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Expansion of Einstein-Yang-Mills amplitude

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ABSTRACT: In this paper, we study from various perspectives the expansion of tree level single trace Einstein-Yang-Mills amplitudes into linear combination of color-ordered Yang-Mills amplitudes. By applying the gauge invariance principle, a programable recursive construction is devised to expand EYM amplitude with arbitrary number of gravitons into EYM amplitudes with fewer gravitons. Based on this recursive technique we write down the complete expansion of any single trace EYM amplitude in the basis of color-order Yang-Mills amplitude. As a byproduct, an algorithm for constructing a polynomial form of the BCJ numerator for Yang-Mills amplitudes is also outlined in this paper. In addition, by applying BCFW recursion relation we show how to arrive at the same EYM amplitude expansion from the on-shell perspective. And we examine the EYM expansion using KLT relations and show how to evaluate the expansion coefficients efficiently.

KEYWORDS: Scattering Amplitudes, Gauge Symmetry

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²The unusual ordering of authors instead of the standard alphabet ordering is for young researchers to get proper recognition of contributions under the current out-dated practice in China.

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1 Introduction

A fairly non-trivial relation between Einstein-Yang-Mills (EYM) amplitude and pure Yang-Mills amplitudes was proposed in [1] recently, where the amplitude of n gluons coupled to a single graviton is expanded as linear sum of $(n+1)$ -point pure gluon amplitudes in an elegant formulation, which is different from the earlier proposed relations that express n -gluon m -graviton amplitudes by $(n+2m)$ -gluon amplitudes [2–6]. It is now widely known that, the non-trivial relations among amplitudes are important both in the practical evaluation and

the analytical study, while the $U(1)$ -relation, Kleiss-Kuijf(KK)relation [7] and especially the Bern-Carrasco-Johansson(BCJ) relations [8] among amplitudes of the same field theory have received considerable investigations in the past few years, and inspired the color-kinematics duality for gravity and Yang-Mills amplitudes [9, 10]. As an analogous scenario, where amplitudes of two originally seemingly unrelated theories take part in novel identity, recall that the famous Kawai-Lewellen-Tye (KLT) relation [11] was proposed quite a long time ago, which formulates a closed string amplitude as products of two open string amplitudes, and in the field theory limit it expands a pure gravity amplitude as bi-linear sum of Yang-Mills amplitudes. The newly proposed linear EYM amplitude relation was also inspired by the study of string theory, where monodromy relations for mixed closed-open string amplitudes, previously been applied to the study of BCJ relations [3, 12, 13], has been considered.

Because of its compact and simple nature, a substantial research interests has been drawn to the study of EYM amplitude relations and to its generalizations [14–19].¹ In particular most of the discussions are based on the Cachazo-He-Yuan (CHY) formulation [21–25], by genuinely reformulating the CHY-integrand in an appropriate form. Notably, explicit expressions for EYM amplitude relations with arbitrary number of gluons coupled to up to three gravitons were provided in [14]. The technique for reformulating the CHY-integrands in these papers developed into a systematic explanation in [26], and it is revealed therein that the cross-ratio identity and other off-shell identities of integrands [27, 28] are crucial tools for deforming CHY-integrands into alternative forms corresponding to different field theories. These powerful tools benefit from the integration rule method [29–32] developed for the purpose of evaluating CHY-integrand without referring to the scattering equations. The idea of integration rule and cross-ratio identity method was to decompose arbitrary CHY-integrand using cross-ratio identities into those corresponding to cubic-scalar Feynman diagrams dressed with kinematic factors. By carefully organizing terms one can identify the resulting CHY-integrands as amplitudes of certain field theories, hence the amplitude relations, as was done in [14, 15]. In fact, there is more about EYM amplitude relations from the perspective of CHY-framework. Starting from CHY-integrand of a theory, it is always possible to reformulate it to another form by cross-ratio and other off-shell relations, for instance the Yang-Mills-scalar (YMs) amplitude can be expanded as linear sum of bi-adjoint cubic-scalar amplitudes. We shall discuss this later in this paper.

As it is very often, on-shell technique can prove to be a powerful tool for the purpose of understanding non-trivial amplitude relations within field theory framework. One such example is the on-shell proof of BCJ relations [33, 34]. The central idea is to deduce physical identities only from general principles such as locality, unitarity and gauge invariance. This is particularly true with the advent of Britto-Cachazo-Feng-Witten(BCFW) on-shell recursion relation [35, 36], which utilizes the first two. In most cases, the BCFW recursion relation computes the amplitude in a way such that only contributions from finite local single poles are summed over, which requires a vanishing behavior in the boundary of

¹Remark that in paper [20], a formula for single trace EYM amplitudes in four dimension for arbitrary many gravitons is provided, although not mentioning the amplitude relations.

BCFW complex parameter plane. This is exactly the case for BCJ relations of Yang-Mills amplitudes. However, for generic situations, the amplitude as a rational function of BCFW parameter z is not vanishing in $z \rightarrow \infty$ and the boundary contributions can not be avoided. This is a problem one would meet when applying BCFW recursions to the EYM amplitude relations, and such subtlety complicates the on-shell proof of EYM amplitude relations. The evaluation of boundary contributions is generically a difficult problem, but many methods have been proposed to deal with it. Noteworthy systematic algorithm has also been proposed recently [37–43] so that at least in principle it is indeed possible to systematically study the EYM amplitude relations using BCFW recursion relations. On the other hand it is also known that very often gauge invariance can become a very handy tool in constraining the specific analytic form of the scattering amplitude. Recent progresses have pushed the gauge invariance principle forward and indicate that, the gauge invariance along with cubic graph expansion are enough to determine the amplitudes [44–49]. In a less but still quite challenging situation, we claim that the gauge invariance should uniquely determine the EYM amplitude relations, and from which we can explicitly write down the expansion for EYM amplitude with arbitrary number of gravitons.

As the number of gravitons increases and that of gluons decreases, in the extremal limit we would come to the amplitude with pure gravitons. This is the important problem of expanding gravity amplitude as pure Yang-Mills amplitudes. Furthermore, with the philosophy of decomposing CHY-integrands, the same argument applies to the Yang-Mills amplitudes which would be expanded as pure bi-adjoint cubic-scalar amplitudes. This is exactly the cubic-graph expansion of Yang-Mills amplitude which makes the color-kinematics duality manifest [26]. The EYM amplitude relation combined with CHY-integrand, more specifically the Pfaffian expansion, would produce the non-trivial expansion for Yang-Mills amplitude as cubic-scalar graphs, as well as expansion for gravity amplitude as pure Yang-Mills amplitudes and eventually the cubic-scalar graphs. This provides a way of computing the BCJ numerators, which is usually considered to be very difficult [46, 50–62]. When KLT relation is in action, the EYM amplitude relation can be connected to the BCJ numerator problem. We will learn more about this in later sections.

In this paper we examine the EYM amplitude relations from the perspectives of CHY-formulation, BCFW on-shell recursion, KLT relation, and through the construction of BCJ numerators. This paper is organized as follows. In section 2, we present the general theoretical playground of non-trivial amplitude relations from the CHY-formulation, and explain the expansion of amplitudes as the expansion of Pfaffian of CHY-integrand. In section 3, we facilitate the principle of gauge invariance to determine the EYM amplitude relations for gluons coupled to arbitrary number of gravitons. In section 4, we generalize the EYM amplitude relations to pure Yang-Mills amplitudes and apply the non-trivial relation to the computation of BCJ numerators. In section 5, we provide the on-shell proof of some EYM amplitude relations by BCFW recursion relations. In section 6 we study in the language of KLT relations. Conclusion is presented in section 7 and some useful backgrounds are summarized in the appendix.

2 Amplitude relations from the perspective of CHY-formulation

The non-trivial relation revealed recently between EYM amplitudes and pure Yang-Mills amplitudes [1, 14, 15] has an intuitive interpretation in the CHY-framework. In fact, the CHY-formulation tells more beyond the EYM amplitudes. In the CHY-formula, it is the so called CHY-integrand $\mathcal{I}^{\text{CHY}}$ that describes specific field theories. The CHY-integrand is an uniform weight-4 rational function of n complex variables z_i for n -point scattering system, i.e., with the $1/z_i^4$ scaling behavior in the $z_i \rightarrow \infty$ limit.

For almost all known theories, the weight-4 CHY-integrand can be factorized as two weight-2 ingredients, formally written as

$$\mathcal{I}^{\text{CHY}} = \mathcal{I}_L \times \mathcal{I}_R. \quad (2.1)$$

Let us then define two new weight-4 CHY integrands as follows

$$\mathcal{I}_L^{\text{CHY}}(\alpha) := \mathcal{I}_L \times \text{PT}(\alpha), \quad \mathcal{I}_R^{\text{CHY}}(\beta) := \mathcal{I}_R \times \text{PT}(\beta), \quad (2.2)$$

where $\text{PT}(\alpha)$ is the Parke-Taylor factor

$$\text{PT}(\alpha) := \frac{1}{(z_{\alpha_1} - z_{\alpha_2}) \cdots (z_{\alpha_{n-1}} - z_{\alpha_n})(z_{\alpha_n} - z_{\alpha_1})}. \quad (2.3)$$

Supposing the two CHY-integrands $\mathcal{I}_L^{\text{CHY}}, \mathcal{I}_R^{\text{CHY}}$ also describe certain physical meaningful field theories and produce the corresponding color-ordered amplitudes $A_L(\alpha), A_R(\beta)$ after CHY-evaluation, then by CHY-construction [21–23] we could arrive at the following generalized KLT relation,

$$A = \sum_{\sigma, \tilde{\sigma} \in S_{n-3}} A_L(n-1, n, \sigma, 1) \mathcal{S}[\sigma|\tilde{\sigma}] A_R(1, \tilde{\sigma}, n-1, n), \quad (2.4)$$

where A is the amplitude of specific field theory determined by the theories of A_L, A_R , while S_n denotes permutations on n elements and $\mathcal{S}[\sigma|\tilde{\sigma}]$ is some kinematic kernel. The summation is over S_{n-3} permutations of sets $\{2, \dots, n-2\}$, depending on our choice of legs k_1, k_{n-1}, k_n being fixed.

The expression (2.4) denotes a general expansion for the original amplitude A defined by CHY-integrand (2.1). If for a specific $\tilde{\sigma}$ ordering, we sum over all S_{n-3} permutations of σ and define the result as

$$\mathcal{C}(\tilde{\sigma}) := \sum_{\sigma \in S_{n-3}} A_L(n-1, n, \sigma, 1) \mathcal{S}[\sigma|\tilde{\sigma}], \quad (2.5)$$

then the original amplitude can be expressed as

$$A = \sum_{\tilde{\sigma} \in S_{n-3}} \mathcal{C}(\tilde{\sigma}) A_R(1, \tilde{\sigma}, n-1, n), \quad (2.6)$$

where $\mathcal{C}(\tilde{\sigma})$ serves as the expansion coefficients. Similarly, if for a specific σ ordering we sum over all S_{n-3} permutations of $\tilde{\sigma}$ and define the summation as

$$\tilde{\mathcal{C}}(\sigma) := \sum_{\tilde{\sigma} \in S_{n-3}} \mathcal{S}[\sigma|\tilde{\sigma}] A_R(1, \tilde{\sigma}, n-1, n), \quad (2.7)$$

then the original amplitude can be expanded as

$$A = \sum_{\sigma \in S_{n-3}} \tilde{C}(\sigma) A_L(n-1, n, \sigma, 1). \quad (2.8)$$

The expressions (2.6) and (2.8) have provided two different expansions of the original theory. There are several general remarks regarding the expansion in above,

- Firstly, the expansion is into a chosen $(n-3)!$ BCJ basis, and the corresponding expansion coefficients $C(\tilde{\sigma})$ and $\tilde{C}(\sigma)$ would also be unique. However, as we will discuss soon, sometimes it is better to expand the original amplitude into the $(n-2)!$ KK basis. Because of the BCJ relations among color-ordered partial amplitudes, the expansion coefficients in the KK basis will not be unique and depend on the *generalized gauge choice* in the BCJ sense.
- Secondly, with the amplitude expansion formula in hand, the next is to compute the expansion coefficients. For this purpose, there are several approaches. The first approach is to use the definitions (2.5) and (2.7) directly. However, in general it is very hard to evaluate the summation for generic n -point situation, and only in certain special case a direct evaluation is possible, which we shall explain later. The second approach seeds back to the expression (2.1), and the major idea is to expand the weight-2 ingredients $\mathcal{I}_L$ or $\mathcal{I}_R$ into the $\text{PT}(\alpha)$ factor of n elements. In fact, this is the approach followed in [14, 15]. The expansion can be systematically achieved by successively applying cross-ratio identities to the CHY-integrands, where in each step a gauge choice should be taken in the cross-ratio identity. In general, such expansion leads to a result with $(n-1)!$ cyclic basis. Then one can use the KK relation to rewrite it into the $(n-2)!$ KK basis. As already mentioned, the gauge dependence remains in the expansion coefficients at each step, and it would disappear only after using the BCJ relations to rewrite all into $(n-3)!$ BCJ basis.

Besides the above two direct evaluation methods for expansion coefficients, there are also some indirect ways. For example, one can propose some ansatz for the expansion coefficients, then prove and generalize it by on-shell recursion relations. One can also use some general considerations, for instance the gauge invariance or the soft behavior, to determine the coefficients [47–49].

In this paper, we will investigate the expansion from these different views.

- Thirdly, although in most theories, the CHY-integrand is given by products of two weight-2 ingredients as (2.1), for some theories the CHY-integrand is defined by the product of four weight-1 ingredients. So there are various combinations of them to form weight-2 parts. In other words, there are possibilities to have more than two expansions given in (2.6) and (2.8). It would be interesting to survey the consequence of different combinations for these theories.

After above general discussions, now we focus on our major topic in this paper, i.e., the single trace part of EYM theory, whose CHY-integrand is defined as

$$\mathcal{I}_{r,s}^{\text{EYM}}(\alpha) = \text{PT}_r(\alpha) \text{Pf } \Psi_s \times \text{Pf}' \Psi_n, \quad (2.9)$$

for scattering system of r gluons and s gravitons with $r + s = n$, and $\alpha = \{\alpha_1, \dots, \alpha_r\}$. We can define two new CHY-integrands as

$$\mathcal{I}_L^{\text{CHY}}(\alpha|\tilde{\sigma}) := \text{PT}_r(\alpha) \text{Pf } \Psi_s \times \text{PT}_n(\tilde{\sigma}), \quad \mathcal{I}_R^{\text{CHY}}(\beta) := \text{Pf}' \Psi_n \times \text{PT}_n(\sigma), \quad (2.10)$$

where $\sigma, \tilde{\sigma} \in S_n$. It is easy to tell that the $\mathcal{I}_L^{\text{CHY}}$ is the CHY-integrand of Yang-Mills-scalar(YMs) theory and $\mathcal{I}_R^{\text{CHY}}$ is the CHY-integrand of Yang-Mills theory. Correspondingly, the amplitude A_L is the color-ordered YMs amplitude $A_{r,s}^{\text{YMs}}$ with r scalars and s gluons, which has two trace structures associated with the two PT-factors, while the amplitude A_R is color-ordered Yang-Mills amplitude A_n^{YM} . One thing to emphasize is that the scalar carries two groups (one gauge group and one flavor group) and has bi-adjoint scalar-cubic interactions.

