{\text{YM}}(\sigma_4)$ inevitably leads to the appearance of $\big(\epsilon_3 \cdot f_s \cdot \epsilon_1\big)\, \mathcal{A}_{\text{YMS}}(1, s, 3; 2|\sigma_4)$. On the other hand, we can derived the following relationship:

$$\mathcal{A}^{(0)_s}_{\text{YMS}}(1, s, 3; 2|\sigma_4) = (\epsilon_2 \cdot k_1)\, \mathcal{A}^{(0)_s}_{\text{BAS}}(1, 2 \sqcup s, 3|\sigma_4).$$

  This equality can be confirmed by substituting the expansion (22) and observing that k_s does not contribute to Y_2 at the leading order. This confirms that the third term in Eq. (34) indeed arises from the sub-leading order soft behavior of $\big(\epsilon_3 \cdot f_s \cdot \epsilon_1\big)\, \mathcal{A}_{\text{YMS}}(1, s, 3; 2|\sigma_4)$.
- $\big(\epsilon_3 \cdot f_2 \cdot f_s \cdot \epsilon_1\big)\, \mathcal{A}^{(0)_s}_{\text{BAS}}(1, s, 2, 3|\sigma_4)$ and $\big(\epsilon_3 \cdot f_s \cdot f_2 \cdot \epsilon_1\big)\, \mathcal{A}^{(0)_s}_{\text{BAS}}(1, 2, s, 3|\sigma_4)$
  Naively, these two terms may come from $\big(\epsilon_3 \cdot f_2' \cdot f_s \cdot \epsilon_1\big)\, \mathcal{A}_{\text{BAS}}(1, s, 2, 3|\sigma_4)$ and $\big(\epsilon_3 \cdot f_s \cdot f_2' \cdot \epsilon_1\big)\, \mathcal{A}_{\text{BAS}}(1, 2, s, 3|\sigma_4)$ respectively, with f_2' defined in (35). However, from the discussion above, we realize that the coefficients in the expansion of $\mathcal{A}_{\text{YM}}(\sigma_4)$ do not involve terms proportional to the square of k_s or higher-order terms. Therefore, these two terms exclusively originate from $\big(\epsilon_3 \cdot f_2 \cdot f_s \cdot \epsilon_1\big)\, \mathcal{A}_{\text{BAS}}(1, s, 2, 3|\sigma_4)$ and $\big(\epsilon_3 \cdot f_s \cdot f_2 \cdot \epsilon_1\big)\, \mathcal{A}_{\text{BAS}}(1, 2, s, 3|\sigma_4)$.

Finally, we observe the desired expansion of four-point amplitude:

$$\begin{aligned}\mathcal{A}^{\text{I}}_{\text{YM}}(\sigma_4) = &\big(\epsilon_3 \cdot \epsilon_1\big)\, \mathcal{A}_{\text{YMS}}(1, 3; s, 2|\sigma_4)\\ &+\big(\epsilon_3 \cdot f_2 \cdot \epsilon_1\big)\, \mathcal{A}_{\text{YMS}}(1, 2, 3; s|\sigma_4)\\ &+\big(\epsilon_3 \cdot f_s \cdot \epsilon_1\big)\, \mathcal{A}_{\text{YMS}}(1, s, 3; 2|\sigma_4)\\ &+\big(\epsilon_3 \cdot f_2 \cdot f_s \cdot \epsilon_1\big)\, \mathcal{A}_{\text{BAS}}(1, s, 2, 3|\sigma_4)\\ &+\big(\epsilon_3 \cdot f_s \cdot f_2 \cdot \epsilon_1\big)\, \mathcal{A}_{\text{BAS}}(1, 2, s, 3|\sigma_4).\end{aligned} \tag{37}$$

It can be seen that this expression (37) remains invariant under the exchange of external legs 2 and s. To obtain the full expression of the four-point Yang–Mills amplitude of tree level, the YMS amplitude in the above equation is expanded into the BAS amplitude, as detailed in Appendix 1.

3.3 General case

In this subsection, we construct the expansion of general color ordered YM amplitudes $\mathcal{A}_{\text{YM}}(\sigma_n)$, by applying the recursive method in the previous Sect. 3.2 iteratively.

The main result of this subsection is the expansion

$$\mathcal{A}^{\text{I}}_{\text{YM}}(\sigma_n) = \sum_{\vec{\boldsymbol{\alpha}}} \big(\epsilon_n \cdot F_{\vec{\boldsymbol{\alpha}}} \cdot \epsilon_1\big)\, \mathcal{A}_{\text{YMS}}(1, \vec{\boldsymbol{\alpha}}, n; \{2, \ldots, n-1\} \backslash \boldsymbol{\alpha}|\sigma_n), \tag{38}$$

where $\boldsymbol{\alpha}$ denotes a subset of external legs in $\{2, \ldots, n-1\}$ which is allowed to be empty, and the ordered set $\vec{\boldsymbol{\alpha}}$ is generated from $\boldsymbol{\alpha}$ by endowing an order among elements in $\boldsymbol{\alpha}$. The tensor $F^{\mu\nu}_{\vec{\boldsymbol{\alpha}}}$ is defined as

$$F^{\mu\nu}_{\vec{\boldsymbol{\alpha}}} \equiv \left(f_{\alpha_k} \cdot f_{\alpha_{k-1}} \cdots f_{\alpha_2} \cdot f_{\alpha_1}\right)^{\mu\nu}, \tag{39}$$

for $\vec{\boldsymbol{\alpha}} = \{\alpha_1, \ldots \alpha_k\}$. The summation in (38) is among all nonequivalent ordered sets $\vec{\boldsymbol{\alpha}}$. In other words, one should sum over all subsets $\boldsymbol{\alpha}$ of $\{2, \ldots, n-1\}$, as well as all un-cyclic permutations of elements in $\boldsymbol{\alpha}$. Evidently, the general formula (38) is satisfied by the expansions of three-point and four-point amplitudes, as shown in (27) and (37). In the remainder of this subsection, we will illustrate that if the formula (38) holds for m-point amplitudes, it also extends to $(m+1)$-point ones. Consequently, we can iteratively ensure the validity of the general expansion (38). This process shares many similarities with the one described in the previous Sect. 3.2, and as such, we will skip various details. An explicit five-point example is provided in Appendix 1.