An immediate consequence from (2.4) reads

$$\begin{aligned} A_{r,s}^{\text{EYM}}(\alpha) &= \sum_{\sigma, \tilde{\sigma} \in S_{n-3}} A_n^{\text{YM}}(n-1, n, \sigma, 1) \mathcal{S}[\sigma|\tilde{\sigma}] A_{r,s}^{\text{YMs}}(\alpha|1, \tilde{\sigma}, n-1, n) \\ &= \sum_{\sigma \in S_{n-3}} \tilde{C}(\alpha|\sigma) A_n^{\text{YM}}(n-1, n, \sigma, 1), \end{aligned} \quad (2.11)$$

with

$$\tilde{C}(\alpha|\sigma) = \sum_{\tilde{\sigma} \in S_{n-3}} \mathcal{S}[\sigma|\tilde{\sigma}] A_{r,s}^{\text{YMs}}(\alpha|1, \tilde{\sigma}, n-1, n). \quad (2.12)$$

The expansion (2.11) is into the BCJ basis with $(n-3)!$ independent Yang-Mills amplitudes. However, as it will be clear soon, an expansion into $(n-2)!$ KK basis is more favorable, and we would present it here as

$$A_{r,s}^{\text{EYM}}(\alpha) = \sum_{\sigma \in S_{n-2}} \tilde{C}'(\alpha|\sigma) A_n^{\text{YM}}(n, \sigma, 1), \quad (2.13)$$

with the expansion coefficients

$$\tilde{C}'(\alpha|\sigma) = \lim_{k_n^2 \rightarrow 0} \frac{1}{k_n^2} \sum_{\tilde{\sigma} \in S_{n-2}} \mathcal{S}[\sigma|\tilde{\sigma}] A_{r,s}^{\text{YMs}}(\alpha|1, \tilde{\sigma}, n). \quad (2.14)$$

The expansion coefficient in (2.13) is the desired quantity we want to compute in this paper. As we have discussed in previous paragraph, these coefficients are determined by only one weight-2 ingredient in the CHY-integrand in (2.1). This means that while keeping the same weight-2 ingredient, we have the freedom to change the other weight-2 ingredient. As an implication of such modification, we could work out the expansion for different field theories but with the same expansion coefficients. This freedom could simplify our investigation of expansion coefficients. For example, in the context of EYM amplitude as Yang-Mills amplitudes, we can change the $\text{Pf}' \Psi_n$ in (2.9) as $\text{PT}_n(\rho)$. The resulting CHY-integrand

$$\mathcal{I}_{r,s}^{\text{YMs}}(\alpha|\rho) = \text{PT}_r(\alpha) \text{Pf } \Psi_s \times \text{PT}_n(\rho) \quad (2.15)$$

describes a Yang-Mills-scalar amplitude with r scalars and s gluons, and the weight-2 ingredients are now $\mathcal{I}_L = \text{PT}_r(\alpha) \text{Pf } \Psi_s$ and $\mathcal{I}_R = \text{PT}_n(\rho)$. With the same philosophy as in (2.10), we can define two new CHY-integrands as

$$\mathcal{I}_L^{\text{CHY}} := \text{PT}_r(\alpha) \text{Pf } \Psi_s \times \text{PT}_n(\gamma), \quad \mathcal{I}_R^{\text{CHY}} := \text{PT}_n(\rho) \times \text{PT}_n(\beta). \quad (2.16)$$

Hence we arrive at the following expansion

$$A_{r,s}^{\text{YMs}}(\alpha|\rho) = \sum_{\sigma \in S_{n-3}} \tilde{C}(\alpha|\sigma) A_n^{\phi^3}(\rho|n-1, n, \sigma, 1), \quad (2.17)$$

with the same expansion coefficients as in (2.12). This non-trivial relation expresses any single trace color-ordered amplitude of Yang-Mills-scalar theory as linear combination of color-ordered amplitude of bi-adjoint scalar ϕ^3 theory.

After studying the expansion of single trace part of EYM theory to YM theory, we will briefly discuss the expansion of gravity theory to YM theory. The CHY-integrand of gravity theory is

$$\mathcal{I}_{r,s}^{\text{G}}(\alpha) = \text{Pf}' \Psi_n \times \text{Pf}' \Psi_n. \quad (2.18)$$

If expanding the reduced Pfaffian

$$\text{Pf}' \Psi_n = \sum_{\sigma \in S_{n-2}} n(1, \sigma, n) \text{PT}_n(1, \alpha, n) \quad (2.19)$$

by cross-ratio identities, we will get

$$A^{\text{G}} = \sum_{\sigma \in S_{n-2}} n(1, \sigma, n) A^{\text{YM}}(1, \sigma, n) \quad (2.20)$$

by (2.18). As already pointed out in papers [23, 54, 57, 63–66], the coefficients $n(1, \sigma, n)$ in the expansion (2.19) (hence also the one in the expansion (2.20)) is nothing but the DDM basis for the BCJ numerator of YM amplitude. While in the expansion (2.8), i.e., $A = \sum_{\sigma \in S_{n-3}} \tilde{C}(\sigma) A_L(n-1, n, \sigma, 1)$, suppose we can rewrite the $(n-3)!$ BCJ basis into $(n-2)!$ KK basis, then identifying the resulting formula with the one given by (2.20), and equating the expansion coefficients of the same KK basis, we will get the BCJ numerator $n(1, \sigma, n)$ as linear combination of $\tilde{C}(\sigma)$. Thus here we provided a new way of computing the BCJ numerators via the computation of amplitude expansion (2.8). Although in (2.20) we have taken gravity amplitude as example, the same consideration can be applied to large number of theories, and the BCJ numerators of those theories can also be identified as the expansion coefficients after rewriting (2.8) into KK basis.

With the above general framework for studying the non-trivial relations among different theories, we will start our exploration from next section. As we will see, these relations encode many surprising structures and connect many important topics, such as the construction of BCJ numerators mentioned above, the boundary contribution of amplitudes under BCFW on-shell recursion relation, the DDM chain and BCJ relations, etc.,

3 The gauge invariance determines the amplitude relations

A physical amplitude should be gauge invariant, i.e., vanishes on the condition $\epsilon_i \rightarrow k_i$. If considering the amplitudes with gravitons and expressing the graviton polarization states as products of two Yang-Mills polarization states $\epsilon_i^\pm \epsilon_i^\pm$, then it should also vanish by setting one of the polarization vector as k_i . The gauge invariance is an important property of amplitude, and of course it is also valid in the amplitude relations. As we have mentioned in previous section, there are different approaches to study expansion coefficients. In this section, we will demonstrate how to use the gauge invariance to fix coefficients, which is the same spirit spelled out in [47–49].

3.1 With single graviton

To motivate our discussion, let us start with the single trace EYM amplitude with one graviton with the known expansion

$$A_{n,1}^{\text{EYM}}(1, 2, \dots, n; p) = \sum_{\sqcup} (\epsilon_p \cdot Y_p) A_{n+1}^{\text{YM}}(1, \{2, \dots, n-1\} \sqcup \{p\}, n), \quad (3.1)$$

where the summation $\sqcup$ is over all shuffles $\sigma \sqcup \tilde{\sigma}$, i.e., all permutation sets of $\sigma \cup \tilde{\sigma}$ while preserving the ordering of each $\sigma, \tilde{\sigma}$. The color-ordering of external legs in A_{n+1}^{YM} has cyclic invariance. However if we conventionally fix the leg 1 in the first position, then every external leg could have a definite position in the color-ordering. In this convention, we can define Y_p (also X_p in the following paragraph) as the sum of momenta of all the gluons at the left hand side (l.h.s.) of leg p , given the definite color-ordering of color-ordered YM amplitudes.

A clarification of the definition Y_p is needed here for the future usage. In the $(n+1)$ -point pure Yang-Mills amplitude, the gluon legs has two different correspondents in the EYM amplitude, i.e., The gluon legs $k_i, i = 1, \dots, n$ are also gluons in EYM amplitude while gluon leg p is originally graviton leg in EYM amplitude. Y_p is specifically defined as the sum of momenta in the gluon subset of EYM amplitude at the l.h.s. of p , while we also define another quantity X_p as the sum of all momenta at the l.h.s. of p no matter it is in the gluon subset or graviton subset of EYM amplitude. X_p, Y_p would be different when considering EYM amplitude with more than one gravitons, but in the current discussion they are the same.

Let us now return to the relation (3.1). In the l.h.s., imposing any gauge condition $\epsilon_i \rightarrow k_i$ for gluon legs would vanish the EYM amplitude, while any Yang-Mills amplitudes in the right hand side (r.h.s.) also vanish under the same gauge condition. For the graviton polarization $\epsilon_p^\pm \epsilon_p^\pm$, setting either $\epsilon_p \rightarrow p$ would vanish the EYM amplitude. In the r.h.s., the graviton polarization is distributed in two places: one is in the Yang-Mills amplitude and the other, in the expansion coefficients. The vanish of r.h.s. for the former case is trivial, while for the latter case, it vanishes due to the fundamental BCJ relations

$$\sum_{\sqcup} (p \cdot Y_p) A_{n+1}^{\text{YM}}(1, \{2, \dots, n-1\} \sqcup \{p\}, n) = 0. \quad (3.2)$$

This consequence is rather interesting. For the non-trivial relation (3.1) to be true and the gauge invariance be not violated, we eventually end up with BCJ relations. On the other

hand, if we assume $A_{n,1}^{\text{EYM}}$ can be expanded as linear combination of Yang-Mills amplitudes in the KK basis for convenience, and the expansion coefficients should be certain sum of $\epsilon_p \cdot k_i$ to compensate the extra graviton polarization,

$$A_{n,1}^{\text{EYM}}(1, \dots, n; p) = \sum_{\alpha \in S_{n-1}} (\epsilon_p \cdot x_p) A_{n+1}^{\text{YM}}(1, \alpha_2, \dots, \alpha_{n-1}, \alpha_p, n), \quad (3.3)$$

then $\sum_{\alpha} (p \cdot x_p) A_{n+1}^{\text{YM}}(1, \alpha_2, \dots, \alpha_{n-1}, \alpha_p, n)$ should be in the BCJ relation form!

The lesson learned from the EYM amplitude with one graviton suggests that, while expressing EYM amplitudes as linear combination of Yang-Mills amplitudes, the gauge invariance strongly constraints the possible form of expansion coefficients. This property motivates us to find the expansion of the single trace multi-graviton EYM amplitude with more than one graviton

$$A_{n,m}^{\text{EYM}}(1, \dots, n; h_1, \dots, h_m), \quad (3.4)$$

by gauge invariance, i.e., we want coefficients to make the expression to zero under each gauge condition $\epsilon_{h_i} \rightarrow h_i$.

In order to construct the non-trivial relations for EYM amplitudes with generic number of gravitons, we start with the following two ansatz,

- **Ansatz 1:** the single trace EYM amplitude $A_{n,m}^{\text{EYM}}$ with m gravitons can always be expanded into EYM amplitudes $A_{n+m-m',m'}^{\text{EYM}}$ with $m' < m$ gravitons.
- **Ansatz 2:** when an EYM amplitude $A_{n,m}^{\text{EYM}}$ is expanded into pure Yang-Mills amplitudes, the terms whose expansion coefficients contains only $\epsilon \cdot k$ but no $\epsilon \cdot \epsilon$ takes the form,²

$$\sum_{\alpha \in S_m} \sum_{\sqcup} (\epsilon_{h_{\alpha_1}} \cdot X_{h_{\alpha_1}}) \cdots (\epsilon_{h_{\alpha_m}} \cdot X_{h_{\alpha_m}}) A_{n+m}^{\text{YM}}(1, \{1, 2, \dots, n\} \sqcup \{\alpha_{h_1}, \dots, \alpha_{h_m}\}, n). \quad (3.5)$$

These two ansatz come from lower-point known results. The first ansatz is in fact a general statement saying that a recursive construction for EYM amplitude expansion exists. While the second ansatz is presented in an explicit expression which has an obvious BCJ-like relation form. The validation of ansatz 2 in fact can be verified by BCFW recursions. In the expression (3.5), we emphasize again that X_{h_i} is defined to be the sum of all momenta in the l.h.s. of leg h_i , no matter those legs representing gluons or gravitons in the EYM amplitude.

Bearing in mind that any EYM amplitude expansion relations should follow the above mentioned two ansatz, we are now ready to extend the introductory one graviton example to EYM amplitudes with arbitrary number of gravitons. However, before presenting the general algorithm, let us familiarize ourselves by studying EYM amplitudes with two and three gravitons.

²We have taken the convention that, for an EYM amplitude we choice the sign of these terms to be (+). It would be possible that for results in other conventions, for instance the CHY results in recent literatures, there could be a sign difference.

3.2 Expressing n -gluon two-graviton EYM amplitudes as Yang-Mills amplitudes

The algorithm for producing general EYM amplitude relations is to expand $A_{n,m}^{\text{EYM}}$ as $A_{n+1,m-1}^{\text{EYM}}$ *successively* until $A_{n+m,0}^{\text{EYM}} \equiv A_{m+n}^{\text{YM}}$. Note that the gravitons are colorless, and it has no color-ordering in EYM amplitudes. But in our construction of EYM amplitude relation by gauge invariance principle, it is necessary to specify a graviton in each step of expansion $A_{n,m}^{\text{EYM}} \rightarrow A_{n+1,m-1}^{\text{EYM}}$, which in the $A_{n,m}^{\text{EYM}}$ amplitude it denotes a graviton but in the $A_{n+1,m-1}^{\text{EYM}}$ amplitude it denotes a gluon, such that we can apply gauge invariance principle with that graviton. Furthermore, it requires us to select one arbitrary graviton to start with.

Now let us outline the arguments that lead to the correct expansion of EYM amplitude with two gravitons $A_{n,2}^{\text{EYM}}(1, 2, \dots, n; p, q)$. In the first step, let us specify the graviton h_p , and following the **Ansatz 1** let us propose the following terms that *would* contribute to the expansion of $A_{n,2}^{\text{EYM}}$,

$$T_1 = \sum_{\sqcup} (\epsilon_p \cdot Y_p) A_{n+1,1}^{\text{EYM}}(1, \{2, \dots, n-1\} \sqcup \{p\}, n; q). \quad (3.6)$$

In fact, these proposed terms (3.6) are reminiscent of the expression (3.1) for expanding the single trace EYM amplitude with one graviton. This is not yet the complete expansion expression for $A_{n,2}^{\text{EYM}}$, but we will explain soon after how to recover the remaining terms. Let us investigate the gauge invariance of gravitons h_p and h_q for the proposed terms (3.6). The gauge invariance for h_q is obvious since $A_{n+1,1}^{\text{EYM}}(\dots; q)$ vanishes under $\epsilon_q \rightarrow q$ gauge condition. However, T_1 is not gauge invariant under $\epsilon_p \rightarrow p$ due to the expansion coefficients $\epsilon_p \cdot Y_p$, and there are some missing terms in order to produce the complete expansion for $A_{n,2}^{\text{EYM}}$. Let us proceed to expand the $A_{n+1,1}^{\text{EYM}}$ in T_1 with the known result (3.1), which gives

$$T_1 = \sum_{\sqcup_1} (\epsilon_p \cdot Y_p) \sum_{\sqcup_2} (\epsilon_q \cdot X_q) A_{n+2}^{\text{YM}}(1, (\{2, \dots, n-1\} \sqcup_1 \{p\}) \sqcup_2 \{q\}, n). \quad (3.7)$$

Note that in the permutation shuffle $\{2, \dots, n-1\} \sqcup \{p\} \sqcup \{q\}$, the position of leg q would be either at the l.h.s. of p or r.h.s. of p . But the leg p denotes a graviton in $A_{n,2}^{\text{EYM}}$. So the expansion coefficient is $\epsilon_q \cdot X_q$ but not $\epsilon_q \cdot Y_q$ (remind that X_q is the sum of all momenta in the l.h.s. of q , while Y_q is the sum of all momenta in the l.h.s. of q excluded the leg p , which means that if p is at the r.h.s. of q , $X_q = Y_q$, but if p is at the l.h.s. of q , $X_q = Y_q + p$).

From the **Ansatz 2** (3.5), we know that in the $A_{n,2}^{\text{EYM}}$ expansion, the correct terms with coefficients $(\epsilon_q \cdot \bullet)(\epsilon_q \cdot \bullet)$ must be

$$\sum_{\sqcup_1} \sum_{\sqcup_2} (\epsilon_p \cdot X_p)(\epsilon_q \cdot X_q) A_{n+2}^{\text{YM}}(1, \{2, \dots, n-1\} \sqcup_1 \{p\} \sqcup_2 \{q\}, n). \quad (3.8)$$

Comparing T_1 (3.7) with the correct result (3.8), it is easy to see that for those terms with p in the l.h.s. of q , $Y_p = X_p$ so that the corresponding terms in T_1 and (3.8) are the same. While for those terms with p in the r.h.s. of q , we have $Y_p + q = X_p$. So in order to reproduce the correct result (3.8), we should add another contribution

$$T_2 = \sum_{\sqcup} (\epsilon_p \cdot q)(\epsilon_q \cdot X_q) A_{n+2}^{\text{YM}}(1, \{2, \dots, n-1\} \sqcup \{q, p\}, n) \quad (3.9)$$

such that

$$T_1 + T_2 = \sum_{\sqcup} (\epsilon_p \cdot Y_p) A_{n+1,1}^{\text{EYM}}(1, \{2, \dots, n-1\} \sqcup \{p\}, n; q) \\ + \sum_{\sqcup} (\epsilon_p \cdot q)(\epsilon_q \cdot X_q) A_{n+2}^{\text{YM}}(1, \{2, \dots, n-1\} \sqcup \{q, p\}, n) \quad (3.10)$$

is exactly equivalent to the correct result (3.8). Remind that **Ansatz 2** gives correct answer for contributing terms without $(\epsilon \cdot \epsilon)$ coefficients for EYM amplitude expansion, and up to now, we have reformulated the correct result as (3.10) which guarantees an easy generalization.