We can denote the external legs of the $(m+1)$-point amplitude as $s \cup 1, \cdots, m$ and investigate the soft behavior associated with the external leg s. The sub-leading order soft behavior of the $(m+1)$-point amplitude is expressed as follows:

$$\begin{aligned}\mathcal{A}^{(1)_s}_{\rm YM}(\sigma_{m+1}) &= S^{(1)_s}_g\, \mathcal{A}^{\rm I}_{\rm YM}(\sigma_{m+1}\backslash s)\\ &= S^{(1)_s}_g \Big[\sum_{\vec{\boldsymbol{\alpha}}} \left(\epsilon_n \cdot F_{\vec{\boldsymbol{\alpha}}} \cdot \epsilon_1\right)\\ &\qquad \mathcal{A}_{\rm YMS}(1, \vec{\boldsymbol{\alpha}}, m; \{2, \ldots, m-1\}\backslash\boldsymbol{\alpha}|\sigma_{m+1}\backslash s)\Big]\\ &= P_1 + P_2,\end{aligned} \tag{40}$$

where P_1 and P_2 are given as

$$\begin{aligned}P_1 = &\sum_{\vec{\boldsymbol{\alpha}}} \left(\epsilon_n \cdot F_{\vec{\boldsymbol{\alpha}}} \cdot \epsilon_1\right) \Big[S^{(1)_s}_g\\ &\mathcal{A}_{\rm YMS}(1, \vec{\boldsymbol{\alpha}}, m; \{2, \ldots, m-1\}\backslash\boldsymbol{\alpha}|\sigma_{m+1}\backslash s)\Big],\end{aligned} \tag{41}$$

and

$$\begin{aligned}P_2 = &\sum_{\vec{\boldsymbol{\alpha}}} \Big[S^{(1)_s}_g \left(\epsilon_n \cdot F_{\vec{\boldsymbol{\alpha}}} \cdot \epsilon_1\right)\Big]\\ &\mathcal{A}_{\rm YMS}(1, \vec{\boldsymbol{\alpha}}, m; \{2, \ldots, m-1\}\backslash\boldsymbol{\alpha}|\sigma_{m+1}\backslash s).\end{aligned} \tag{42}$$

The soft theorem (15) leads to

$$\begin{aligned}P_1 = &\sum_{\vec{\boldsymbol{\alpha}}} \left(\epsilon_n \cdot F_{\vec{\boldsymbol{\alpha}}} \cdot \epsilon_1\right)\\ &\mathcal{A}^{(1)_s}_{\rm YMS}(1, \vec{\boldsymbol{\alpha}}, m; s \cup \{2, \ldots, m-1\}\backslash\boldsymbol{\alpha}|\sigma_{m+1}).\end{aligned} \tag{43}$$

The block P_2 can be calculated as

$$\begin{aligned}P_2 = &\sum_{\vec{\boldsymbol{\alpha}}} \left(\epsilon_n \cdot F_{\vec{\boldsymbol{\alpha}}\sqcup s} \cdot \epsilon_1\right)\left(\frac{\delta_{s_l s}}{s_{s_l s}} + \frac{\delta_{s s_r}}{s_{s r}}\right)\\ &\mathcal{A}_{\rm YMS}(1, \vec{\boldsymbol{\alpha}}, m; \{2, \cdots, m-1\}\backslash\boldsymbol{\alpha}|\sigma_{m+1}\backslash s),\end{aligned} \tag{44}$$

by using relations in (20) and (21). The notation s_l denotes the adjacent leg of s which is at the l.h.s of s in $\vec{\boldsymbol{\alpha}} \sqcup s$, while s_r denotes the r.h.s one. Using the argument the same as that from previous subsection, we arrive at

$$\begin{aligned}P_2 = &\sum_{\vec{\boldsymbol{\alpha}}} \left(\epsilon_n \cdot F_{\vec{\boldsymbol{\alpha}}\sqcup s} \cdot \epsilon_1\right)\\ &\mathcal{A}^{(0)_s}_{\rm YMS}(1, \vec{\boldsymbol{\alpha}} \sqcup s, m; \{2, \ldots, m-1\}\backslash\boldsymbol{\alpha}|\sigma_{m+1}).\end{aligned} \tag{45}$$

Combining (43) and (45) together leads to

$$\begin{aligned}\mathcal{A}^{(1)_s}_{\rm YM}(\sigma_{m+1}) = &\sum_{\vec{\boldsymbol{\alpha}}} \left(\epsilon_n \cdot F_{\vec{\boldsymbol{\alpha}}} \cdot \epsilon_1\right)^{(0)_s}\\ &\quad\mathcal{A}^{(1)_s}_{\rm YMS}(1, \vec{\boldsymbol{\alpha}}, m; s \cup \{2, \cdots, m-1\}\backslash\boldsymbol{\alpha}|\sigma_{m+1})\\ &+\sum_{\vec{\boldsymbol{\alpha}}} \left(\epsilon_n \cdot F_{\vec{\boldsymbol{\alpha}}\sqcup s} \cdot \epsilon_1\right)^{(0)_s}\\ &\quad\mathcal{A}^{(0)_s}_{\rm YMS}(1, \vec{\boldsymbol{\alpha}} \sqcup s, m; \{2, \ldots, m-1\}\backslash\boldsymbol{\alpha}|\sigma_{m+1}),\end{aligned} \tag{46}$$

which indicates the expansion

$$\begin{aligned}\mathcal{A}_{\rm YM}(\sigma_{m+1}) = &\sum_{\vec{\boldsymbol{\alpha}}} \left(\epsilon_n \cdot F_{\vec{\boldsymbol{\alpha}}} \cdot \epsilon_1\right)\\ &\quad\mathcal{A}_{\rm YMS}(1, \vec{\boldsymbol{\alpha}}, m; s \cup \{2, \ldots, m-1\}\backslash\boldsymbol{\alpha}|\sigma_{m+1})\\ &+\sum_{\vec{\boldsymbol{\alpha}}} \left(\epsilon_n \cdot F_{\vec{\boldsymbol{\alpha}}\sqcup s} \cdot \epsilon_1\right)\\ &\quad\mathcal{A}_{\rm YMS}(1, \vec{\boldsymbol{\alpha}} \sqcup s, m; \{2, \ldots, m-1\}\backslash\boldsymbol{\alpha}|\sigma_{m+1})\\ = &\sum_{\vec{\boldsymbol{\alpha}}''} \left(\epsilon_n \cdot F_{\vec{\boldsymbol{\alpha}}''} \cdot \epsilon_1\right)\\ &\quad\mathcal{A}_{\rm YMS}(1, \vec{\boldsymbol{\alpha}}'', m; s \cup \{2, \ldots, m-1\}\backslash\boldsymbol{\alpha}''|\sigma_{m+1}).\end{aligned} \tag{47}$$

The final line in (47) corresponds to the expanded formula (38) applicable to the $(m+1)$-point case. It's worth noting that each set $\boldsymbol{\alpha}$ in (47) represents a subset of $\{2, \ldots, m-1\}$ excluding the leg s, while each $\boldsymbol{\alpha}''$ denotes a subset of $s \cup \{2, \ldots, m-1\}$.