Of course, (3.10) is still not yet the complete expansion for $A_{n,2}^{\text{EYM}}$, since those terms with coefficient $(\epsilon_p \cdot \epsilon_q)$ are still missing. Let us propose that the complete expansion takes the form

$$A_{n,2}^{\text{EYM}}(1, 2, \dots, n; p, q) = T_1 + T_2 + (\epsilon_p \cdot \epsilon_q) T_3, \quad (3.11)$$

and the remaining task is to determine T_3 . It can be determined either by gauge condition $\epsilon_p \rightarrow p$ or by $\epsilon_q \rightarrow q$, however the latter is much more convenient since T_1 is already manifestly gauge invariant for leg q . Setting $\epsilon_q \rightarrow q$, we have

$$0 = \left(T_1 + T_2 + (\epsilon_p \cdot \epsilon_q) T_3 \right) \Big|_{\epsilon_q \rightarrow q} = (\epsilon_p \cdot q) \left(\sum_{\sqcup} (q \cdot X_q) A_{n+2}^{\text{YM}}(1, \{2, \dots, n-1\} \sqcup \{q, p\}, n) + T_3 \right), \quad (3.12)$$

which has a solution

$$T_3 = - \sum_{\sqcup} (q \cdot X_q) A_{n+2}^{\text{YM}}(1, \{2, \dots, n-1\} \sqcup \{q, p\}, n). \quad (3.13)$$

Hence we get the non-trivial relation for EYM amplitude with two gravitons as

$$A_{n,2}^{\text{EYM}}(1, 2, \dots, n; p, q) = \sum_{\sqcup} (\epsilon_p \cdot Y_p) A_{n+1,1}^{\text{EYM}}(1, \{2, \dots, n-1\} \sqcup \{p\}, n; q) \\ + \sum_{\sqcup} (\epsilon_p \cdot q)(\epsilon_q \cdot X_q) A_{n+2}^{\text{YM}}(1, \{2, \dots, n-1\} \sqcup \{q, p\}, n) \\ - \sum_{\sqcup} (\epsilon_p \cdot \epsilon_q)(q \cdot X_q) A_{n+2}^{\text{YM}}(1, \{2, \dots, n-1\} \sqcup \{q, p\}, n). \quad (3.14)$$

If we define the tensor

$$F_q^{\mu\nu} := q^\mu \epsilon_q^\nu - \epsilon_q^\mu q^\nu, \quad (3.15)$$

the above EYM amplitude expansion can be reformulated in a more compact form as

$$A_{n,2}^{\text{EYM}}(1, 2, \dots, n; p, q) = \sum_{\sqcup} (\epsilon_p \cdot Y_p) A_{n+1,1}^{\text{EYM}}(1, \{2, \dots, n-1\} \sqcup \{p\}, n; q) \\ + \sum_{\sqcup} (\epsilon_p \cdot F_q \cdot X_q) A_{n+2}^{\text{YM}}(1, \{2, \dots, n-1\} \sqcup \{q, p\}, n). \quad (3.16)$$

From expression (3.16) we can infer some important features. Firstly, for terms in the first line, leg p denotes a gluon and leg q denotes a graviton, while for terms in the

second line, leg q denotes gluon instead of graviton. This difference leads to the difference of expansion coefficient, such that the Y_p factor in the first line has been replaced by the factor $F_q \cdot X_q$. Or we can say a factor F_q is inserted. As we would see shortly after, this is a general pattern for EYM amplitudes involving more gravitons.

Secondly, in the expression (3.16), the gauge invariance for leg q is manifest, while gauge invariance for leg p is not manifest and requires further checking. Although it can be checked directly, we will follow another approach. Note that the whole result should be symmetric under switching $p \leftrightarrow q$. For the terms with kinematic factors $(\epsilon \cdot k)(\epsilon \cdot k)$, this symmetry is manifest since it is given by (3.8). For the terms with kinematic factors $(\epsilon_p \cdot \epsilon_q)$, the result is not manifestly symmetric. In order to show the symmetry, we need to use the generalized BCJ relation. Let us divide the set $\{2, \dots, n-1\}$ into two ordered subsets $\alpha = \{\alpha_1, \dots, \alpha_m\}$ and $\beta = \{\beta_1, \dots, \beta_t\}$ such that $m+t = n-2$, then the general BCJ relation is given by [12, 34]

$$\sum_{\sqcup} \left(\sum_{i=1}^t k_{\beta_i} \cdot X_{\beta_i} \right) A(1, \alpha \sqcup \beta, n) = 0, \quad (3.17)$$

where the first summation is over all shuffles, and X_{β_i} is the summation of all momenta of legs at the l.h.s. of leg β_i . Using (3.17) with $\beta = \{q, p\}$ it is easy to see that

$$\begin{aligned} (\epsilon_q \cdot \epsilon_p) \sum_{\sqcup} (q \cdot X_q) A(1, \{2, \dots, n-1\} \sqcup \{q, p\}, n) \\ = -(\epsilon_q \cdot \epsilon_p) \sum_{\sqcup} (p \cdot X_p) A(1, \{2, \dots, n-1\} \sqcup \{q, p\}, n). \end{aligned} \quad (3.18)$$

Next, we use the general BCJ relation (3.17) with the choice $\beta = \{p\}$ (i.e., the fundamental BCJ relation) to reach

$$(\epsilon_q \cdot \epsilon_p) \sum_{\sqcup} (p \cdot X_p) A(1, \{2, \dots, n-1\} \sqcup \{p, q\}, n). \quad (3.19)$$

Hence the symmetry of legs q, p for the terms with factor $(\epsilon_p \cdot \epsilon_q)$ is apparent. Since the gauge invariance for leg q is satisfied, by the symmetry, the gauge invariance for leg p is also satisfied.

The above discussion allows a systematical generalization to EYM amplitude with any number of gravitons. Before doing so, let us introduce a new quantity which would be useful in later discussions. Assuming the gravitons have been split into two subsets α, β , where α is the ordered length- m_1 set in the gluon side and β is a length- m_2 set in the graviton side whose ordering is not relevant, we define

$$\mathcal{T}[\alpha|\beta] = \sum_{\sqcup} \left(\prod_{i=1}^{m_1-1} \epsilon_{\alpha_i} \cdot k_{\alpha_{i+1}} \right) (\epsilon_{\alpha_{m_1}} \cdot Y_{\alpha_{m_1}}) A_{n+m_1, m_2}^{\text{EYM}}(1, \{2, \dots, n-1\} \sqcup \{\alpha_{m_1}, \dots, \alpha_1\}, n; \beta). \quad (3.20)$$

For example, if $\alpha = \{p\}, \beta = \{q\}$, we have $m_1 = m_2 = 1$, and

$$\mathcal{T}[\{p\}|\{q\}] = \sum_{\sqcup} (\epsilon_p \cdot Y_p) A_{n+1, 1}^{\text{EYM}}(1, \{2, \dots, n-1\} \sqcup \{p\}, n; q), \quad (3.21)$$

which is in fact the first line of (3.14). While if $\alpha = \{q, p\}, \beta = \emptyset, m_1 = 2, m_2 = 0$, and we have

$$\mathcal{T}[\{q, p\}|\emptyset] = \sum_{\sqcup} (\epsilon_p \cdot q)(\epsilon_q \cdot Y_q) A_{n+2}^{\text{YM}}(1, \{2, \dots, n-1\} \sqcup \{q, p\}, n), \quad (3.22)$$

which reproduces the second line of (3.14).

3.3 Expressing n -gluon three-graviton EYM amplitudes as Yang-Mills amplitudes

Now let us explore the details by the EYM amplitude with three gravitons $A_{n,3}^{\text{EYM}}(1, \dots, n; p, q, r)$. Our purpose is to construct a recursive algorithm for EYM amplitude expansion which is manifestly gauge invariant in each step for gravitons (except the initial one), and the terms without $(\epsilon_{h_i} \cdot \epsilon_{h_j})$ factor matches the **Ansatz 2** (3.5). In the current case it is

$$\sum_{\sqcup_1} \sum_{\sqcup_2} \sum_{\sqcup_3} (\epsilon_p \cdot X_p)(\epsilon_q \cdot X_q)(\epsilon_r \cdot X_r) A_{n+3}^{\text{YM}}(1, \{2, \dots, n-1\} \sqcup_1 \{p\} \sqcup_2 \{q\} \sqcup_3 \{r\}, n). \quad (3.23)$$

Again, the starting point is specifying an arbitrary graviton for expanding $A_{n,3}^{\text{EYM}} \rightarrow A_{n+1,2}^{\text{EYM}}$ and without loss of generality we choose p . The proposed contributing terms are

$$\mathcal{T}[\{p\}|\{q, r\}] = \sum_{\sqcup} (\epsilon_p \cdot Y_p) A_{n+1,2}^{\text{EYM}}(1, \{2, \dots, n-1\} \sqcup \{p\}, n; q, r). \quad (3.24)$$

Note that q, r are manifestly gauge invariant in $\mathcal{T}[\{p\}|\{q, r\}]$, and legs q, r denote gravitons.

To match the correct result (3.23), we need to add terms where leg q or r is at the l.h.s. of p . This means that we need to add terms $A_{n+2,1}^{\text{EYM}}$ where leg q or leg r now denotes gluon and its position is at the l.h.s. of leg p . For $A_{n+2,1}^{\text{EYM}}$ terms where leg p, q are gluons but leg r is graviton, the added term should be

$$\mathcal{T}[\{q, p\}|\{r\}] = \sum_{\sqcup} (\epsilon_p \cdot q)(\epsilon_q \cdot Y_q) A_{n+2,1}^{\text{EYM}}(1, \{2, \dots, n-1\} \sqcup \{q, p\}, n; r). \quad (3.25)$$

These terms introduce the missing terms for $\mathcal{T}[\{p\}|\{q, r\}]$ in order to match the result (3.23), however the gauge invariance for q is still broken. In order to keep gauge invariance for legs q, r at every step, we should further modify (3.25) by adding terms with $(\epsilon_p \cdot \epsilon_q)$ coefficients, and the resulting terms should not alter the matching with result (3.23). From experiences gained in the previous subsection, we can propose the following modification

$$\begin{aligned} \mathcal{G}[\{q, p\}|\{r\}] &= \sum_{\sqcup} (\epsilon_p \cdot q)(\epsilon_q \cdot Y_q) A_{n+2,1}^{\text{EYM}}(1, \{2, \dots, n-1\} \sqcup \{q, p\}, n; r) \\ &\quad - \sum_{\sqcup} (\epsilon_p \cdot \epsilon_q)(q \cdot Y_q) A_{n+2,1}^{\text{EYM}}(1, \{2, \dots, n-1\} \sqcup \{q, p\}, n; r) \\ &= \sum_{\sqcup} (\epsilon_p \cdot F_q \cdot Y_q) A_{n+2,1}^{\text{EYM}}(1, \{2, \dots, n-1\} \sqcup \{q, p\}, n; r), \end{aligned} \quad (3.26)$$

which are manifestly gauge invariant for q, r .

Similarly, for $A_{n+2,1}^{\text{EYM}}$ terms where legs p, r are gluons but leg q is graviton, the proposed gauge invariant term should be

$$\mathcal{G}[\{r, p\}|\{q\}] = \sum_{\sqcup} (\epsilon_p \cdot F_r \cdot Y_r) A_{n+2,1}^{\text{EYM}}(1, \{2, \dots, n-1\} \sqcup \{r, p\}, n; q). \quad (3.27)$$

Emphasize again that the above proposals are based on the gauge invariant principle, the **Ansatz 1** and the **Ansatz 2**.

Notice that in (3.26) and (3.27), we have $(\epsilon_q \cdot Y_q)$ or $(\epsilon_r \cdot Y_r)$ instead of $(\epsilon_{q,r} \cdot X_{q,r})$. So in order to arrive at a complete matching with result (3.23), we should further add $A_{n+3,0}^{\text{EYM}}$ terms where all p, q, r are gluon legs. For $\mathcal{G}[\{q, p\}|\{r\}]$, the **Ansatz 1** guides us to propose additional terms as

$$\sum_{\sqcup} (\epsilon_p \cdot F_q \cdot r)(\epsilon_r \cdot Y_r) A_{n+3}^{\text{EYM}}(1, \{2, \dots, n-1\} \sqcup \{r, q, p\}, n). \quad (3.28)$$

However, these terms are not gauge invariant for leg r , and according to gauge invariance principle we need to modify (3.28) as

$$\begin{aligned} \mathcal{G}[\{r, q, p\}|\emptyset] &= \sum_{\sqcup} (\epsilon_p \cdot F_q \cdot r)(\epsilon_r \cdot Y_r) A_{n+3}^{\text{YM}}(1, \{2, \dots, n-1\} \sqcup \{r, q, p\}, n) \\ &\quad - \sum_{\sqcup} (\epsilon_p \cdot F_q \cdot \epsilon_r)(r \cdot Y_r) A_{n+3}^{\text{YM}}(1, \{2, \dots, n-1\} \sqcup \{r, q, p\}, n) \\ &= \sum_{\sqcup} (\epsilon_p \cdot F_q \cdot F_r \cdot Y_r) A_{n+3}^{\text{YM}}(1, \{2, \dots, n-1\} \sqcup \{r, q, p\}, n), \end{aligned} \quad (3.29)$$

which reproduces the correct result (3.23) yet is gauge invariant manifestly. The $(\epsilon_p \cdot F_q \cdot \epsilon_r)$ coefficient in the second line of (3.29) is

$$(\epsilon_p \cdot F_q \cdot \epsilon_r) = (\epsilon_p \cdot q)(\epsilon_q \cdot \epsilon_r) - (\epsilon_p \cdot \epsilon_q)(q \cdot \epsilon_r), \quad (3.30)$$

so we can see clearly that, the second line of (3.29) only introduces terms with $(\epsilon_{h_i} \cdot \epsilon_{h_j})$ factor which will not contribute to the (3.23) terms.

Similarly, for $\mathcal{G}[\{r, p\}|\{q\}]$, we need to add the following gauge invariant terms

$$\mathcal{G}[\{q, r, p\}|\emptyset] = \sum_{\sqcup} (\epsilon_p \cdot F_r \cdot F_q \cdot Y_q) A_{n+3}^{\text{YM}}(1, \{2, \dots, n-1\} \sqcup \{q, r, p\}, n). \quad (3.31)$$

Summarizing all parts together, we have

$$\begin{aligned} A_{n,3}^{\text{EYM}}(1, \dots, n; p, q, r) &= \mathcal{T}[\{p\}|\{q, r\}] + \mathcal{G}[\{q, p\}|\{r\}] + \mathcal{G}[\{r, p\}|\{q\}] + \mathcal{G}[\{r, q, p\}|\emptyset] + \mathcal{G}[\{q, r, p\}|\emptyset] \\ &= \sum_{\sqcup} (\epsilon_p \cdot Y_p) A_{n+1,2}^{\text{EYM}}(1, \{2, \dots, n-1\} \sqcup \{p\}, n; q, r) \\ &\quad + \sum_{\sqcup} (\epsilon_p \cdot F_q \cdot Y_q) A_{n+2,1}^{\text{EYM}}(1, \{2, \dots, n-1\} \sqcup \{q, p\}, n; r) \\ &\quad + \sum_{\sqcup} (\epsilon_p \cdot F_r \cdot Y_r) A_{n+2,1}^{\text{EYM}}(1, \{2, \dots, n-1\} \sqcup \{r, p\}, n; q) \\ &\quad + \sum_{\sqcup} (\epsilon_p \cdot F_q \cdot F_r \cdot Y_r) A_{n+3}^{\text{YM}}(1, \{2, \dots, n-1\} \sqcup \{r, q, p\}, n) \\ &\quad + \sum_{\sqcup} (\epsilon_p \cdot F_r \cdot F_q \cdot Y_q) A_{n+3}^{\text{YM}}(1, \{2, \dots, n-1\} \sqcup \{q, r, p\}, n). \end{aligned} \quad (3.32)$$

Expression (3.32) has demonstrated the recursive construction pattern more clearly, i.e., expanding the EYM amplitude successively and keep the gauge invariance in each step by introducing additional terms. The starting point is to specify an arbitrary graviton and propose the contributing terms $\mathcal{T}[\{p\}|\{q, r\}]$, which are terms of $A_{n+1,2}^{\text{EYM}}$. It reproduces a part of the correct result (3.23) from **Ansatz 2**, and another part would come from $A_{n+2,1}^{\text{EYM}}$ terms. Specifying graviton q , we can propose the contributing terms $\mathcal{G}[\{q, p\}|\{r\}]$, deduced from gauge invariance principle, **Ansatz 1** and the matching of **Ansatz 2**. While specifying graviton r , we can propose $\mathcal{G}[\{r, p\}|\{q\}]$. The remaining part could be proposed by specifying the last graviton, which gives $\mathcal{G}[\{r, q, p\}|\emptyset]$, $\mathcal{G}[\{q, r, p\}|\emptyset]$. The correctness of terms without $(\epsilon_{h_i} \cdot \epsilon_{h_j})$ is guaranteed by construction, while the terms with $(\epsilon_{h_i} \cdot \epsilon_{h_j})$ factor are determined by gauge invariance in each step. The gauge invariance for q, r is then manifest at each term, except for the leg p . It is also easy to see that, in each step when leg h_i in the amplitude denotes a gluon while in the previous step it denotes a graviton, the corresponding gauge invariant term is just to insert a F_{h_i} into the kinematic factor in an appropriate position. It corresponds to replacing $k_{h_i}^\mu \epsilon_{h_i}^\nu$ as $F_{h_i}^{\mu\nu}$. So similar to the definition of $\mathcal{T}[\alpha|\beta]$ in (3.20), we can define a new quantity

$$\mathcal{G}[\alpha|\beta] = \sum_{\sqcup} (\epsilon_{\alpha_1} \cdot F_{\alpha_2} \cdot F_{\alpha_3} \cdots F_{\alpha_{m_1}} \cdot Y_{\alpha_{m_1}}) A_{n+m_1, m_2}^{\text{EYM}}(1, \{2, \dots, n-1\} \sqcup \{\alpha_{m_1}, \dots, \alpha_1\}, n; \beta). \quad (3.33)$$

Note that when $m_1 = 1$, $\mathcal{T}[\alpha|\beta] = \mathcal{G}[\alpha|\beta]$.

Before presenting the algorithm for general EYM amplitude relations, we give a remark on the gauge invariance of p . It is not apparent, but one can show the full S_3 symmetry among three gravitons after using various BCJ relations. Hence the gauge invariance of leg p should be indicated by the symmetry.

3.4 A constructive algorithm for producing general EYM amplitude relations

The basic idea of constructive algorithm for producing general EYM amplitude relations $A_{n,m}^{\text{EYM}}$ is to write down the contributing terms $A_{n+1, m-1}^{\text{EYM}}, A_{n+2, m-2}^{\text{EYM}}, \dots, A_{n+m, 0}^{\text{EYM}}$ successively, and the explicit expression corresponding to $A_{n+m', m-m'}^{\text{EYM}}$ relies on $A_{n+m'-1, m-m'+1}^{\text{EYM}}$ recursively. Briefly speaking, provided we have written down the contribution of $A_{n-m_2, m_2}^{\text{EYM}}$, where the gravitons in this EYM amplitude are labeled as $\beta = \{\beta_1, \dots, \beta_{m_2}\}$. Then by specifying a graviton, say h_{β_i} ,

$$\beta_i \in \beta = \{\beta_1, \dots, \beta_{m_2}\},$$

we can directly write down a gauge invariant contributing term $A_{n-m_2+1, m_2-1}^{\text{EYM}}$ as $\mathcal{G}[\{\beta_i\} \cup \alpha|\beta/\{\beta_i\}]$, whose coefficients are obtained by replacing $Y_{\alpha_{m_1}} \rightarrow F_{\beta_i} \cdot Y_{\beta_i}$ in the coefficients of $A_{n-m_2, m_2}^{\text{EYM}}$.

Now let us describe the algorithm for generic EYM amplitude relations. For the EYM amplitude with m gravitons

$$A_{n,m}^{\text{EYM}}(1, 2, \dots, n; h_1, h_2, \dots, h_m), \quad (3.34)$$

- **Step 1:** specify arbitrary one graviton, say h_1 , and record the contribution

$$\mathcal{G}[\{h_1\}|\{h_2, \dots, h_m\}]. \quad (3.35)$$

- **Step 2:** from the previous step, specify one graviton $h'_2 \in \{h_2, \dots, h_m\}$, and record the corresponding contribution

$$\mathcal{G}[\{h'_2, h_1\}|\{h_2, \dots, h_m\}/\{h'_2\}] , \quad h'_2 \in \{h_2, \dots, h_m\} . \quad (3.36)$$

- **Step 3:** for each $\mathcal{G}$ in the previous step, specify one graviton $h'_3 \in \{h_2, \dots, h_m\}/\{h'_2\}$ and record the corresponding contribution

$$\mathcal{G}[\{h'_3, h'_2, h_1\}|\{h_2, \dots, h_m\}/\{h'_2, h'_3\}] , \quad h'_2 \in \{h_2, \dots, h_m\} , \quad h'_3 \in \{h_2, \dots, h_m\}/\{h'_2\} . \quad (3.37)$$

•

- **Step m:** for each $\mathcal{G}$ in the previous step, specify one graviton $h'_m = \{h_2, \dots, h_m\}/\{h'_2, \dots, h'_{m-1}\}$ and record the contribution

$$\mathcal{G}[\{h'_m, h'_{m-1}, \dots, h'_2, h_1\}|\emptyset] , \quad h'_i \in \{h_2, \dots, h_m\}/\{h'_2, \dots, h'_{i-1}\} \text{ for } i = 2, \dots, m . \quad (3.38)$$

Summing over all the recorded contributions, we get the relation for generic EYM amplitude expansion as

$$A_{n,m}^{\text{EYM}}(1, 2, \dots, n; h_1, h_2, \dots, h_m) = \sum_{|H|=0}^{m-1} \sum_{H \subset \{h_2, \dots, h_m\}} \sum_{\sigma \in S_{|H|}} \mathcal{G}[\{\sigma_H, h_1\}|\{h_2, \dots, h_m/H\}] , \quad (3.39)$$

where H is a subset of $\{h_2, \dots, h_m\}$, and $|H|$ is the length of set H . Explicitly writing down, we have

$$\begin{aligned} & A_{n,m}^{\text{EYM}}(1, 2, \dots, n; h_1, h_2, \dots, h_m) \\ &= \mathcal{G}[\{h_1\}|\{h_2, \dots, h_m\}] + \left(\sum_{h'_2 \in \{h_2, \dots, h_m\}} \mathcal{G}[\{h'_2, h_1\}|\{h_2, \dots, h_m\}/\{h'_2\}] \right) \\ &+ \dots + \left(\sum_{\{h'_2, \dots, h'_k\} \subset \{h_2, \dots, h_m\}} \sum_{\sigma \in S_{k-1}} \mathcal{G}[\{\sigma_{h'_2}, \dots, \sigma_{h'_k}, h_1\}|\{h_2, \dots, h_m\}/\{h'_2, \dots, h'_k\}] \right) \\ &+ \dots + \left(\sum_{\sigma \in S_{m-1}} \mathcal{G}[\{\sigma_{h'_2}, \dots, \sigma_{h'_m}, h_1\}|\emptyset] \right) . \end{aligned} \quad (3.40)$$

Since $\mathcal{G}[\alpha|\beta]$ is well-defined in (3.33), the explicit expression for (3.39) can be readily written down. Note that relation (3.39) expands an EYM amplitude with m gravitons as linear combination of EYM amplitudes with $m' < m$ gravitons and Yang-Mills amplitudes. In this expression (3.40), the gauge invariance is manifest for $(m-1)$ gravitons $\{h_2, \dots, h_m\}$, since by construction, each contributing term $\mathcal{G}[\alpha|\beta]$ that building up the expansion relation is gauge invariant for $\{h_2, \dots, h_m\}$. For the leg h_1 , the gauge invariance is not manifest. However, as argued in [47–49], for n -point Yang-Mills amplitudes, manifest gauge invariance for $(n-1)$ points will be enough to guarantee the correctness of the result, so the gauge

invariance of the n -th point. We believe the same conclusion can be made for EYM theory by similar argument. If we buy this argument, result (3.39) must be the right expression.

As a demonstration, let us briefly present the non-trivial relations for EYM amplitude with four gravitons $A_{n,4}^{\text{EYM}}(1, \dots, n; h_1, h_2, h_3, h_4)$. The contributions in each step are abbreviated as follows,

$$[\{h_1\}|\{h_2, h_3, h_4\}] \rightarrow \left\{ \begin{array}{l} [\{h_2, h_1\}|\{h_3, h_4\}] \rightarrow \left\{ \begin{array}{l} [\{h_3, h_2, h_1\}|\{h_4\}] \rightarrow [\{h_4, h_3, h_2, h_1\}|\{\emptyset\}] \\ [\{h_4, h_2, h_1\}|\{h_3\}] \rightarrow [\{h_3, h_4, h_2, h_1\}|\{\emptyset\}] \end{array} \right. \\ \\ [\{h_3, h_1\}|\{h_2, h_4\}] \rightarrow \left\{ \begin{array}{l} [\{h_2, h_3, h_1\}|\{h_4\}] \rightarrow [\{h_4, h_2, h_3, h_1\}|\{\emptyset\}] \\ [\{h_4, h_3, h_1\}|\{h_2\}] \rightarrow [\{h_2, h_4, h_3, h_1\}|\{\emptyset\}] \end{array} \right. \\ \\ [\{h_4, h_1\}|\{h_2, h_3\}] \rightarrow \left\{ \begin{array}{l} [\{h_2, h_4, h_1\}|\{h_3\}] \rightarrow [\{h_3, h_2, h_4, h_1\}|\{\emptyset\}] \\ [\{h_3, h_4, h_1\}|\{h_2\}] \rightarrow [\{h_2, h_3, h_4, h_1\}|\{\emptyset\}] \end{array} \right. \end{array} \right. .$$

The first vertical line corresponds to the contributions of $A_{n+1,3}^{\text{EYM}}$, where we have specified leg h_1 as the gluon leg in $A_{n+1,3}^{\text{EYM}}$ amplitude. The second vertical line corresponds to the contributions of $A_{n+2,2}^{\text{EYM}}$, and seen from the first vertical line, we can specify either h_2, h_3 or h_4 as gluon leg in $A_{n+2,2}^{\text{EYM}}$ amplitudes. Thus we get three contributions. The third vertical line corresponds to the contributions of $A_{n+3,1}^{\text{EYM}}$, deduced from the second vertical line by specifying a graviton leg in $A_{n+2,2}^{\text{EYM}}$ as gluon leg in $A_{n+3,1}^{\text{EYM}}$. And so arrives at the fourth vertical line. Each one in the above table corresponds to a gauge invariant term $\mathcal{G}$ defined in (3.33), and summing over all contributions we get the expansion for EYM amplitude with four gravitons,

$$\begin{aligned} & A_{n,4}^{\text{EYM}}(1, \dots, n; h_1, h_2, h_3, h_4) \\ &= \sum_{\sqcup} (\epsilon_{h_1} \cdot Y_{h_1}) A_{n+1,3}^{\text{EYM}}(1, \{2, \dots, n-1\} \sqcup \{h_1\}, n; h_2, h_3, h_4) \\ &+ \sum_{i=2,3,4} \sum_{\sqcup} (\epsilon_{h_1} \cdot F_{h_i} \cdot Y_{h_i}) A_{n+2,2}^{\text{EYM}}(1, \{2, \dots, n-1\} \sqcup \{h_i, h_1\}, n; \{h_2, h_3, h_4\} / \{h_i\}) \\ &+ \sum_{\substack{2 \leq i, j \leq 4 \\ i \neq j}} \sum_{\sqcup} (\epsilon_{h_1} \cdot F_{\sigma_{h_i}} \cdot F_{\sigma_{h_j}} \cdot Y_{\sigma_{h_j}}) A_{n+3,1}^{\text{EYM}}(1, \{2, \dots, n-1\} \sqcup \{\sigma_{h_j}, \sigma_{h_i}, h_1\}, n; \{h_2, h_3, h_4\} / \{h_i, h_j\}) \\ &+ \sum_{\sigma \in S_3} \sum_{\sqcup} (\epsilon_{h_1} \cdot F_{\sigma_{h_2}} \cdot F_{\sigma_{h_3}} \cdot F_{\sigma_{h_4}} \cdot Y_{\sigma_{h_4}}) A_{n+4}^{\text{YM}}(1, \{2, \dots, n-1\} \sqcup \{\sigma_{h_2}, \sigma_{h_3}, \sigma_{h_4}, h_1\}, n). \end{aligned} \tag{3.41}$$

3.5 Expanding to pure Yang-Mills amplitudes: ordered splitting formula

The recursive construction given in (3.39) is easy to implement and one can eventually get an expansion with pure Yang-Mills amplitudes. In this subsection, we will present the related discussion.

To familiarize ourselves with this problem, let us start with some examples. The first example is the one with two gravitons. After substituting (3.1) into the first term of (3.16),

we get

$$\begin{aligned}
 A_{n,2}^{\text{EYM}}(1, 2, \dots, n; p, q) &= \sum_{\sqcup_1, \sqcup_2} (\epsilon_p \cdot Y_p)(\epsilon_q \cdot X_q) A_{n+2}^{\text{YM}}(1, \{2, \dots, n-1\} \sqcup_1 \{p\} \sqcup_2 \{q\}, n) \\
 &\quad + \sum_{\sqcup} (\epsilon_p \cdot F_q \cdot X_q) A_{n+2}^{\text{YM}}(1, \{2, \dots, n-1\} \sqcup \{q, p\}, n), \quad (3.42)
 \end{aligned}$$

where it is crucial to use X_q instead of Y_q in the first term of the expansion, since to the leg q , leg p is actually a gluon. Although the expression (3.42) is very suggestive, the pattern is still not clear, so we go ahead to the examples with three gravitons (3.32). Doing similar manipulations, we arrive at

$$\begin{aligned}
 A_{n,3}^{\text{EYM}}(1, \dots, n; p, q, r) &\quad (3.43) \\
 &= \sum_{\sqcup} (\epsilon_p \cdot Y_p)(\epsilon_q \cdot Z_q)(\epsilon_r \cdot Z_r) A_{n+3}^{\text{YM}}(1, \{2, \dots, n-1\} \sqcup \{p\} \sqcup \{q\} \sqcup \{r\}, n) \\
 &\quad + \sum_{\sqcup} (\epsilon_p \cdot Y_p)(\epsilon_q \cdot F_r \cdot Z_r) A_{n+3}^{\text{YM}}(1, \{2, \dots, n-1\} \sqcup \{p\} \sqcup \{r, q\}, n) \\
 &\quad + \sum_{\sqcup} (\epsilon_p \cdot F_q \cdot Y_q)(\epsilon_r \cdot Z_r) A_{n+3}^{\text{YM}}(1, \{2, \dots, n-1\} \sqcup \{q, p\} \sqcup \{r\}, n) \\
 &\quad + \sum_{\sqcup} (\epsilon_p \cdot F_r \cdot Y_r)(\epsilon_q \cdot Z_q) A_{n+3}^{\text{YM}}(1, \{2, \dots, n-1\} \sqcup \{r, p\} \sqcup \{q\}, n) \\
 &\quad + \sum_{\sqcup} (\epsilon_p \cdot F_q \cdot F_r \cdot Y_r) A_{n+3}^{\text{YM}}(1, \{2, \dots, n-1\} \sqcup \{r, q, p\}, n) \\
 &\quad + \sum_{\sqcup} (\epsilon_p \cdot F_r \cdot F_q \cdot Y_q) A_{n+3}^{\text{YM}}(1, \{2, \dots, n-1\} \sqcup \{q, r, p\}, n).
 \end{aligned}$$

Some explanations for (3.43) are in order. Firstly, when expanding $A_{n+1,2}^{\text{EYM}}(1, \{2, \dots, n-1\} \sqcup \{p\}, n; q, r)$ we need to specify a graviton leg which would be the gluon leg in $A_{n+2,1}^{\text{EYM}}$, and our choice is leg q . Secondly, we have defined a new notation Z_{h_i} . To define Z_{h_i} , we shall introduce a new concept, i.e., the *ordered splitting of m elements*. To define the ordered splitting, we must first define an ordering of m elements, for example, $h_1 \prec h_2 \prec \dots \prec h_m$ (we will call it *ordered gauge*). Once the *ordered gauge* is fixed, the ordered splitting is then defined by the following *ordered set* of subsets $\{\alpha_1, \dots, \alpha_t\}$ satisfying following conditions,

- Each subset $\alpha_i \subset \{h_1, \dots, h_m\}$ is ordered,
- $\text{Join}[\{\alpha_1, \dots, \alpha_t\}] = \{h_1, \dots, h_m\}$,
- Denoting R_{α_i} as the last element of the ordered subset α_i (or named the pivot), then $R_{\alpha_1} \prec R_{\alpha_2} \prec \dots \prec R_{\alpha_t}$ according to the *ordered gauge* (it defines the ordering of subset α_i in the set $\{a_1, \dots, a_t\}$),
- In each subset, all other elements must be larger than R_{α_i} according to the *ordered gauge*. However, there is no ordering requirement for all other elements.

To better understand the definition of ordered splitting, we take the set $\{p, q, r\}$ with *ordered gauge* $p \prec q \prec r$ as an example to write down all ordered splitting,

- With only one subset, we can have two cases: $\{r, q, p\}$ and $\{q, r, p\}$,
- With two subsets, we can have three cases: $\{\{p\}, \{r, q\}\}$, $\{\{r, p\}, \{q\}\}$ and $\{\{q, p\}, \{r\}\}$,
- With three subsets, we have only one case $\{\{p\}, \{q\}, \{r\}\}$.

Now let us define the notation Z_{h_i} . It is easy to notice that, the six lines in (3.43) are one-to-one mapped to the six ordered splitting of $\{p, q, r\}$ with *ordered gauge* $p \prec q \prec r$. The Z_{h_i} is the sum of momenta of legs satisfying the following two conditions: (1) legs at the l.h.s. of the leg h_i in the color-ordered Yang-Mills amplitudes, (2) legs at the l.h.s. of the label chain defined by the ordered splitting. The label chain for a given ordered splitting is the ordered set $\{1, 2, \dots, n-1, \alpha_1, \dots, \alpha_t, n\}$. For instance, for the ordered splitting $\{\{p\}, \{q\}, \{r\}\}$ in the first line of (3.43), the label chain is $\{1, 2, \dots, n-1, p, q, r, n\}$, and for $\{\{p\}, \{r, q\}\}$ in the second line of (3.43), the label chain is $\{1, 2, \dots, n-1, p, r, q, n\}$.