Hence, the general expansion formula (38) is proven to be valid for $(m+1)$-point amplitudes when it has been established for m-point amplitudes and demonstrated for three-point and four-point amplitudes. This conclusion is derived through a mathematical induction argument.

4 Manifests the gauge invariance

The expansion presented in (38) does not inherently exhibit gauge invariance for all polarizations, including ϵ_1 and ϵ_n. In this section, we establish an expansion that explicitly maintains gauge invariance through two distinct approaches. The first approach, detailed in Sect. 4.1, involves a direct modification of (38), incorporating the gauge invariance condition. While this approach requires the imposition of gauge invariance rather than its proof, it serves as a valuable starting point. To address the logical concern associated with the first construction, we introduce the second approach in Sect. 4.2. In this approach, we utilize the recursive technique established in the previous Sect. 3. The key difference lies in the modification of the starting point of the recursion,i.e, the three-point amplitude, ensuring that the expression at this initial stage exhibits explicit gauge invariance. Subsequently, at each step of the recursion, we insert soft particles while maintaining this manifest gauge invariance. Ultimately, this process allows us to construct an expansion that ensures gauge invariance without the need for explicit requirements.

4.1 Direct construction

In the expansion (38), gauge invariance is manifest for polarizations ϵ_i with $i \in \{2, \ldots, n-1\}$ because the tensor $f_i^{\mu\nu}$ automatically vanishes under the replacement $\epsilon_i \to k_i$. However, ensuring gauge invariance for polarizations ϵ_1 and ϵ_n is not as straightforward. To obtain an expansion formula that also explicitly demonstrates gauge invariance for ϵ_1 and ϵ_n, one can impose the following gauge invariance conditions:

$$
\begin{aligned}
A_n &= \sum_{\vec{\boldsymbol{\alpha}}} \left(\epsilon_n \cdot F_{\vec{\boldsymbol{\alpha}}} \cdot k_1\right) \\
&\quad \mathcal{A}_{\mathrm{YMS}}(1, \vec{\boldsymbol{\alpha}}, n; \{2, \ldots, n-1\} \backslash \boldsymbol{\alpha} | \sigma_n) = 0, \\
B_n &= \sum_{\vec{\boldsymbol{\alpha}}} \left(k_n \cdot F_{\vec{\boldsymbol{\alpha}}} \cdot \epsilon_1\right) \\
&\quad \mathcal{A}_{\mathrm{YMS}}(1, \vec{\boldsymbol{\alpha}}, n; \{2, \ldots, n-1\} \setminus \boldsymbol{\alpha} | \sigma_n) = 0, \\
C_n &= \sum_{\vec{\boldsymbol{\alpha}}} \left(k_n \cdot F_{\vec{\boldsymbol{\alpha}}} \cdot k_1\right) \\
&\quad \mathcal{A}_{\mathrm{YMS}}(1, \vec{\boldsymbol{\alpha}}, n; \{2, \ldots, n-1\} \setminus \boldsymbol{\alpha} | \sigma_n) = 0,
\end{aligned} \tag{48}
$$

which are obtained from (38) by replacing ϵ_1 or ϵ_n with k_1 or k_n, respectively. These conditions lead to the following new formula,

$$
\mathcal{A}^{\mathrm{II}}_{\mathrm{YM}}(\sigma_n) = -\sum_{\vec{\boldsymbol{\alpha}}} \frac{\mathrm{tr}\left(f_n \cdot F_{\vec{\boldsymbol{\alpha}}} \cdot f_1\right)}{k_n \cdot k_1} \mathcal{A}_{\mathrm{YMS}}(1, \vec{\boldsymbol{\alpha}}, n; \{2, \ldots, n-1\} \backslash \boldsymbol{\alpha} | \sigma_n), \tag{49}
$$

since

$$
\mathcal{A}^{\mathrm{II}}_{\mathrm{YM}}(\sigma_n) = \mathcal{A}^{\mathrm{I}}_{\mathrm{YM}}(\sigma_n) - \frac{k_n \cdot \epsilon_1}{k_n \cdot k_1} A_n - \frac{\epsilon_n \cdot k_1}{k_n \cdot k_1} B_n + \frac{\epsilon_n \cdot \epsilon_1}{k_n \cdot k_1} C_n, \tag{50}
$$

where $\mathcal{A}^{\mathrm{I}}_{\mathrm{YM}}(\sigma_n)$ is the expanded formula in (38). The explicit four-point and five-point examples for the expansion (49) are given in Appendix A.

In the above construction, we required the gauge invariance for polarizations ϵ_1 and ϵ_n, namely, $A_n = B_n = C_n = 0$. However, it is quite non-trivial to prove this property for general n. To ensure this gauge invariance condition, one must derive the expansion (38) from a manifestly gauge invariant framework, such as Lagrangian or CHY formalism. Thus, if we insist the spirit of constructing YM amplitudes recursively from lowest-point ones, without respecting other frameworks, the above construction is not so satisfactory.

4.2 Recursive derivation

For the expansion of the simplest three-point amplitudes in (27), the gauge invariance for polarization ϵ_1 or ϵ_3 is easy to be observed. For example, replacing ϵ_3 by k_3 in (38) yields

$$
\begin{aligned}
\mathcal{A}^{\mathrm{I}}_{\mathrm{YM}}(\sigma_3)\Big|_{\epsilon_3 \to k_3} &= \left(k_3 \cdot \epsilon_1\right) \mathcal{A}_{\mathrm{YMS}}(1, 3; 2|\sigma_3) \\
&\quad - \left(k_3 \cdot \epsilon_2\right) \left(k_2 \cdot \epsilon_1\right) \mathcal{A}_{\mathrm{BAS}}(1, 2, 3|\sigma_3),
\end{aligned} \tag{51}
$$

where we have used $k_3 \cdot k_2 = 0$ due to momentum conservation and on-shell condition. By utilizing (22) to expand $\mathcal{A}_{\mathrm{YMS}}(1, 3; 2|\sigma_3)$ into the BAS amplitude $\mathcal{A}_{\mathrm{BAS}}(1, 2, 3|\sigma_3)$, we can readily verify that $\mathcal{A}^{\mathrm{I}}_{\mathrm{YM}}(\sigma_3)\Big|\epsilon_3 \to k_3 = 0$. This corresponds to the gauge invariance condition stated in the second line of (48) for the case of three-point amplitudes. Similar verifications apply to the other two conditions in (48). Consequently, we can transform the expansion (27) into a new formulation denoted as $\mathcal{A}^{\mathrm{II}}_{\mathrm{YM}}(\sigma_3)$, which is expressed as:

$$
\begin{aligned}
\mathcal{A}^{\mathrm{II}}_{\mathrm{YM}}(\sigma_3) &= -\frac{\mathrm{tr}\left(f_3 \cdot f_1\right)}{k_3 \cdot k_1} \mathcal{A}_{\mathrm{YMS}}(1, 3; 2|\sigma_3) \\
&\quad - \frac{\mathrm{tr}\left(f_3 \cdot f_2 \cdot f_1\right)}{k_3 \cdot k_1} \mathcal{A}_{\mathrm{BAS}}(1, 2, 3|\sigma_3).
\end{aligned} \tag{52}
$$