With the understanding of Z_{h_i} , it is easy to see that all Y_{h_i} appearing in (3.43) is equal to Z_{h_i} , so we can rewrite (3.43) as

$$\begin{aligned}
 A_{n,3}^{\text{EYM}}(1, \dots, n; p, q, r) & \quad (3.44) \\
 = & \sum_{\sqcup} (\epsilon_p \cdot Z_p)(\epsilon_q \cdot Z_q)(\epsilon_r \cdot Z_r) A_{n+3}^{\text{YM}}(1, \{2, \dots, n-1\} \sqcup \{p\} \sqcup \{q\} \sqcup \{r\}, n) \\
 & + \sum_{\sqcup} (\epsilon_p \cdot Z_p)(\epsilon_q \cdot F_r \cdot Z_r) A_{n+3}^{\text{YM}}(1, \{2, \dots, n-1\} \sqcup \{p\} \sqcup \{r, q\}, n) \\
 & + \sum_{\sqcup} (\epsilon_p \cdot F_q \cdot Z_q)(\epsilon_r \cdot Z_r) A_{n+3}^{\text{YM}}(1, \{2, \dots, n-1\} \sqcup \{q, p\} \sqcup \{r\}, n) \\
 & + \sum_{\sqcup} (\epsilon_p \cdot F_r \cdot Z_r)(\epsilon_q \cdot Z_q) A_{n+3}^{\text{YM}}(1, \{2, \dots, n-1\} \sqcup \{r, p\} \sqcup \{q\}, n) \\
 & + \sum_{\sqcup} (\epsilon_p \cdot F_q \cdot F_r \cdot Z_r) A_{n+3}^{\text{YM}}(1, \{2, \dots, n-1\} \sqcup \{r, q, p\}, n) \\
 & + \sum_{\sqcup} (\epsilon_p \cdot F_r \cdot F_q \cdot Z_q) A_{n+3}^{\text{YM}}(1, \{2, \dots, n-1\} \sqcup \{q, r, p\}, n).
 \end{aligned}$$

We have numerically checked the above relation, by comparing with $A_{n,3}^{\text{EYM}}$ directly evaluated with the CHY definition and found agreements in the lower-point examples up to $A_{3,3}^{\text{EYM}}$. In addition, when expanding the amplitude $A_{n,3}^{\text{EYM}}(1, \dots, n; p, q, r)$ into terms of pure Yang-Mills ones by (3.44), (3.42) and (3.1) and considering BCJ relations, we obtain the same result proposed in [14].

With the above result (3.44), it is ready to outline the rule for generalizing (3.43) for arbitrary number of gravitons,

- Decide an *ordered gauge* a priori, and write down all possible ordered splitting.
- For each ordered splitting $\{\alpha_1, \alpha_2, \dots, \alpha_t\}$, write down a factor $(\epsilon_{e_1} \cdot F_{e_2} \cdots F_{e_{|\alpha_i|-1}} \cdot F_{e_{|\alpha_i|}} \cdot Z_{e_{|\alpha_i|}})$ for each subset $\alpha_i = \{e_{|\alpha_i|}, \dots, e_2, e_1\}$, and product the factors for all α_i 's in the ordered splitting. This is the desired coefficients for the color-ordered amplitudes with color-ordering defined by the corresponding ordered splitting.

- Sum over the results from all possible ordered splitting, and we get the desired expansion of EYM amplitudes into pure Yang-Mills amplitudes.

A final remark says that, because of the choice of *ordered gauge* a priori, in the expansion the gauge invariance of gravitons is not as obvious as the one given by the recursive expansion in the previous subsection.

3.6 Expanding to pure Yang-Mills amplitudes: KK basis formula

The formula (3.44) and its generalizations provide an expansion of EYM amplitudes into Yang-Mills amplitudes in the framework of ordered splitting. However, to get the explicit expression for BCJ numerators, we need an expansion based on KK basis. From the framework of ordered splitting to the KK basis is somehow straightforward, and the only problem is to identify all the corresponding ordered splitting that can produce the desired KK basis. More explicitly, we need to reconstruct the ordered splitting from a given color-ordering in KK basis. It is easy to propose such algorithm, and we would like to demonstrate with a six-graviton example.

Assuming the *ordered gauge* is $h_1 \prec h_2 \prec h_3 \prec h_4 \prec h_5 \prec h_6$, and the color-ordering in KK basis is $\{\dots h_5 \dots h_4 \dots h_1 \dots h_2 \dots h_6 \dots h_3 \dots\}$, we reconstruct the coefficient of KK basis as follows,

- Start with the lowest element in the *ordered gauge*, here h_1 , and write down all possible subsets $\alpha_i \subset \{h_1, \dots, h_6\}$ which contains h_1 as its last element respecting the given color-ordering in KK basis. Since h_5, h_4 are at the l.h.s. of h_1 , we can write down four subsets,

$$\alpha_{h_1,1} = \{h_1\}, \quad \alpha_{h_1,2} = \{h_5, h_1\}, \quad \alpha_{h_1,3} = \{h_4, h_1\}, \quad \alpha_{h_1,4} = \{h_5, h_4, h_1\}. \quad (3.45)$$

- For each $\alpha_{h_1,i}$, we then drop its element in $\{h_1, \dots, h_6\}$ and re-do the step one for the remaining elements $\{h_1, \dots, h_6\}/\{\alpha_{h_1,i}\}$ with the lowest element therein. For instance, for $\alpha_{h_1,2} = \{h_5, h_1\}$, its complement regarding $\{h_1, \dots, h_6\}$ is $\{h_2, h_3, h_4, h_6\}$, and the lowest element is h_2 . Now the color-ordering $\{\dots h_5 \dots h_4 \dots h_1 \dots h_2 \dots h_6 \dots h_3 \dots\}$ becomes $\{\dots h_4 \dots h_2 \dots h_6 \dots h_3\}$ after dropping elements in $\alpha_{h_1,2}$. Repeating the step one, we get two possible subsets $\alpha_{h_2,1} = \{h_2\}$ and $\alpha_{h_2,2} = \{h_4, h_2\}$.
- Repeat until we get the complete ordered splitting.

For our current example, we can write the recursive construction starting from $\alpha_{h_1,4}$ as follows,

$$\alpha_{h_1,4} = \{h_5, h_4, h_1\} \rightarrow \alpha_{h_2,1} = \{h_2\} \rightarrow \begin{cases} \alpha_{h_3,1} = \{h_3\} \\ \alpha_{h_3,2} = \{h_6, h_3\} \end{cases} \rightarrow \alpha_{h_6,1} = \{h_6\}. \quad (3.46)$$

This gives two ordered splitting.

After generating all possible ordered splitting regarding the given color-ordering in KK basis, we can readily write down its coefficient in KK basis as the sum of those from the

ordered splitting. However, we remark that, the definition of Z_{h_i} relies on the ordered splitting, so the explicit expression of Z_{h_i} in different ordered splitting is different. Thus we need to be careful when summing over results of all possible ordered splitting.

Finally, let us present an complete example with three gravitons to demonstrate the algorithm, which is shown as follows,

- Choose the *ordered gauge* as $p \prec q \prec r$.
- For the color-ordering $\{\dots p \dots q \dots r \dots\}$ in the KK basis, the only possible ordered splitting is $\{\{p\}, \{q\}, \{r\}\}$. Thus its coefficient is

$$(\epsilon_p \cdot Z_p)(\epsilon_q \cdot Z_q)(\epsilon_r \cdot Z_r)|_{\{\{p\}, \{q\}, \{r\}\}}, \quad (3.47)$$

where for Z_{h_i} to be clearly defined, we have explicitly write down the ordered splitting for reference.

- For the color-ordering $\{\dots p \dots r \dots q \dots\}$ in the KK basis, the only possible ordered splitting are $\{\{p\}, \{q\}, \{r\}\}$ and $\{\{p\}, \{r, q\}\}$. Thus its coefficient is

$$(\epsilon_p \cdot Z_p)(\epsilon_q \cdot Z_q)(\epsilon_r \cdot Z_r)|_{\{\{p\}, \{q\}, \{r\}\}} + (\epsilon_p \cdot Z_p)(\epsilon_q \cdot F_r \cdot Z_r)|_{\{\{p\}, \{r, q\}\}}. \quad (3.48)$$

- For the color-ordering $\{\dots q \dots p \dots r \dots\}$ in the KK basis, the only possible ordered splitting are $\{\{p\}, \{q\}, \{r\}\}$ and $\{\{q, p\}, \{r\}\}$. Thus its coefficient is

$$(\epsilon_p \cdot Z_p)(\epsilon_q \cdot Z_q)(\epsilon_r \cdot Z_r)|_{\{\{p\}, \{q\}, \{r\}\}} + (\epsilon_p \cdot F_q \cdot Z_q)(\epsilon_r \cdot Z_r)|_{\{\{q, p\}, \{r\}\}}. \quad (3.49)$$

- For the color-ordering $\{\dots r \dots p \dots q \dots\}$ in the KK basis, the only possible ordered splitting are $\{\{p\}, \{q\}, \{r\}\}$, $\{\{p\}, \{r, q\}\}$ and $\{\{r, p\}, \{q\}\}$. Thus the coefficient is

$$\begin{aligned} & (\epsilon_p \cdot Z_p)(\epsilon_q \cdot Z_q)(\epsilon_r \cdot Z_r)|_{\{\{p\}, \{q\}, \{r\}\}} \\ & + (\epsilon_p \cdot Z_p)(\epsilon_q \cdot F_r \cdot Z_r)|_{\{\{p\}, \{r, q\}\}} + (\epsilon_p \cdot F_r \cdot Z_r)(\epsilon_q \cdot Z_q)|_{\{\{r, p\}, \{q\}\}}. \end{aligned} \quad (3.50)$$

As we have emphasized, Z_q has different meaning in the first and third terms. It will contain k_r in the third term, but not in the first term.

- For the color-ordering $\{\dots q \dots r \dots p \dots\}$ in the KK basis, the only possible ordered splitting are $\{\{p\}, \{q\}, \{r\}\}$, $\{\{q, p\}, \{r\}\}$, $\{\{r, p\}, \{q\}\}$ and $\{q, r, p\}$. Thus its coefficient is

$$\begin{aligned} & (\epsilon_p \cdot Z_p)(\epsilon_q \cdot Z_q)(\epsilon_r \cdot Z_r)|_{\{\{p\}, \{q\}, \{r\}\}} + (\epsilon_p \cdot F_q \cdot Z_q)(\epsilon_r \cdot Z_r)|_{\{\{q, p\}, \{r\}\}} \\ & + (\epsilon_p \cdot F_r \cdot Z_r)(\epsilon_q \cdot Z_q)|_{\{\{r, p\}, \{q\}\}} + (\epsilon_p \cdot F_r \cdot F_q \cdot Z_q)|_{\{q, r, p\}}. \end{aligned} \quad (3.51)$$

- For the color-ordering $\{\dots r \dots q \dots p \dots\}$ in the KK basis, the only possible ordered splitting are $\{\{p\}, \{q\}, \{r\}\}$, $\{\{q, p\}, \{r\}\}$, $\{\{r, p\}, \{q\}\}$, $\{\{p\}, \{r, q\}\}$ and $\{r, q, p\}$. Thus its coefficient is

$$\begin{aligned} & (\epsilon_p \cdot Z_p)(\epsilon_q \cdot Z_q)(\epsilon_r \cdot Z_r)|_{\{\{p\}, \{q\}, \{r\}\}} + (\epsilon_p \cdot F_q \cdot Z_q)(\epsilon_r \cdot Z_r)|_{\{\{q, p\}, \{r\}\}} \\ & + (\epsilon_p \cdot F_r \cdot Z_r)(\epsilon_q \cdot Z_q)|_{\{\{r, p\}, \{q\}\}} + (\epsilon_p \cdot Z_p)(\epsilon_q \cdot F_r \cdot Z_r)|_{\{\{p\}, \{r, q\}\}} + (\epsilon_p \cdot F_q \cdot F_r \cdot Z_r)|_{\{r, q, p\}}. \end{aligned} \quad (3.52)$$

The above example clearly shows how to reproduce the EYM amplitude expansion from the ordered splitting formula to the KK basis. Although for EYM amplitudes with many gravitons the procedure would be quite involved, but with the help of computer, it would not be a serious problem. And the expansion in KK basis is ideal for the study of BCJ numerators, which we will mention in the next section.

4 The BCJ numerator of Yang-Mills theory

In this section, we will apply the story of EYM theory to pure Yang-Mills theory, to provide an algorithmic construction of BCJ numerators for Yang-Mills amplitudes. Let us start from some necessary backgrounds. In paper [67], an expansion of Pfaffian is introduced as,

$$\text{Pf } \Psi = (-1)^{\frac{1}{2}n(n+1)} \sum_{p \in S_n} (-1)^{\text{sign}(p)} \Psi_I \Psi_J \cdots \Psi_K, \quad (4.1)$$

where the sum is over permutations S_n , and $I, J, \dots, K$ are closed cycles from splitting of the permutation. The factor Ψ_I is defined as

$$\Psi_I = \frac{F_I}{z_I} = \frac{\frac{1}{2} \text{Tr}(F_{i_1} \cdot F_{i_2} \cdots F_{i_{|I|}})}{z_{i_1 i_2} z_{i_2 i_3} \cdots z_{i_{|I|} i_1}}, \quad F_i^{\mu\nu} = k_i^\mu \epsilon_i^\nu - \epsilon_i^\nu k_i^\mu \quad (4.2)$$

for I containing more than one z'_i s, and

$$\Psi_{(i)} = C_{ii} = - \sum_{j \neq i} \frac{\epsilon_i \cdot k_j}{z_{ij}}. \quad (4.3)$$

for I containing only one z_i , which is explicitly the diagonal term of C matrix. Although the definition (4.1) is proposed for the full $2n \times 2n$ Pfaffian matrix, it is also valid for the sub-matrix of Pfaffian. In the case of Yang-Mills theory, we are interested in the reduced Pfaffian,

$$\text{Pf}' \Psi_{\lambda\nu}^{\lambda\nu} = -2^{n-3} \sum'_{p \in S_n} (-1)^{\text{sign}(p)} \frac{W_I}{z_I} \Psi_J \cdots \Psi_K, \quad (4.4)$$

where the λ and ν -th rows and columns in Ψ have been removed. The prime in the $\sum$ indicates that the sum is taken over all $p \in S_n$ permutation such that ν is changed into λ , which we call constraint permutation. The constraint permutation p has been decomposed to closed cycles $I, J, \dots, K$. In this paper, we take $1, n$ as the gauge choice, so the constraint permutation is the closed cycle $I = (1 i_2 i_3 \cdots i_{|I|} n)$, and

$$W_I = \epsilon_1 \cdot F_{i_2} \cdot F_{i_3} \cdots F_{i_{|I|-1}} \cdot \epsilon_n, \quad (4.5)$$

With above gauge choice, we can decompose the constraint permutation sum in (4.4) as three summations. The first summation is the summation of splitting $\{2, 3, \dots, n-1\}$ into a gluon subset A and a graviton subset B , while both subsets could be empty. The second summation is the permutation over gluon subset A . The third summation is the

permutation over graviton subset B . This gives³

$$\begin{aligned}
 \text{Pf}'\Psi &= -2^{n-3} \sum_{\text{split}} \left[\sum_{\rho \in S_A} (-)^{\text{sign}(\rho)} \frac{W_{(1\rho(A)n)}}{z_{(1\rho(A)n)}} \right] \left[\sum_{\tilde{\rho} \in S_B} (-)^{\text{sign}(\tilde{\rho})} \Psi_J \dots \Psi_K \right] \\
 &= -2^{n-3} \sum_{\text{split}} \left[\sum_{\rho \in S_A} (-)^{\text{sign}(\rho)} \frac{W_{(1\rho(A)n)}}{z_{(1\rho(A)n)}} \right] \text{Pf}\Psi_B \\
 &= -2^{n-3} \sum_{\text{split}} \sum_{\rho \in S_A} (-)^{\text{sign}(\rho)} W_{(1\rho(A)n)} \left\{ \frac{1}{z_{(1\rho(A)n)}} \text{Pf}\Psi_B \right\}, \tag{4.6}
 \end{aligned}$$

where in the second line we have used (4.1).

If we multiply (4.6) by another copy of reduced Pfaffian, then the expression in the curly bracket in the third line of (4.6) can be identified as CHY-integrand of single trace EYM amplitude with gluon legs $\{1, A, n\}$ and graviton legs B . Thus the above relation between reduced Pfaffian and Pfaffians for fewer points, exactly establishes the same relation between Einstein gravity and EYM/Yang-Mills amplitudes. As already pointed out in section 2, the relation between gravity and YM amplitudes shares the same kinematic coefficients for relations between Yang-Mills amplitude and cubic-scalar amplitudes. Since we have already worked out the EYM amplitude relations in the previous section, we can use the known results for EYM amplitude to directly write down the basis of BCJ numerators for Yang-Mills theory, without going through again the expansion of Yang-Mills amplitudes into cubic-scalar amplitudes.

Now we present the algorithm for finding the BCJ numerator of one KK basis with the color-ordered $A^{\text{YM}}(1, h_2, h_3, \dots, h_{n-1}, n)$. The key idea is again to reconstruct related ordered splitting in (4.6) from the given ordering $\{h_2, \dots, h_{n-1}\}$,

- Firstly, we reconstruct the $\rho(A)$. The length of subset $\rho(A)$ could be values from 0 to $n-2$, so we can explicitly get

$$\begin{aligned}
 n_{\rho(A)} = 0 : \quad & \rho(A) = \emptyset, \\
 n_{\rho(A)} = 1 : \quad & \rho(A) = \{h_i\}, \quad i = 2, \dots, n-1, \\
 n_{\rho(A)} = 2 : \quad & \rho(A) = \{h_i, h_j\}, \quad 2 \leq i < j \leq n-1, \\
 & \dots \quad \dots \\
 n_{\rho(A)} = k : \quad & \rho(A) = \{h_{i_1}, h_{i_2}, \dots, h_{i_k}\}, \quad 2 \leq i_1 < i_2 < \dots < i_k \leq n-1.
 \end{aligned}$$

- With the knowledge of $\rho(A)$, we generate an ordered subset $\mathcal{O}(B) = \{h_2, \dots, h_{n-1}\}/\rho(A)$. Then we choose the standard *ordered gauge* $2 \prec 3 \prec \dots \prec n-1$, and reconstruct the ordered splitting as the story in (3.46). Each ordered splitting contributes a factor $\mathcal{C}_i$.

³Naively, there will be a sign factor $(-)^{\frac{1}{2}n_B(n_B+1)}$ if using the result (4.1). However, comparing with our explicit example and the argument using the BCFW on-shell recursion relation, it seems this sign factor should not be there.

- Collecting results for all possible ordered splitting, we get the coefficient,

$$\sum_{\rho(A)} (-)^{n_A} 2^{n-3} W_{(1\rho(A)n)} \times \left\{ \sum_{\text{Ordered Splitting}(\mathcal{O}(B))} \mathcal{C}_i \right\}. \quad (4.7)$$

As a demonstration of above algorithm, let us compute the KK basis of BCJ numerators for four-point Yang-Mills amplitude. For the numerator $n_{(1|23|4)}$, we can generate the following terms,

$$\begin{aligned} \rho(A) = \emptyset, \quad \text{Split}\mathcal{O}[\{2, 3\}] = \{\{2\}, \{3\}\} &\implies + 2(\epsilon_1 \cdot \epsilon_4)(\epsilon_2 \cdot k_1)(\epsilon_3 \cdot k_{12}), \\ \rho(A) = \{2\}, \quad \text{Split}\mathcal{O}[\{3\}] = \{3\} &\implies - 2(\epsilon_1 \cdot F_2 \cdot \epsilon_4)(\epsilon_3 \cdot k_{12}), \\ \rho(A) = \{3\}, \quad \text{Split}\mathcal{O}[\{2\}] = \{2\} &\implies - 2(\epsilon_1 \cdot F_3 \cdot \epsilon_4)(\epsilon_2 \cdot k_1), \\ \rho(A) = \{2, 3\}, \quad \text{Split}\mathcal{O}[\emptyset] = \emptyset &\implies + 2(\epsilon_1 \cdot F_2 \cdot F_3 \cdot \epsilon_4). \end{aligned}$$

Summing over all the results, we get

$$\begin{aligned} n_{(1|23|4)} &= 2(\epsilon_1 \cdot \epsilon_4)(\epsilon_2 \cdot k_1)(\epsilon_3 \cdot k_{12}) - 2(\epsilon_1 \cdot F_2 \cdot \epsilon_4)(\epsilon_3 \cdot k_{12}) \\ &\quad - 2(\epsilon_1 \cdot F_3 \cdot \epsilon_4)(\epsilon_2 \cdot k_1) + 2(\epsilon_1 \cdot F_2 \cdot F_3 \cdot \epsilon_4). \end{aligned} \quad (4.8)$$

Similarly, for $n_{(1|32|4)}$ we can reconstruct the following terms,

$$\begin{aligned} \rho(A) = \emptyset, \quad \text{Split}\mathcal{O}[\{3, 2\}] = \{\{2\}, \{3\}\}, \{3, 2\} &\implies + 2(\epsilon_1 \cdot \epsilon_4)[(\epsilon_2 \cdot k_1)(\epsilon_3 \cdot k_1) + \epsilon_2 \cdot F_3 \cdot k_1], \\ \rho(A) = \{2\}, \quad \text{Split}\mathcal{O}[\{3\}] = \{3\} &\implies - 2(\epsilon_1 \cdot F_2 \cdot \epsilon_4)(\epsilon_3 \cdot k_1), \\ \rho(A) = \{3\}, \quad \text{Split}\mathcal{O}[\{2\}] = \{2\} &\implies - 2(\epsilon_1 \cdot F_3 \cdot \epsilon_4)(\epsilon_2 \cdot k_{13}), \\ \rho(A) = \{2, 3\}, \quad \text{Split}\mathcal{O}[\emptyset] = \emptyset &\implies + 2(\epsilon_1 \cdot F_2 \cdot F_3 \cdot \epsilon_4). \end{aligned}$$

Summing over all results, we get

$$\begin{aligned} n_{(1|32|4)} &= 2(\epsilon_1 \cdot \epsilon_4)[(\epsilon_2 \cdot k_1)(\epsilon_3 \cdot k_1) + \epsilon_2 \cdot F_3 \cdot k_1] \\ &\quad - 2(\epsilon_1 \cdot F_2 \cdot \epsilon_4)(\epsilon_3 \cdot k_1) - 2(\epsilon_1 \cdot F_3 \cdot \epsilon_4)(\epsilon_2 \cdot k_{13}) + 2(\epsilon_1 \cdot F_2 \cdot F_3 \cdot \epsilon_4). \end{aligned} \quad (4.9)$$

In paper [26], the BCJ numerators for four-point Yang-Mills are computed by directly manipulating the $\text{Pf}'\Psi$ using cross-ratio identities, and the result is given by

$$\begin{aligned} n_{(1|23|4)} &= -W_{(1234)} + W_{(124)}(-(\epsilon_3 \cdot k_4)) + W_{(134)}(\epsilon_2 \cdot k_1) \\ &\quad + (\epsilon_1 \cdot \epsilon_4) \{t \{(\epsilon_2 \cdot \epsilon_3)(k_4 \cdot k_3) - (\epsilon_2 \cdot k_4)(\epsilon_3 \cdot k_4) - (\epsilon_2 \cdot k_3)(\epsilon_3 \cdot k_4)\} + (1-t)(\epsilon_3 \cdot k_4)(\epsilon_2 \cdot k_1)\}, \\ n_{(1|32|4)} &= -W_{(1324)} + W_{(124)}(\epsilon_3 \cdot k_1) - W_{(134)}(\epsilon_2 \cdot k_4) \\ &\quad + (\epsilon_1 \cdot \epsilon_4) \{t(\epsilon_2 \cdot k_4)(\epsilon_3 \cdot k_1) + (1-t) \{(\epsilon_2 \cdot \epsilon_3)(k_4 \cdot k_2) - (\epsilon_3 \cdot k_4)(\epsilon_2 \cdot k_4) - (\epsilon_3 \cdot k_2)(\epsilon_2 \cdot k_4)\}\}, \end{aligned}$$

where t is the gauge choice in cross-ratio identities. If taking $t = 1/2$, we get the relabeling symmetric expression between $2 \leftrightarrow 3$. While if taking $t = 0$, we get

$$\begin{aligned} n_{(1|23|4)} &= -W_{(1234)} + W_{(124)}(\epsilon_3 \cdot k_{12}) + W_{(134)}(\epsilon_2 \cdot k_1) - (\epsilon_1 \cdot \epsilon_4)(\epsilon_3 \cdot k_{12})(\epsilon_2 \cdot k_1), \\ n_{(1|32|4)} &= -W_{(1324)} + W_{(124)}(\epsilon_3 \cdot k_1) + W_{(134)}(\epsilon_2 \cdot k_{13}) - (\epsilon_1 \cdot \epsilon_4)[(\epsilon_2 \cdot k_1)(\epsilon_3 \cdot k_1) + \epsilon_2 \cdot F_3 \cdot k_1], \end{aligned}$$

which has a perfect agreement with results (4.8) and (4.9) up to a factor -2 .

Although only four-point example is explicitly displayed, this algorithm can directly be applied to obtain BCJ numerators for tree level Yang-Mills amplitudes with more than four points.

5 Inspecting the amplitude relations through BCFW recursions

Using gauge invariance, we have determined the non-trivial relations between any EYM amplitudes and Yang-Mills amplitudes, with the formula as shown in (3.39) for general EYM amplitudes. However, it would be interesting to inspect it again by BCFW recursions. As mentioned before, the relation between color-ordered EYM amplitudes and color-ordered Yang-Mills amplitudes is the same as that between color-ordered Yang-Mills-scalar amplitudes and pure scalar amplitudes. So for simplicity, we would use BCFW recursion to inspect the following two non-trivial relations,

$$A_{n,1}^{\text{YMs}}(1, \dots, n; p) = \sum_{\sqcup} (\epsilon_p \cdot Y_p) A_{n+1}^{\phi^3}(1, \{2, \dots, n-1\} \sqcup \{p\}, n), \quad (5.1)$$

$$\begin{aligned} A_{n,2}^{\text{YMs}}(1, \dots, n; p, q) &= \sum_{\sqcup} (\epsilon_p \cdot Y_p) A_{n+1,1}^{\text{YMs}}(1, \{2, \dots, n-1\} \sqcup \{p\}, n; q) \\ &\quad + \sum_{\sqcup} (\epsilon_p \cdot F_q \cdot Y_q) A_{n+2}^{\phi^3}(1, \{2, \dots, n-1\} \sqcup \{q, p\}, n). \end{aligned} \quad (5.2)$$

For more complicated relations where $A_{n,m}^{\text{YMs}}$ with $m > 2$, of course we can also investigate them by BCFW recursions. While $m \geq 2$, we need to consider both contribution from finite poles and boundary contribution, and although for $m > 2$ cases the analysis would be more involved, the techniques for computing boundary contribution are no more than the $m = 2$ case. Hence their analysis is similar to the relations of $A_{n,2}^{\text{YMs}}$.

In fact, verify the relation (5.1) by BCFW recursion is trivial. We only need to apply BCFW on both sides of (5.1), while a $\hat{k}_1, \hat{k}_n$ shifting is sufficient to detect all the contributions for $A_{n,1}^{\text{YMs}}$ and $A_{n+1}^{\phi^3}$. By using the relation (5.1) for $A_{n',1}^{\text{YMs}}$ with $n' < n$, we can prove it inductively. While the starting point of induction, i.e., the relation for $A_{2,1}^{\text{YMs}}$, can be verified explicitly.

For the two-scalar one-gluon amplitude $A_{2,1}^{\text{YMs}}(1, 2; p)$, we explicitly have

$$A_{2,1}^{\text{YMs}}(1, 2; p) = f^{a'_1 a'_2 a'_p} \left(-\frac{i}{\sqrt{2}} \right) (k_1 - k_2) \cdot \epsilon_p = (\epsilon_p \cdot k_1) \left(i\sqrt{2} f^{a'_1 a'_p a'_2} \right) = (\epsilon_p \cdot k_1) A_3^{\phi^3}(1, p, 2), \quad (5.3)$$

where $A_3^{\phi^3}(1, p, 2)$ is the three-point scalar amplitude with cubic vertex defined as $f^{a'_1 a'_p a'_2}$. We have absorbed the factor $i\sqrt{2}$ into ϵ_p . This operation just changes the normalization factor and will not affect the following discussions.

We will not repeat the trivial proof of (5.1) here, but jump to the more typical one (5.2). While applying BCFW deformation, for (5.1) only residues of finite poles will contribute, but for (5.2) the boundary contribution is un-avoidable. So we need to compare both sides of (5.2) with the finite pole contributions as well as boundary contribution, and the later will be computed by analyzing Feynman diagrams [68–70].

Now let us study the relation for $A_{n,2}^{\text{YMs}}(1, \dots, n; p, q)$ with two gluons by BCFW recursion. We shift the momenta of two scalars k_1 and k_n , i.e.,

$$k_1 \rightarrow \hat{k}_1 = k_1 + zq, \quad k_n \rightarrow \hat{k}_n = k_n - zq, \quad (5.4)$$

where q satisfies $k_1 \cdot q = k_n \cdot q = q^2 = 0$. We shall emphasize that the on-shell condition of scalar k_n is not really used in the following proof, thus this relation is also valid for

amplitudes with k_n off-shell. As the standard BCFW recursion arguments, under this deformation, amplitude A as a rational function of z can be written as

$$A = \sum_{\text{Finite Poles}} \text{Res} \frac{A(z)}{z} + \text{Boundary terms.} \quad (5.5)$$

To prove the relation (5.2), we should confirm, (1) the sums over finite poles for the l.h.s. and r.h.s. of (5.2) match with each other, (2) the boundary terms for the l.h.s. and r.h.s. of (5.2) match with each other.

5.1 Contributions of finite poles

Let us first treat the contributions from finite poles. According to BCFW recursion, the contribution in the l.h.s. of (5.2) can be written as

$$\begin{aligned} A_{n,2}^{\text{YMs}}(1, \dots, n; p, q) &= \sum_{i=1}^{n-1} A(\widehat{1}, 2, \dots, i; p \mid i+1, \dots, \widehat{n}; q) + \sum_{i=1}^{n-1} A(\widehat{1}, 2, \dots, i; q \mid i+1, \dots, \widehat{n}; p) \\ &\quad + \sum_{i=1}^{n-2} A(\widehat{1}, 2, \dots, i; p, q \mid i+1, \dots, \widehat{n}) + \sum_{i=2}^{n-1} A(\widehat{1}, 2, \dots, i \mid i+1, \dots, \widehat{n}; p, q), \end{aligned} \quad (5.6)$$

where $A(\alpha|\beta)$ is short for $A_L(\alpha, P_\alpha) \frac{i}{P_\alpha^2} A_R(-P_\alpha, \beta)$, and P_α is the sum of all momenta in set α , which is the propagator in between the left and right sub-amplitudes. The contribution from the finite poles in the r.h.s. of (5.2) can be given by the sum of $\mathcal{F}_1, \mathcal{F}_2$ defined as

$$\mathcal{F}_1 = \sum_{i=1}^{n-1} \sum_{\sqcup} (\epsilon_p \cdot \widehat{Y}_p) A(\widehat{1}, \{2, \dots, i\} \sqcup \{p\} \mid i+1, \dots, \widehat{n}; q) \quad (5.7)$$

$$+ \sum_{i=2}^{n-1} \sum_{\sqcup} (\epsilon_p \cdot \widehat{Y}_p + \epsilon_p \cdot \widehat{P}_{1\dots i}) A(\widehat{1}, 2, \dots, i \mid \{i+1, \dots, n-1\} \sqcup \{p\}, \widehat{n}; q) \quad (5.8)$$

$$+ \sum_{i=1}^{n-2} \sum_{\sqcup} (\epsilon_p \cdot \widehat{Y}_p) A(\widehat{1}, \{2, \dots, i\} \sqcup \{p\}; q \mid i+1, \dots, \widehat{n}) \quad (5.9)$$

$$+ \sum_{i=1}^{n-1} \sum_{\sqcup} (\epsilon_p \cdot \widehat{Y}_p + \epsilon_p \cdot \widehat{P}_{1\dots i}) A(\widehat{1}, 2, \dots, i; q \mid \{i+1, \dots, n-1\} \sqcup \{p\}, \widehat{n}), \quad (5.10)$$

and

$$\mathcal{F}_2 = \sum_{i=1}^{n-2} \sum_{\sqcup} (\epsilon_p \cdot F_q \cdot \widehat{Y}_q) A(\widehat{1}, \{2, \dots, i\} \sqcup \{q, p\} \mid i+1, \dots, \widehat{n}) \quad (5.11)$$

$$+ \sum_{i=2}^{n-1} \sum_{\sqcup} (\epsilon_p \cdot F_q \cdot (\widehat{Y}_q + \widehat{P}_{1\dots i})) A(\widehat{1}, 2, \dots, i \mid \{i+1, \dots, n-1\} \sqcup \{q, p\}, \widehat{n}) \quad (5.12)$$

$$+ \sum_{i=1}^{n-1} \sum_{\sqcup_1, \sqcup_2} (\epsilon_p \cdot F_q \cdot \widehat{Y}_q) A(\widehat{1}, \{2, \dots, i\} \sqcup_1 \{q\} \mid \{i+1, \dots, n-1\} \sqcup_2 \{p\}, \widehat{n}), \quad (5.13)$$

where remind again Y_p is defined as the sum of the momenta at the l.h.s. of p in its corresponding sub-amplitude which has scalar origin in $A_{n,2}^{\text{YMs}}$. While p is the right sub-amplitude A_R , the intermediate propagator P_α appears as the first leg of A_R which is at the l.h.s. of p , and we write it explicitly out of $\hat{Y}_p$ to avoid ambiguity.