Next, we will start from expression (52) and repeat the procedure outlined in Sect. (3.3) to iteratively construct an alternative expansion form of $\mathcal{A}^{\mathrm{II}}_{\mathrm{YM}}(\sigma_n)$ using lower-point amplitudes. Simultaneously, we will recursively observe that $A_n = B_n = C_n = 0$ in (48) holds for any n, which establishes the gauge invariance for polarizations ϵ_1 and ϵ_n in the expansion (38).

First, let's make the following inductive assumption: (A) The expansion (49) that maintains manifestness of all polarization vectors is valid for all $n \leq m$. (B) The gauge invariance condition (48) $A_n = B_n = C_n = 0$ holds for all $n \leq m$. As shown above, these two conditions hold when $n = 3$. Therefore, we have obtained the starting point for the inductive proof. We need to prove that these two conditions hold for $n = m + 1$ as well. The sub-leading soft behavior of $\mathcal{A}^{\mathrm{II}}_{\mathrm{YM}}(\sigma_{m+1})$ can be expressed as

$$
\begin{aligned}
\mathcal{A}^{(1)_s}_{\mathrm{YM}}(\sigma_{m+1}) &= S^{(1)_s}_g \mathcal{A}^{\mathrm{II}}_{\mathrm{YM}}(\sigma_{m+1} \backslash s) \\
&= S^{(1)_s}_g \Bigg[-\sum_{\vec{\boldsymbol{\alpha}}} \frac{\mathrm{tr}\left(f_m \cdot F_{\vec{\boldsymbol{\alpha}}} \cdot f_1\right)}{k_m \cdot k_1} \\
&\quad \mathcal{A}_{\mathrm{YMS}}(1, \vec{\boldsymbol{\alpha}}, m; \{2, \ldots, m-1\} \backslash \boldsymbol{\alpha} | \sigma_{m+1} \backslash s) \Bigg] \\
&= P_1 + P_2,
\end{aligned} \tag{53}
$$

where

$$P_1 = -\sum_{\vec{\boldsymbol{\alpha}}} \frac{\mathrm{tr}\left(f_m \cdot F_{\vec{\boldsymbol{\alpha}}} \cdot f_1\right)}{k_m \cdot k_1} \mathcal{A}^{(1)_s}_{\mathrm{YMS}}(1, \vec{\boldsymbol{\alpha}}, m; s \cup \{2, \ldots, m-1\} \backslash \boldsymbol{\alpha} | \sigma_{m+1}) \tag{54}$$

is obtained by acting the operator $S^{(1)_s}_g$ on YMS amplitudes, while P_2 is obtained by acting $S^{(1)_s}_g$ on coefficients. The block P_2 can be evaluated as

$$\begin{aligned} P_2 = &-\sum_{\vec{\boldsymbol{\alpha}}} \frac{\mathrm{tr}\left(f_m \cdot F_{\vec{\boldsymbol{\alpha}} \sqcup s} \cdot f_1\right)}{k_m \cdot k_1} \left(\frac{\delta_{s_l s}}{s_{s_l s}} + \frac{\delta_{s s_r}}{s_{s s_r}}\right) \\ &\mathcal{A}_{\mathrm{YMS}}(1, \vec{\boldsymbol{\alpha}}, m; \{2, \ldots, m-1\} \backslash \boldsymbol{\alpha} | \sigma_{m+1} \backslash s) \\ &-\sum_{\vec{\boldsymbol{\alpha}}} \frac{\mathrm{tr}\left(f_m \cdot F_{\vec{\boldsymbol{\alpha}}} \cdot f_1 \cdot f_s\right)}{k_m \cdot k_1} \left(\frac{\delta_{ms}}{s_{ms}} + \frac{\delta_{s1}}{s_{s1}}\right) \\ &\mathcal{A}_{\mathrm{YMS}}(1, \vec{\boldsymbol{\alpha}}, m; \{2, \ldots, m-1\} \backslash \boldsymbol{\alpha} | \sigma_{m+1} \backslash s) \\ &+\frac{k_m \cdot f_s \cdot k_1}{k_m \cdot k_1} \left(\frac{\delta_{1s}}{s_{1s}} + \frac{\delta_{sm}}{s_{sm}}\right) \Big[\sum_{\vec{\boldsymbol{\alpha}}} \frac{\mathrm{tr}\left(f_m \cdot F_{\vec{\boldsymbol{\alpha}}} \cdot f_1\right)}{k_m \cdot k_1} \\ &\mathcal{A}_{\mathrm{YMS}}(1, \vec{\boldsymbol{\alpha}}, m; \{2, \ldots, m-1\} \backslash \boldsymbol{\alpha} | \sigma_{m+1} \backslash s) \Big], \end{aligned} \tag{55}$$

notice that the last line arises from acting the soft operator on the denominator $k_n \cdot k_1$ in (53). The first line in (55) can be recognized as

$$P_{21} = -\sum_{\vec{\boldsymbol{\alpha}}} \frac{\mathrm{tr}\left(f_m \cdot F_{\vec{\boldsymbol{\alpha}} \sqcup s} \cdot f_1\right)}{k_m \cdot k_1} \mathcal{A}^{(0)_s}_{\mathrm{YMS}}(1, \vec{\boldsymbol{\alpha}} \sqcup s, m; \{2, \ldots, m-1\} \backslash \boldsymbol{\alpha} | \sigma_{m+1}), \tag{56}$$

via the technique from (44) to (45). Then we combine the second and third lines in (55) and regroup them as

$$\begin{aligned} P_{22} = &\mathcal{C}_1 \Big[\sum_{\vec{\boldsymbol{\alpha}}} \left(\epsilon_m \cdot F_{\vec{\boldsymbol{\alpha}}} \cdot \epsilon_1\right) \\ &\mathcal{A}_{\mathrm{YMS}}(1, \vec{\boldsymbol{\alpha}}, m; \{2, \ldots, m-1\} \backslash \boldsymbol{\alpha} | \sigma_{m+1} \backslash s) \Big] \\ &+\mathcal{C}_2 \Big[\sum_{\vec{\boldsymbol{\alpha}}} \left(\epsilon_m \cdot F_{\vec{\boldsymbol{\alpha}}} \cdot k_1\right) \\ &\mathcal{A}_{\mathrm{YMS}}(1, \vec{\boldsymbol{\alpha}}, m; \{2, \ldots, m-1\} \backslash \boldsymbol{\alpha} | \sigma_{m+1} \backslash s) \Big] \\ &+\mathcal{C}_3 \Big[\sum_{\vec{\boldsymbol{\alpha}}} \left(k_m \cdot F_{\vec{\boldsymbol{\alpha}}} \cdot \epsilon_1\right) \\ &\mathcal{A}_{\mathrm{YMS}}(1, \vec{\boldsymbol{\alpha}}, m; \{2, \ldots, m-1\} \backslash \boldsymbol{\alpha} | \sigma_{m+1} \backslash s) \Big] \\ &+\mathcal{C}_4 \Big[\sum_{\vec{\boldsymbol{\alpha}}} \left(k_m \cdot F_{\vec{\boldsymbol{\alpha}}} \cdot k_1\right) \\ &\mathcal{A}_{\mathrm{YMS}}(1, \vec{\boldsymbol{\alpha}}, m; \{2, \ldots, m-1\} \backslash \boldsymbol{\alpha} | \sigma_{m+1} \backslash s) \Big], \end{aligned} \tag{57}$$

where coefficients $\mathcal{C}_i$ with $i \in \{1, \cdots, 4\}$ are independent of ordered sets $\vec{\boldsymbol{\alpha}}$. Using $\delta_{ab} = \delta_{ba}$ and $k_m \cdot f_s \cdot k_1 = -k_1 \cdot f_s \cdot k_m$, we find $\mathcal{C}_1 = 0$. Then remaining three lines in (57) vanish automatically, due to the gauge invariance conditions in (48) for m-point amplitudes by the condition (A) of the induction hypothesis. Thus we obtain

$$\begin{aligned} \mathcal{A}^{(1)_s}_{\mathrm{YM}}(\sigma_{m+1}) = &\ P_1 + P_{21} \\ = &-\sum_{\vec{\boldsymbol{\alpha}}} \frac{\mathrm{tr}\left(f_m \cdot F_{\vec{\boldsymbol{\alpha}}} \cdot f_1\right)}{k_m \cdot k_1} \\ &\mathcal{A}^{(1)_s}_{\mathrm{YMS}}(1, \vec{\boldsymbol{\alpha}}, m; s \cup \{2, \ldots, m-1\} \setminus \boldsymbol{\alpha} | \sigma_{m+1}) \\ &-\sum_{\vec{\boldsymbol{\alpha}}} \frac{\mathrm{tr}\left(f_m \cdot F_{\vec{\boldsymbol{\alpha}} \sqcup s} \cdot f_1\right)}{k_m \cdot k_1} \\ &\mathcal{A}^{(0)_s}_{\mathrm{YMS}}(1, \vec{\boldsymbol{\alpha}} \sqcup s, m; \{2, \ldots, m-1\} \backslash \boldsymbol{\alpha} | \sigma_{m+1}), \end{aligned} \tag{58}$$

which indicates

$$\begin{aligned} \mathcal{A}^{\mathrm{II}}_{\mathrm{YM}}(\sigma_{m+1}) = &-\sum_{\vec{\boldsymbol{\alpha}}} \frac{\mathrm{tr}\left(f_m \cdot F_{\vec{\boldsymbol{\alpha}}} \cdot f_1\right)}{k_m \cdot k_1} \\ &\mathcal{A}_{\mathrm{YMS}}(1, \vec{\boldsymbol{\alpha}}, m; s \cup \{2, \cdots, m-1\} \setminus \boldsymbol{\alpha} | \sigma_{m+1}) \\ &-\sum_{\vec{\boldsymbol{\alpha}}} \frac{\mathrm{tr}\left(f_m \cdot F_{\vec{\boldsymbol{\alpha}} \sqcup s} \cdot f_1\right)}{k_m \cdot k_1} \\ &\mathcal{A}_{\mathrm{YMS}}(1, \vec{\boldsymbol{\alpha}} \sqcup s, m; \{2, \cdots, m-1\} \setminus \boldsymbol{\alpha} | \sigma_{m+1}) \\ = &-\sum_{\vec{\boldsymbol{\alpha}}'} \frac{\mathrm{tr}\left(f_m \cdot F_{\vec{\boldsymbol{\alpha}}'} \cdot f_1\right)}{k_m \cdot k_1} \\ &\mathcal{A}_{\mathrm{YMS}}(1, \vec{\boldsymbol{\alpha}}', m; s \cup \{2, \ldots, m-1\} \setminus \boldsymbol{\alpha}' | \sigma_{m+1}). \end{aligned} \tag{59}$$

In the formula (59), $\boldsymbol{\alpha}$ denotes subsets of $\{2, \cdots, m-1\}$ that do not include the leg s, while $\boldsymbol{\alpha}'$ represents subsets of $s \cup \{2, \cdots, m-1\}$. The expansion (59) is essentially the expanded formula $\mathcal{A}^{\mathrm{II}}_{\mathrm{YM}}(\sigma_n)$ as seen in (49), applied to the $(m+1)$-point case. It is important to recall that $\mathcal{A}^{\mathrm{II}}_{\mathrm{YM}}(\sigma_{m+1})$ and $\mathcal{A}^{\mathrm{I}}_{\mathrm{YM}}(\sigma_{m+1})$ are two distinct forms of expansion derived using the same method. As a result, we arrive at the conclusion that $\mathcal{A}^{\mathrm{II}}_{\mathrm{YM}}(\sigma_{m+1}) = \mathcal{A}^{\mathrm{I}}_{\mathrm{YM}}(\sigma_{m+1})$, leading to

$$-\frac{k_m \cdot \epsilon_1}{k_m \cdot k_1} A_{m+1} - \frac{\epsilon_m \cdot k_1}{k_m \cdot k_1} B_{m+1} + \frac{\epsilon_m \cdot \epsilon_1}{k_m \cdot k_1} C_{m+1} = 0, \tag{60}$$

where A_{m+1}, B_{m+1}, and C_{m+1} are defined in (48) with $(m+1)$ replacing n. Consequently, we conclude that the gauge invariance conditions $A_{m+1} = B_{m+1} = C_{m+1} = 0$ hold for the $(m+1)$-point amplitudes, as each coefficient associated with the independent variables $k_m \cdot \epsilon_1$, $\epsilon_m \cdot k_1$, and $\epsilon_m \cdot \epsilon_1$ must vanish individually.