Let us now compare the result in (5.6) and $\mathcal{F}_1, \mathcal{F}_2$. From inductive assumption, we know $A_{n,1}^{\text{YMs}}$ for any n and the lower-point amplitude $A_{n',2}^{\text{YMs}}$ with $n' < n$ satisfy (5.1), (5.2). So we have,

1. The sum of A_L in (5.7) is equal to the A_L in the first term of (5.6) by relations of YMs amplitude with one gluon.

2. In the (5.13), $(\epsilon_p \cdot F_q \cdot \hat{Y}_q) = (\epsilon_p \cdot q)(\epsilon_q \cdot \hat{Y}_q) - (\epsilon_p \cdot \epsilon_q)(q \cdot \hat{Y}_q)$, while for the latter factor,

$$\sum_{\sqcup_1} (q \cdot \hat{Y}_q) A_L(\hat{1}, \{2, \dots, i\} \sqcup_1 \{q\}, \hat{P}_{1\dots i, q}) = 0$$

due to BCJ relation. For the former factor,

$$\begin{aligned} & \sum_{\sqcup_1} (\epsilon_p \cdot q)(\epsilon_q \cdot \hat{Y}_q) A(\hat{1}, \{2, \dots, i\} \sqcup_1 \{q\} \Big| \{i+1, \dots, n-1\} \sqcup_2 \{p\}, \hat{n}) \\ &= (\epsilon_p \cdot q) A(\hat{1}, 2, \dots, i; q \Big| \{i+1, \dots, n-1\} \sqcup_2 \{p\}, \hat{n}). \end{aligned}$$

Noting that this term plus (5.10), and that $\epsilon_p \cdot \hat{P}_{1\dots i} + \epsilon_p \cdot q = \epsilon_p \cdot \hat{P}_{1\dots i, q}$, we get

$$\sum_{\sqcup} (\epsilon_p \cdot Y_p + \epsilon_p \cdot \hat{P}_{1\dots i, q}) A_L(\hat{1}, 2, \dots, i, -\hat{P}_{1\dots i, q}; q) \frac{i}{P_{1\dots i, q}^2} A_R(\hat{P}_{1\dots i, q}, \{i+1, \dots, n-1\} \sqcup \{p\}, \hat{n}),$$

which is equal to the second term of (5.6) by relations of YMs amplitude with one gluon for A_R .

3. The A_L in (5.9) and (5.11) sums to,

$$\begin{aligned} & \sum_{\sqcup} (\epsilon_p \cdot \hat{Y}_p) A_L(\hat{1}, \{2, \dots, i\} \sqcup \{p\}, -\hat{P}_{1\dots i, p, q}; q) \frac{i}{P_{1\dots i, p, q}^2} A_R(\hat{P}_{1\dots i, p, q}, i+1, \dots, \hat{n}) \\ & + \sum_{\sqcup} (\epsilon_p \cdot F_q \cdot \hat{Y}_q) A_L(\hat{1}, \{2, \dots, i\} \sqcup \{q, p\}, -\hat{P}_{1\dots i, p, q}) \frac{i}{\hat{P}_{1\dots i, p, q}^2} A_R(\hat{P}_{1\dots i, p, q}, i+1, \dots, \hat{n}), \end{aligned}$$

which equals to the third term of (5.6) by relations of lower-point YMs amplitudes with two gluons.

4. The A_R in (5.8) and (5.12) sums to

$$\begin{aligned} & \sum_{\sqcup} (\epsilon_p \cdot (\hat{Y}_p + \hat{P}_{1\dots i})) A_L(\hat{1}, 2, \dots, i, -\hat{P}_{1\dots i}) \frac{i}{P_{1\dots i}^2} A_R(\hat{P}_{1\dots i}, \{i+1, \dots, n-1\} \sqcup \{p\}, \hat{n}; q) \\ & + \sum_{\sqcup} (\epsilon_p \cdot F_q \cdot (\hat{Y}_q + \hat{P}_{1\dots i})) A_L(\hat{1}, 2, \dots, i, -\hat{P}_{1\dots i}) \frac{i}{\hat{P}_{1\dots i}^2} A_R(\hat{P}_{1\dots i}, \{i+1, \dots, n-1\} \sqcup \{q, p\}, \hat{n}), \end{aligned}$$

which equals to the fourth term of (5.6) by relations of lower-point YMs amplitude with two gluons.

Hence, all contributions of finite poles in the l.h.s. and r.h.s. of (5.2) under (k_1, k_n) -shifting match with each other.

Figure 1. Boundary of the left hand side of relation for amplitudes with more than two scalars and two gluons.

5.2 The boundary contributions

Now let us discuss the boundary contributions. We would consider the situations with $n > 2$ and $n = 2$ separately, since there are more subtleties in the latter situation.

The case with $n > 2$: in this case, the boundary term of the BCFW recursion under (k_1, k_n) -deformation comes from the diagram as shown in figure 1.a. In the l.h.s. of (5.2), it is given by

$$f^{a'_n a'_1 e} \frac{i}{s_{1n}} \tilde{A}_{n-1,2}^{\text{YMs}}(2, \dots, n-1, P_{1,n}^e; p, q), \quad (5.14)$$

where $\tilde{A}_{n-1,2}^{\text{YMs}}(P_{1,n}^e, 2, \dots, n-1; p, q)$ denotes sum of all possible diagrams with one off-shell scalar line $P_{1,n}^e$, $(n-2)$ on-shell scalars $k_2, \dots, k_{n-1}$ as well as two on-shell gluons p, q . In the r.h.s. of (5.2), it is given by

$$\begin{aligned} & \sum_{\sqcup} (\epsilon_p \cdot Y_p) f^{a'_n a'_1 e} \frac{i}{s_{1n}} \tilde{A}_{n,1}^{\text{YMs}}(\{2, \dots, n-1\} \sqcup \{p\}, P_{1,n}^e; q) \\ & + \sum_{\sqcup} (\epsilon_p \cdot F_q \cdot Y_q) f^{a'_n a'_1 e} \frac{i}{s_{1n}} \tilde{A}_{n+1}^{\phi^3}(\{2, \dots, n-1\} \sqcup \{q, p\}, P_{1,n}^e). \end{aligned} \quad (5.15)$$

By the use of generalized U(1)-decoupling identity [71]

$$\sum_{\sqcup} \tilde{A}_{n+m,k}^{\text{YMs}}(\{1, \dots, n-1\} \sqcup \{\alpha_1, \dots, \alpha_m\}, -P_{1\dots n-1, \alpha_1 \dots \alpha_m, h_1 \dots h_k}; h_1, \dots, h_k) = 0, \quad (5.16)$$

we re-express the boundary term in the r.h.s. of (5.2) as

$$\begin{aligned} & \sum_{\sqcup} (\epsilon_p \cdot Y_p) f^{a'_n a'_1 e} \frac{i}{s_{1n}} \tilde{A}_{n,1}^{\text{YMs}}(2, \{3, \dots, n-1\} \sqcup \{p\}, P_{1,n}^e; q) \\ & + \sum_{\sqcup} (\epsilon_p \cdot F_q \cdot Y_q) f^{a'_n a'_1 e} \frac{i}{s_{1n}} \tilde{A}_{n+1}^{\phi^3}(2, \{3, \dots, n-1\} \sqcup \{q, p\}, P_{1,n}^e). \end{aligned} \quad (5.17)$$

Remind that our proof of (5.2) does not rely on the on-shell condition of the right-most scalar k_n , hence (5.2) is also valid for amplitudes with off-shell k_n . Assuming the validation of (5.2) for YMs amplitude with $n' < n$ gluons, we simply get the sum (5.17) as $f^{a'_n a'_1 e} \frac{i}{s_{1n}} \tilde{A}_{n-1,2}^{\text{YMs}}(2, \dots, n-1, P_{1,n}^e; p, q)$, which is identical to the boundary contribution in the l.h.s. of (5.2).

The case with $n = 2$: this case is much more subtle. The boundary contributions in the l.h.s. of (5.2) come from the diagrams as shown in figure 1.b, figure 1.c, while the boundary contributions in the r.h.s. of (5.2) come from the diagrams as shown in figure 1.d, figure 1.e, figure 1.f.

According to the Feynman rules for Yang-Mills-scalar amplitudes, we can compute the three terms for the r.h.s. of (5.2) as

$$\text{Figure 1.d} = f^{a'_2 a'_1 e} f^{e a'_p a'_q} \frac{i}{s_{12}} (\sqrt{2}i)^2 (\epsilon_q \cdot p) (\epsilon_p \cdot k_1), \quad (5.18)$$

$$\text{Figure 1.e} = f^{a'_2 a'_1 e} f^{e a'_q a'_p} \frac{i}{s_{12}} (\sqrt{2}i)^2 (\epsilon_p \cdot F_q \cdot k_1), \quad (5.19)$$

$$\text{Figure 1.f} = -f^{a'_1 a'_q e} f^{e a'_p a'_2} (\sqrt{2}i)^2 \frac{i}{2} (\epsilon_p \cdot \epsilon_q). \quad (5.20)$$

On the other hand, we can compute the two terms for l.h.s. of (5.2) as

$$\begin{aligned} \text{Figure 1.b} &= f^{a'_2 a'_1 e} f^{e a'_p a'_q} \frac{i}{s_{12}} (\sqrt{2}i)^2 [(\epsilon_q \cdot p)(\epsilon_p \cdot k_1) - (\epsilon_p \cdot q)(\epsilon_q \cdot k_1) + (\epsilon_p \cdot \epsilon_q)(q \cdot k_1)] \\ &+ (-i) f^{a'_2 a'_1 e} f^{e a'_p a'_q} \frac{1}{2} (\epsilon_p \cdot \epsilon_q). \\ \text{Figure 1.c} &= f^{a'_1 a'_p e} f^{e a'_q a'_2} \frac{i}{2} (\epsilon_p \cdot \epsilon_q) + f^{a'_1 a'_q e} f^{e a'_p a'_2} \frac{i}{2} (\epsilon_p \cdot \epsilon_q). \end{aligned} \quad (5.21)$$

If we re-write the second line in the result of figure 1.b by Jacobi identity

$$f^{a'_2 a'_1 e} f^{e a'_p a'_q} = f^{a'_1 a'_p e} f^{e a'_q a'_2} - f^{a'_1 a'_q e} f^{e a'_p a'_2},$$

then the matching of boundary contribution in both sides of (5.2) can be easily checked.

With above discussions, we have confirmed the non-trivial relations between YMs amplitude and pure scalar amplitudes (hence the EYM amplitude and Yang-Mills amplitudes) by BCFW recursion relations. The proof of relations for YMs amplitude with more than two gluons requires more labors, but the strategy is similar, which includes comparing the contributions from finite poles and boundary contributions. We will not discuss it further.

6 Inspecting the amplitude relations through KLT relation

In the following discussions we will demonstrate that, at least in the first few simplest scenarios, the newly discovered multi-graviton relations [1, 14, 15] can be readily understood from the perspective of KLT relations. It was demonstrated in [72] that the KLT relation provides a much more perturbation-friendly construction of the EYM amplitudes, which would be otherwise difficult to calculate in viewing of the infinite vertices that constitute the linearized gravity Feynman rules. In this setting, EYM amplitude factorizes into a copy of pure gluon amplitude and a copy that gluon interacts with scalars, through which the color dependence is introduced. To have simpler expression, we will use the $(n-2)!$ symmetric KLT relation first introduced in [73–75],

$$\begin{aligned} A^{\text{EYM}}(1, 2, \dots, n) &= \lim_{k_n^2 \rightarrow 0} \frac{1}{k_n^2} \sum_{\alpha, \beta \in S_{n-2}} A^{\text{YM}}(n, \alpha, 1) S[\alpha|\beta] A^{\text{YMs}}(1, \beta, n) \\ &= \sum_{\alpha \in S_{n-2}} A^{\text{YM}}(1, \alpha, n) n(1, \alpha, n). \end{aligned} \quad (6.1)$$

where the numerator in the expression defined using gluon scalar currents

$$n(1, \alpha, n) = \sum_{\beta \in S_{n-2}} \mathcal{S}[\alpha|\beta] J^{\text{YMs}}(1, \beta, n) \quad (6.2)$$

carries both kinematic and color factors. The formula defined in (6.2) has provided a way of evaluating the numerator $n(1, \alpha, n)$. However, it is obvious that, directly calculating all currents and then making the sum is not an efficient method. There are two alternative methods to compute the coefficients $n(1, \alpha, n)$. The first is to carry out the summation step by step as was done in [61, 71]. The idea is to divide the full S_{n-2} permutation sums appearing in (6.2) into $(n-2)$ blocks of S_{n-3} permutation sums, such that in each block we can pull out a format of BCJ sums. Then one can use the Fundamental BCJ relation for currents to simplify the expression and arrive at a similar sum as the one given in (6.2) but with only S_{n-3} permutation sums. Iterating this procedure several times, we can finally compute the coefficients. Establishing the Fundamental BCJ relation for currents is a crucial point for this method, and we will show how to do this in the later sections. The second method is, however, less straightforward. When expanding the amplitude into KK basis with the formulation given in the second line of (6.1), it is shown in [23, 54, 57, 66] that, the coefficients $n(1, \alpha, n)$ are nothing but the numerators of Del Duca-Dixon-Maltoni (DDM) basis provided we write the whole $A^{\text{YMs}}(1, \beta, n)$ amplitude into BCJ form (i.e., numerators satisfying the Jacobi relations). Using this aspect, the problem is translated to computing the BCJ numerators of DDM basis by any conventional methods.

The purpose of this section is to show that, the newly discovered EYM amplitude relations can also be fitted in the framework of KLT relations. The methods that developed in the computation of BCJ numerators in various theories [61, 71] are also well-suited in the analysis of EYM amplitude expansion, with only a few modification. This connects the problem of EYM amplitude expansion with many other theories. In the following discussions, we will use both methods developed years ago for computing the BCJ numerators to address the problem of constructing the expansion coefficients $n(1, \alpha, n)$.

6.1 The case with single gluon

For the purpose of being self-contained we list the color-ordered Feynman rules for gluon-scalar interaction presented in [72] in the appendix A. Consider first the scalar Yang-Mills amplitudes when there is only one gluon. Note that a (color-stripped) gluon propagator does not transmit the color/flavor of scalars attached to its two ends, so that for single trace part of the partial amplitude, gluon lines cannot be internal or the color factors carried by the scalars at its two ends factorize. A consequence is that all single gluon amplitudes are consisting of cubic graphs. For example at four points when, say leg 3, is the gluon line there are only three cubic graphs in the KK sector, up to anti-symmetry of the three-vertices,

It is very important to notice that the color-kinematics duality is ensured by the vanishing of the sum of their numerators (even at the off-shell level)

$$f^{a_1 a_2 a_4} (k_1 + k_2 + k_4) \cdot \epsilon_3 \sim k_3 \cdot \epsilon_3 = 0. \quad (6.3)$$

This observation (i.e., only cubic vertex is allowed and the gauge invariance), when generalized to higher points, indicates that the Feynman diagrams provide the desired BCJ form. In particular, an n -point DDM half-ladder numerator $n(1, 2, 3, \dots, i, p_g, i+1, \dots, n)$ is therefore given by the corresponding Feynman diagrams as

$$k_{12}^2 k_{123}^2 \dots \overline{1 \left| \begin{array}{c} | \\ 2 \end{array} \right| \left| \begin{array}{c} | \\ 3 \end{array} \right| \dots \left| \begin{array}{c} | \\ i \end{array} \right| \left| \begin{array}{c} | \\ p \end{array} \right| \left| \begin{array}{c} | \\ i+1 \end{array} \right| \dots \left| \begin{array}{c} | \\ n-1 \end{array} \right|}^n = \left[f^{1,2,*} f^{*,3,*} \dots f^{*,i,a} \times \delta^{ab} \times f^{b,i+1,*} \dots f^{*,n-1,n} \right] \\ \times \sqrt{2}^{n-2} (-1)^{n+1} i \epsilon_p \cdot (k_1 + \dots + k_i). \quad (6.4)$$

So what are the allowed DDM numerators? The Yang-Mills-scalar theory has a gauge group and a flavor group. The flavor ordering fixes the ordering of scalars, thus the only allowed freedom is the location of gluon leg along the DDM-chain. In other words, the desired expansion coefficients in (6.1) are nothing but the one given in (6.4) with all possible insertions of gluon legs,

$$A_{n,1}^{\text{EYM}}(1, 2, \dots, n; p) = \sqrt{2}^{n-2} (-1)^{n+1} i \sum_{\sqcup} (\epsilon_p \cdot X_p) A^{\text{YM}}(1, \{2, \dots, n-1\} \sqcup \{p\}, n), \quad (6.5)$$

and we find agreement with the new single graviton relation (up to an overall factor).