In summary, if the expansion (49) and the gauge invariance conditions (48) hold for m-point amplitudes, they automatically hold for $(m+1)$-point amplitudes. Given that the three-point amplitudes $\mathcal{A}_{\mathrm{YM}}(\sigma_3)$ satisfy both the expansion (49) and the gauge invariance conditions (48), we can apply this result iteratively to conclude that (49) and (48) are valid for any YM amplitude $\mathcal{A}_{\mathrm{YM}}(\sigma_n)$. In other words, we have presented an alternative expression (49) that explicitly maintains gauge invariance for all polarization vectors constructed from lower-point amplitudes. Additionally, we've verified that the expansions derived in the previous section, as outlined in (3.3), also preserve gauge invariance for both ϵ_1 and ϵ_n.

5 Summary

In this paper, we have enhanced the recursive method based on the sub-leading soft theorem for external gluons, as previously employed in [43]. With our new approach, we have developed two types of expansions from YM amplitudes to YMS amplitudes. The first type does not exhibit manifest gauge invariance for each polarization, while the second type does. As detailed in Sects. 1 and 2, the sub-leading soft theorem for gluons effectively "grows" a soft gluon in a manifestly gauge-invariant manner. Consequently, as long as our recursive starting point is manifestly gauge-invariant, any intermediate result obtained during the recursion process remains explicitly gauge-invariant.

According to the methodology presented in this paper, we can also make the following two extensions:

- Based on the double copy structure, one can replace YM (YMS) by GR (EYM) in (38) and (49) to obtain the expansion of GR amplitudes to EYM ones as follows,

$$\mathcal{A}^{\mathrm{I}}_{\mathrm{GR}}(n) = \sum_{\vec{\boldsymbol{\alpha}}} \left(\epsilon_n \cdot F_{\vec{\boldsymbol{\alpha}}} \cdot \epsilon_1\right) \mathcal{A}_{\mathrm{EYM}}(1, \vec{\boldsymbol{\alpha}}, n; \{2, \ldots, n-1\} \setminus \boldsymbol{\alpha}), \tag{61}$$

$$\mathcal{A}^{\mathrm{II}}_{\mathrm{GR}}(n) = -\sum_{\vec{\boldsymbol{\alpha}}} \frac{\mathrm{tr}\left(f_n \cdot F_{\vec{\boldsymbol{\alpha}}} \cdot f_1\right)}{k_n \cdot k_1} \mathcal{A}_{\mathrm{EYM}}(1, \vec{\boldsymbol{\alpha}}, n; \{2, \ldots, n-1\} \setminus \boldsymbol{\alpha}). \tag{62}$$

  Then, we perform a similar replacement for (24),

$$\mathcal{A}_{\mathrm{EYM}}(1, \cdots, n; \{p_1, \cdots, p_m\}) = \sum_{\vec{\boldsymbol{\alpha}}} \frac{k_r \cdot F_{\vec{\boldsymbol{\alpha}}} \cdot Y_{\vec{\boldsymbol{\alpha}}}}{k_r \cdot k_{p_1 \cdots p_m}} \mathcal{A}_{\mathrm{EYM}}(1, \{2, \cdots, n-1\} \shuffle \vec{\boldsymbol{\alpha}}, n; \{p_1, \ldots, p_m\} \setminus \boldsymbol{\alpha}). \tag{63}$$

  Starting from (62), iteratively using (63), one arrives at the expansions of pure GR amplitudes to pure YM amplitudes, whose coefficients manifest the gauge invariance for each polarization. Thus the manifestly gauge invariant BCJ numerators are found.
- The gauge invariant expansion can be extended to the 1-loop level straightforwardly. One can first use (38) to expand the $(n+2)$-point tree YM amplitude as

$$\mathcal{A}_{\mathrm{YM}}(+, \sigma_n, -) = \sum_{\vec{\boldsymbol{\alpha}}} (\epsilon_- \cdot F_{\vec{\boldsymbol{a}}} \cdot \epsilon_+) \mathcal{A}_{\mathrm{YMS}}(+, \vec{\boldsymbol{\alpha}}, -; \{1, \ldots, n\} \setminus \boldsymbol{\alpha} | +, \sigma_n, -), \tag{64}$$

  where two fixed legs are encoded as $+$, $-$, and $\boldsymbol{\alpha}$ denotes subsets of $\{1, \cdots, n\}$. The 1-loop amplitude can be generated by taking the forward limit of (65) for legs $+$ and $-$, namely, setting $k_+ = -k_- = \ell$, then gluing two legs $+$ and $-$ together by identifying ϵ_+, ϵ_-, and summing over all possible states [45–49]. This manipulation leads to the expansion at amplitude level,

$$\mathcal{A}^{1-\mathrm{loop}}_{\mathrm{YM}}(\sigma_n) = \sum_{\vec{\boldsymbol{\alpha}}} \left(\mathrm{Tr}\ F_{\vec{\boldsymbol{a}}}\right) \times \mathcal{A}^{1-\mathrm{loop}}_{\mathrm{sYMS}}(\vec{\boldsymbol{\alpha}}; \{1, \cdots, n\} \setminus \boldsymbol{\alpha} | \sigma_n), \tag{65}$$

  which manifests the gauge invariance. Here the subscript s in $\mathcal{A}^{1-\mathrm{loop}}_{\mathrm{sYMS}}$ denotes the special type of 1-loop YMS amplitudes those the virtual particle propagating in the loop is a scalar. At the integrand level, one can employ (24) to expand sYMS integrands iteratively, end with pure BAS integrands. Since $Y_{\vec{\boldsymbol{\alpha}}}$ should include the loop momentum ℓ when applying (24) to the 1-loop level, the obtained gauge invariant expansion to pure BAS ones does not hold at the amplitude level.

Moreover, in Sect. 1, we also pointed out that the explicit formulas of soft factors can be regarded as the consequence of the universality of soft behaviors, without respecting any top down derivation. When referring to universality, we mean the soft factor for BAS scalars observed from pure BAS amplitudes holds for BAS scalars in general YMS amplitudes, and the soft factors for gluons derived from YMS amplitudes with only one external gluon also hold for general YMS amplitudes. From the traditional perspective, such universality is the consequence of the symmetries. For example, the universal soft behavior of gravitons are ensured by the asymptotic Bondi–Metzner–Sachs (BMS) symmetries of flat space time at null infinity [50–56]. From the bottom up perspective, universality of soft behaviors can be taken as the basic principle, and the associated symmetries are hard to be observed. Thus, a natural question is, can we reproduce the corresponding underlying symmetries from the bottom up perspective? This is an interesting future direction.

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Appendix A: Examples of expansions

In this section, we give some explicit examples of expansion.

A.1 Explicit expression of four-point Yang–Mills (YM) amplitude

Consider the four-point YM amplitude $\mathcal{A}_{\rm YM}(\sigma_4)$ with the ordering σ_4 among external lines. Substituting expansions in (22) into the expansion of YM amplitude in (38), we get the following full expansion to the BAS KK basis,

$$\begin{aligned}\mathcal{A}_{\rm YM}(\sigma_4)=&\Big[(\epsilon_4\cdot\epsilon_1)(\epsilon_2\cdot k_1)(\epsilon_3\cdot k_{12})+(\epsilon_4\cdot f_2\cdot\epsilon_1)(\epsilon_3\cdot k_{12})\\&+(\epsilon_4\cdot f_3\cdot\epsilon_1)(\epsilon_2\cdot k_1)\\&+\epsilon_4\cdot f_3\cdot f_2\cdot\epsilon_1\Big]\mathcal{A}_{\rm BAS}(1,2,3,4|\sigma_4)\\&+\Big[(\epsilon_4\cdot\epsilon_1)(\epsilon_2\cdot k_1)(\epsilon_3\cdot k_1)\\&+(\epsilon_4\cdot\epsilon_1)(\epsilon_2\cdot f_3\cdot k_1)+(\epsilon_4\cdot f_2\cdot\epsilon_1)(\epsilon_3\cdot k_1)\\&+(\epsilon_4\cdot f_3\cdot\epsilon_1)(\epsilon_2\cdot k_{12})\\&+\epsilon_4\cdot f_2\cdot f_3\cdot\epsilon_1\Big]\mathcal{A}_{\rm BAS}(1,3,2,4|\sigma_4).\end{aligned}\tag{66}$$

This expansion manifests the locality while breaking the explicit gauge invariance and the symmetry among legs 2 and 3.

One can also use the expansion in (49) to expand $\mathcal{A}_{\rm YM}(\sigma_4)$ to single-trace YMS amplitudes

$$\begin{aligned}\mathcal{A}_{\rm YM}(\sigma_4)=&-\frac{{\rm tr}(f_4\cdot f_1)}{k_4\cdot k_1}\mathcal{A}_{\rm YMS}(1,4;\{2,3\}|\sigma_4)\\&-\frac{{\rm tr}(f_4\cdot f_2\cdot f_1)}{k_4\cdot k_1}\mathcal{A}_{\rm YMS}(1,2,4;3|\sigma_4)\\&-\frac{{\rm tr}(f_4\cdot f_3\cdot f_1)}{k_4\cdot k_1}\mathcal{A}_{\rm YMS}(1,3,4;2|\sigma_4)\\&-\frac{{\rm tr}(f_4\cdot f_3\cdot f_2\cdot f_1)}{k_4\cdot k_1}\mathcal{A}_{\rm BAS}(1,2,3,4|\sigma_4)\\&-\frac{{\rm tr}(f_4\cdot f_2\cdot f_3\cdot f_1)}{k_4\cdot k_1}\mathcal{A}_{\rm BAS}(1,3,2,4|\sigma_4).\end{aligned}\tag{67}$$

Substituting (24), we get

$$\begin{aligned}\mathcal{A}_{\rm YM}(\sigma_4)=&-\Big[\frac{{\rm tr}(f_4\cdot f_1)}{k_4\cdot k_1}\frac{k_q\cdot f_2\cdot k_1}{k_q\cdot k_{23}}\frac{k_q\cdot f_3\cdot k_{12}}{k_q\cdot k_3}\\&+\frac{{\rm tr}(f_4\cdot f_1)}{k_4\cdot k_1}\frac{k_q\cdot f_3\cdot k_1}{k_q\cdot k_{23}}\frac{k_q\cdot f_2\cdot k_1}{k_q\cdot k_3}\\&+\frac{{\rm tr}(f_4\cdot f_1)}{k_4\cdot k_1}\frac{k_q\cdot f_3\cdot f_2\cdot k_1}{k_q\cdot k_{23}}\\&+\frac{{\rm tr}(f_4\cdot f_2\cdot f_1)}{k_4\cdot k_1}\frac{k_q\cdot f_3\cdot k_{12}}{k_q\cdot k_3}\\&+\frac{{\rm tr}(f_4\cdot f_3\cdot f_1)}{k_4\cdot k_1}\frac{k_q\cdot f_2\cdot k_1}{k_q\cdot k_2}\\&+\frac{{\rm tr}(f_4\cdot f_3\cdot f_2\cdot f_1)}{k_4\cdot k_1}\Big]\mathcal{A}_{\rm BAS}(1,2,3,4|\sigma_4)\\&+2\leftrightarrow 3,\end{aligned}\tag{68}$$

where k_q is an arbitrary reference massless momentum. The symbol $2\leftrightarrow 3$ in the last line means exchange 2 and 3 in coefficients and the first order $(1,2,3,4)$, without altering σ_4. This formula manifests the gauge invariance among legs 2 and 3. If we fix $\sigma_4=(1,2,3,4)$, the BAS amplitudes can be evaluated as

$$\begin{aligned}\mathcal{A}_{\rm BAS}(1,2,3,4|1,2,3,4)&=\frac{1}{s_{12}}+\frac{1}{s_{14}},\\\mathcal{A}_{\rm BAS}(1,3,2,4|1,2,3,4)&=-\frac{1}{s_{14}}.\end{aligned}\tag{69}$$

Then we get

$$\begin{aligned}\mathcal{A}_{\rm YM}(\sigma_4)=&-\Big[\frac{{\rm tr}(f_4\cdot f_1)}{k_4\cdot k_1}\frac{k_q\cdot f_2\cdot k_1}{k_q\cdot k_{23}}\frac{k_q\cdot f_3\cdot k_{12}}{k_q\cdot k_3}\\&+\frac{{\rm tr}(f_4\cdot f_1)}{k_4\cdot k_1}\frac{k_q\cdot f_3\cdot k_1}{k_q\cdot k_{23}}\frac{k_q\cdot f_2\cdot k_1}{k_q\cdot k_3}\\&+\frac{{\rm tr}(f_4\cdot f_1)}{k_4\cdot k_1}\frac{k_q\cdot f_3\cdot f_2\cdot k_1}{k_q\cdot k_{23}}\\&+\frac{{\rm tr}(f_4\cdot f_2\cdot f_1)}{k_4\cdot k_1}\frac{k_q\cdot f_3\cdot k_{12}}{k_q\cdot k_3}\\&+\frac{{\rm tr}(f_4\cdot f_3\cdot f_1)}{k_4\cdot k_1}\frac{k_q\cdot f_2\cdot k_1}{k_q\cdot k_2}\\&+\frac{{\rm tr}(f_4\cdot f_3\cdot f_2\cdot f_1)}{k_4\cdot k_1}\Big]\left(\frac{1}{s_{12}}+\frac{1}{s_{14}}\right)\\&-\Big[\frac{{\rm tr}(f_4\cdot f_1)}{k_4\cdot k_1}\frac{k_q\cdot f_3\cdot k_1}{k_q\cdot k_{23}}\frac{k_q\cdot f_2\cdot k_{13}}{k_q\cdot k_2}\\&+\frac{{\rm tr}(f_4\cdot f_1)}{k_4\cdot k_1}\frac{k_q\cdot f_2\cdot k_1}{k_q\cdot k_{23}}\frac{k_q\cdot f_3\cdot k_1}{k_q\cdot k_2}\\&+\frac{{\rm tr}(f_4\cdot f_1)}{k_4\cdot k_1}\frac{k_q\cdot f_2\cdot f_3\cdot k_1}{k_q\cdot k_{23}}\end{aligned}$$

$$
\begin{aligned}
&+\frac{\mathrm{tr}(f_4\cdot f_3\cdot f_1)}{k_4\cdot k_1}\frac{k_q\cdot f_2\cdot k_{13}}{k_q\cdot k_2}\\
&+\frac{\mathrm{tr}(f_4\cdot f_2\cdot f_1)}{k_4\cdot k_1}\frac{k_q\cdot f_3\cdot k_1}{k_q\cdot k_3}\\
&+\frac{\mathrm{tr}(f_4\cdot f_2\cdot f_3\cdot f_1)}{k_4\cdot k_1}\Big]\left(-\frac{1}{s_{14}}\right).
\end{aligned} \tag{70}
$$

The manifest locality is broken by spurious poles such as $(k_1\cdot k_4)^2$, $k_q\cdot k_i$.

A.2 Expansion of five-point amplitude to YMS ones

Using the expansion in (38), we can expand the YM amplitude $\mathcal{A}_{\mathrm{YM}}(\sigma_5)$ to YMS ones:

$$
\begin{aligned}
\mathcal{A}_{\mathrm{YM}}(\sigma_5) = &(\epsilon_5\cdot\epsilon_1)\,\mathcal{A}_{\mathrm{YMS}}(1,5;\{2,3,4\}|\sigma_5)\\
&+(\epsilon_5\cdot f_2\cdot\epsilon_1)\,\mathcal{A}_{\mathrm{YMS}}(1,2,5;\{3,4\}|\sigma_5)\\
&+2\leftrightarrow 3+2\leftrightarrow 4\\
&+(\epsilon_5\cdot f_3\cdot f_2\cdot\epsilon_1)\,\mathcal{A}_{\mathrm{YMS}}(1,2,3,5;4|\sigma_5)\\
&+2\leftrightarrow 3\\
&+(\epsilon_5\cdot f_4\cdot f_2\cdot\epsilon_1)\,\mathcal{A}_{\mathrm{YMS}}(1,2,4,5;3|\sigma_5)\\
&+2\leftrightarrow 4\\
&+(\epsilon_5\cdot f_4\cdot f_3\cdot\epsilon_1)\,\mathcal{A}_{\mathrm{YMS}}(1,3,4,5;2|\sigma_5)\\
&+3\leftrightarrow 4\\
&+(\epsilon_5\cdot f_4\cdot f_3\cdot f_2\cdot\epsilon_1)\,\mathcal{A}_{\mathrm{BAS}}(1,2,3,4,5|\sigma_5)\\
&+\mathcal{S}_3(2,3,4),
\end{aligned} \tag{71}
$$

where $\mathcal{S}_3(2,3,4)$ denotes permutations among legs 2, 3 and 4. Again, any $i\leftrightarrow j$ in the above representation does not alter σ_5. This expansion manifests the locality while breaking the explicit gauge invariance for ϵ_1 and ϵ_5.

One can also use the expansion in (38) to expand the YM amplitude $\mathcal{A}_{\mathrm{YM}}(\sigma_5)$ to YMS ones as

$$
\begin{aligned}
\mathcal{A}_{\mathrm{YM}}(\sigma_5) = &\frac{\mathrm{tr}(f_5\cdot f_1)}{k_5\cdot k_1}\,\mathcal{A}_{\mathrm{YMS}}(1,5;\{2,3,4\}|\sigma_5)\\
&+\frac{\mathrm{tr}(f_5\cdot f_2\cdot f_1)}{k_5\cdot k_1}\,\mathcal{A}_{\mathrm{YMS}}(1,2,5;\{3,4\}|\sigma_5)\\
&+2\leftrightarrow 3+2\leftrightarrow 4\\
&+\frac{\mathrm{tr}(f_5\cdot f_3\cdot f_2\cdot f_1)}{k_5\cdot k_1}\,\mathcal{A}_{\mathrm{YMS}}(1,2,3,5;4|\sigma_5)\\
&+2\leftrightarrow 3\\
&+\frac{\mathrm{tr}(f_5\cdot f_4\cdot f_2\cdot f_1)}{k_5\cdot k_1}\,\mathcal{A}_{\mathrm{YMS}}(1,2,4,5;3|\sigma_5)\\
&+2\leftrightarrow 4\\
&+\frac{\mathrm{tr}(f_5\cdot f_4\cdot f_3\cdot f_1)}{k_5\cdot k_1}\,\mathcal{A}_{\mathrm{YMS}}(1,3,4,5;2|\sigma_5)\\
&+3\leftrightarrow 4\\
&+\frac{\mathrm{tr}(f_5\cdot f_4\cdot f_3\cdot f_2\cdot f_1)}{k_5\cdot k_1}\,\mathcal{A}_{\mathrm{BAS}}(1,2,3,4,5|\sigma_5)\\
&+\mathcal{S}_3(2,3,4).
\end{aligned} \tag{72}
$$

This expansion manifests the gauge invariance for ϵ_1 and ϵ_5, and breaks the explicit locality by introducing an extra $1/k_5\cdot k_1$. In a similar manner, we can substitute the expression for YMS, as expanded into BAS from Eq. (24), into the calculation. Then, by following the method detailed in Sect. 2.1 of Sect. 2, we can determine the corresponding BAS amplitude. This process ultimately yields the final specific expression. Due to space constraints, we will not provide a detailed expansion here.

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