6.2 The four-point gluon-scalar amplitude involving two gluons

Next we consider Yang-Mills-scalar amplitudes involving two gluons. For this case, since Feynman diagrams will involve the four-point vertex, the BCJ form will not be manifest for

Feynman diagrams and the computation will be more complicated. Thus in this subsection, we will follow the method of summing over the color-ordered KK basis.

At four points we have the following two KK basis amplitudes,

$$A_{2,2}^{\text{YMs}}(1, 2_g, 3_g, 4) = \frac{n_s}{s_{12}} - \frac{n_t}{s_{23}} + n_4 = \text{diagram}_s + \text{diagram}_t + \text{diagram}_4, \quad (6.6)$$

$$A_{2,2}^{\text{YMs}}(1, 3_g, 2_g, 4) = -\frac{n_u}{s_{13}} + \frac{n_t}{s_{23}} + n_4 = \text{diagram}_u + \text{diagram}_t + \text{diagram}_4, \quad (6.7)$$

where n_s , n_t , n_u and n_4 denote the factors

$$n_s = k_{12}^2 \text{diagram}_s = \left(((k_3 + k_4) - k_1) \cdot \epsilon_2 \right) \left((k_4 - (k_1 + k_2)) \cdot \epsilon_3 \right) \times \delta^{a_1 a_4} \left(\frac{-i}{\sqrt{2}} \right)^2 i, \quad (6.8)$$

$$n_t = k_{23}^2 \text{diagram}_t = \left((\epsilon_2 \cdot \epsilon_3) ((k_3 - k_2) \cdot (k_4 - k_1)) + ((k_4 - k_1) \cdot \epsilon_3) (((k_1 + k_4) - k_3) \cdot \epsilon_2) \right. \\ \left. + ((k_4 - k_1) \cdot \epsilon_2) ((k_2 - (k_1 + k_4)) \cdot \epsilon_3) \right) \times \delta^{a_1 a_4} \left(\frac{i}{\sqrt{2}} \right) \left(\frac{-i}{\sqrt{2}} \right) i, \quad (6.9)$$

$$n_u = (-1) k_{13}^2 \text{diagram}_u = (-1) \left(((k_2 + k_4) - k_1) \cdot \epsilon_3 \right) \left((k_4 - (k_1 + k_3)) \cdot \epsilon_2 \right) \times \delta^{a_1 a_4} \left(\frac{-i}{\sqrt{2}} \right)^2 i, \quad (6.10)$$

and

$$n_4 = \text{diagram}_4 = \frac{i}{2} \delta^{a_1 a_4} (\epsilon_2 \cdot \epsilon_3). \quad (6.11)$$

Now that with quartic graph present, the original Jacobi identity inevitably needs to be modified if color-kinematics duality is to remain holding. To better keep track of how this is done we write the BCJ sum of the two KK basis amplitudes in terms of the factors just introduced so that every term appears in the sum has a clear graphical interpretation. Also for future reference we analytically continue one of the scalar legs, say leg 4, and write

$$s_{21} A_{2,2}^{\text{YMs}}(1, 2_g, 3_g, 4) + (s_{21} + s_{23}) A_{2,2}^{\text{YMs}}(1, 3_g, 2_g, 4) \\ = s_{12} \left(\frac{n_s}{s_{12}} - \frac{n_t}{s_{23}} + n_4 \right) + (s_{21} + s_{23}) \left(-\frac{n_u}{s_{13}} + \frac{n_t}{s_{23}} + n_4 \right) \\ = (n_s + n_t + n_u + (s_{12} - s_{13}) n_4) + k_4^2 \left(-\frac{n_u}{s_{13}} + n_4 \right). \quad (6.12)$$

The fact that BCJ sum vanishes in the on-shell limit suggests that the Jacobi identity is modified as $n_s + n_t + n_u + (s_{12} - s_{13})n_4 = 0$ up to terms proportional to k_4^2 . A careful inspection shows that these terms actually cancel completely. Plugging equations (6.8) to (6.11) into the left hand side of this modified Jacobi sum, we see that (neglecting an overall factor $(-i)\delta^{a_1 a_4}/2$),

$$\begin{aligned}
 (\epsilon_2 \cdot \epsilon_3) \text{ part :} & \quad - (k_3 - k_2) \cdot (k_4 - k_1) + (s_{12} - s_{13}) = 0, & (6.13) \\
 (\epsilon_2 \cdot k)(\epsilon_3 \cdot k) \text{ part :} & \quad 2^2 (k_1 \cdot \epsilon_2) ((k_1 + k_2) \cdot \epsilon_3), & \leftarrow \text{contribution from } n_s, \\
 & \quad + 2^2 (-1) ((k_1 + k_3) \cdot \epsilon_2) (k_1 \cdot \epsilon_3), & \leftarrow \text{contribution from } n_u, \\
 & \quad + 2 \left((k_3 \cdot \epsilon_2) ((2k_1 + k_2) \cdot \epsilon_3) - ((2k_1 + k_3) \cdot \epsilon_2) (k_2 \cdot \epsilon_3) \right), & \leftarrow \text{contribution from } n_t, \\
 & \quad = 0. & (6.14)
 \end{aligned}$$

We obtain the numerator by feeding the off-shell continued BCJ sum just computed into the KLT inspired prescription (6.2), taking the modified Jacobi identity into account, yielding

$$\begin{aligned}
 n(13_g 2_g 4) &= \frac{1}{k_4^2} s_{31} \left[s_{21} A_{2,2}^{\text{YMs}}(1, 2_g, 3_g, 4) + (s_{21} + s_{23}) A_{2,2}^{\text{YMs}}(1, 3_g, 2_g, 4) \right] \\
 &= -n_u + s_{13} n_4 = 1 \overline{\text{graph}}_1 + s_{13} \overline{\text{graph}}_2,
 \end{aligned}$$

where by an abuse of notation we neglected factors of inverse propagators so that the graphs appear in the equation above should be understood as representing the corresponding numerators rather than the original Feynman graphs. In the following discussions we shall not distinguish numerators from Feynman graphs unless it is not apparent from the context. The other two gluon numerator at four points can be readily obtained by swapping labels $(2 \leftrightarrow 3)$. Inserting the half-ladder numerators back into KLT relation and we find agreement with the two graviton relation (equation (4) in [14]).

$$A_{2,2}^{\text{EYM}}(1, 4; h_2, h_3) = (-2i) \left((\epsilon_2 \cdot X_2)(\epsilon_3 \cdot X_3) - \frac{1}{4}(\epsilon_2 \cdot \epsilon_3) s_{21} \right) A_4^{\text{YM}}(1, 2, 3, 4) + (2 \leftrightarrow 3). \quad (6.15)$$

Note that the above relation is not exactly the same as (5.1), but equivalent to it after using certain BCJ relations, and note particularly that the new $\epsilon_2 \cdot \epsilon_3$ term came from the quartic graph contribution.

Off-shell continued Jacobi identity. The key point of the above calculation is the modified Jacobi identity when some of the legs becoming off-shell, e.g., $n_s + n_t + n_u + (s_{12} - s_{13})n_4 = 0$. This modification will lead to modified fundamental BCJ relations, to be discussed later. When considering situations for higher points, one note that the color dependency will factorize when the scalars are connected by an internal gluon line, thus the single trace part of a two-gluon partial amplitude can only contain graphs derivable from those appearing at four-point case by welding pure scalar currents to their two scalar legs. Therefore we only need to consider analytically continuing the two scalar lines of the modified Jacobi identity when two gluons are present. Careful inspection of (6.14)

shows that the $(\epsilon \cdot k)(\epsilon \cdot k)$ part of the Jacobi sum is a pair-wise cancelation, up to terms proportional to $(\epsilon_2 \cdot k_2)$ or $(\epsilon_3 \cdot k_3)$, and therefore remains valid even when scalars become off-shell. The only modification comes from the $(\epsilon_2 \cdot \epsilon_3)$ part. To completely cancel the $(k_2 - k_3) \cdot (k_1 - k_4)$ factor produced by n_t , we see that the quartic graph needs to be multiplied by the same factor. The off-shell continued identity we need for all two gluon amplitudes is then

$$\begin{array}{c} 1 \\ \diagdown \\ \text{---} \\ \diagup \\ 2 \end{array} \begin{array}{c} 4 \\ \diagup \\ \text{---} \\ \diagdown \\ 3 \end{array} + \begin{array}{c} 1 \\ \diagdown \\ \text{---} \\ \diagup \\ 3 \end{array} \begin{array}{c} 4 \\ \diagup \\ \text{---} \\ \diagdown \\ 2 \end{array} - \begin{array}{c} 1 \\ \diagdown \\ \text{---} \\ \diagup \\ 3 \end{array} \begin{array}{c} 4 \\ \diagup \\ \text{---} \\ \diagdown \\ 2 \end{array} + (k_2 - k_3) \cdot (k_1 - k_4) \begin{array}{c} 1 \\ \diagdown \\ \text{---} \\ \diagup \\ 2 \end{array} \begin{array}{c} 4 \\ \diagup \\ \text{---} \\ \diagdown \\ 3 \end{array} = 0, \quad (6.16)$$

and we will be using this identity in the following discussions.

6.3 The five-point YMs amplitudes with two gluons

Having presented the example of four points with two gluons, we further show an example of five-point amplitude with two gluons. Again, we will use the method of summing over color-ordered KK basis.

At five points the number of graphs increases considerably. Recall from [8] that there are 15 different graphs in total in the KK sector at five points if the amplitudes are to be described by cubic graphs only, 6 of them are independent when Jacobi identities are taken into account. Similarly we label the cubic graphs as $n_1, n_2, \dots, n_{15}$, and we regard the quartic graphs as additional corrections n_{16}, n_{17}, n_{18} . The amplitudes are given by

$$A_{3,2}^{\text{YMs}}(1, 2_g, 3_g, 4, 5) = \frac{n_1}{s_{12}s_{45}} + \frac{n_2}{s_{23}s_{15}} + \frac{n_3}{s_{34}s_{12}} + \frac{n_4}{s_{45}s_{23}} + \frac{n_5}{s_{15}s_{34}} + \frac{n_{16}}{s_{45}} + \frac{n_{17}}{s_{15}}, \quad (6.17)$$

$$A_{3,2}^{\text{YMs}}(1, 4, 3_g, 2_g, 5) = \frac{n_6}{s_{14}s_{25}} + \frac{n_5}{s_{34}s_{15}} + \frac{n_7}{s_{23}s_{14}} + \frac{n_8}{s_{25}s_{34}} + \frac{n_2}{s_{15}s_{23}} + \frac{n_{18}}{s_{14}} + \frac{n_{17}}{s_{15}}, \quad (6.18)$$

$$A_{3,2}^{\text{YMs}}(1, 3_g, 4, 2_g, 5) = \frac{n_9}{s_{13}s_{25}} - \frac{n_5}{s_{34}s_{15}} + \frac{n_{10}}{s_{24}s_{13}} - \frac{n_8}{s_{25}s_{34}} + \frac{n_{11}}{s_{15}s_{24}} - 2\frac{n_{17}}{s_{15}}, \quad (6.19)$$

$$A_{3,2}^{\text{YMs}}(1, 2_g, 4, 3_g, 5) = \frac{n_{12}}{s_{12}s_{35}} + \frac{n_{11}}{s_{24}s_{15}} - \frac{n_3}{s_{34}s_{12}} + \frac{n_{13}}{s_{35}s_{24}} - \frac{n_5}{s_{15}s_{34}} - 2\frac{n_{17}}{s_{15}}, \quad (6.20)$$

$$A_{3,2}^{\text{YMs}}(1, 4, 2_g, 3_g, 5) = \frac{n_{14}}{s_{14}s_{35}} - \frac{n_{11}}{s_{24}s_{15}} - \frac{n_7}{s_{23}s_{14}} - \frac{n_{13}}{s_{35}s_{24}} - \frac{n_2}{s_{15}s_{23}} + \frac{n_{18}}{s_{14}} + \frac{n_{17}}{s_{15}}, \quad (6.21)$$

$$A_{3,2}^{\text{YMs}}(1, 3_g, 2_g, 4, 5) = \frac{n_{15}}{s_{13}s_{45}} - \frac{n_2}{s_{23}s_{15}} - \frac{n_{10}}{s_{24}s_{13}} - \frac{n_4}{s_{45}s_{23}} - \frac{n_{11}}{s_{15}s_{24}} + \frac{n_{16}}{s_{45}} + \frac{n_{17}}{s_{15}}. \quad (6.22)$$

Together there are 15 cubic graphs and 3 quartic graphs in the two gluon scalar Yang-Mills amplitudes at five points, which we list below,

$$\begin{array}{ccccc}
 n_1 = \begin{array}{c} 1 \\ \diagdown \\ \text{---} \\ \diagup \\ 2 \end{array} \begin{array}{c} 5 \\ \diagup \\ \text{---} \\ \diagdown \\ 4 \end{array}, & n_2 = \begin{array}{c} 2 \\ \diagdown \\ \text{---} \\ \diagup \\ 3 \end{array} \begin{array}{c} 1 \\ \diagup \\ \text{---} \\ \diagdown \\ 5 \end{array}, & n_3 = \begin{array}{c} 3 \\ \diagdown \\ \text{---} \\ \diagup \\ 4 \end{array} \begin{array}{c} 2 \\ \diagup \\ \text{---} \\ \diagdown \\ 1 \end{array}, & n_4 = \begin{array}{c} 4 \\ \diagdown \\ \text{---} \\ \diagup \\ 5 \end{array} \begin{array}{c} 3 \\ \diagup \\ \text{---} \\ \diagdown \\ 2 \end{array}, & n_5 = \begin{array}{c} 5 \\ \diagdown \\ \text{---} \\ \diagup \\ 1 \end{array} \begin{array}{c} 4 \\ \diagup \\ \text{---} \\ \diagdown \\ 3 \end{array}, \\
 n_6 = \begin{array}{c} 1 \\ \diagdown \\ \text{---} \\ \diagup \\ 4 \end{array} \begin{array}{c} 5 \\ \diagup \\ \text{---} \\ \diagdown \\ 3 \end{array}, & n_7 = \begin{array}{c} 3 \\ \diagdown \\ \text{---} \\ \diagup \\ 2 \end{array} \begin{array}{c} 4 \\ \diagup \\ \text{---} \\ \diagdown \\ 1 \end{array}, & n_8 = \begin{array}{c} 2 \\ \diagdown \\ \text{---} \\ \diagup \\ 5 \end{array} \begin{array}{c} 3 \\ \diagup \\ \text{---} \\ \diagdown \\ 4 \end{array}, & n_9 = \begin{array}{c} 1 \\ \diagdown \\ \text{---} \\ \diagup \\ 3 \end{array} \begin{array}{c} 5 \\ \diagup \\ \text{---} \\ \diagdown \\ 2 \end{array}, & n_{10} = \begin{array}{c} 4 \\ \diagdown \\ \text{---} \\ \diagup \\ 2 \end{array} \begin{array}{c} 3 \\ \diagup \\ \text{---} \\ \diagdown \\ 1 \end{array},
 \end{array}$$

$$\begin{aligned}
 n_{11} &= \text{diagram 1}, & n_{12} &= \text{diagram 2}, & n_{13} &= \text{diagram 3}, & n_{14} &= \text{diagram 4}, & n_{15} &= \text{diagram 5}, \\
 n_{16} &= \text{diagram 6}, & n_{17} &= \text{diagram 7}, & n_{18} &= \text{diagram 8}.
 \end{aligned} \tag{6.23}$$

As in the case of a cubic theory, not all graphs are independent. Together there are seven Jacobi identities derived from cyclic permutations involving one gluon, one of the identities obtainable as a linear combination of the others,

$$\begin{aligned}
 n_3 - n_5 + n_8 &= 0, & n_3 - n_1 + n_{12} &= 0, & n_4 - n_2 + n_7 &= 0, \\
 n_8 - n_6 + n_9 &= 0, & n_{10} - n_9 + n_{15} &= 0, & n_{10} - n_{11} + n_{13} &= 0, & (n_{13} - n_{12} + n_{14} &= 0).
 \end{aligned}$$

In addition there are three more modified Jacobi identities where two gluons participate the permutations, and therefore contains quartic graphs,

$$n_4 - n_1 + n_{15} - (s_{21} - s_{31})n_{16} = 0, \tag{6.24}$$

$$n_5 - n_2 + n_{11} + (s_{34} - s_{24})n_{17} = 0, \quad n_7 - n_6 + n_{14} + (s_{35} - s_{25})n_{18} = 0. \tag{6.25}$$

The above constraints allows us to trade $n_7, n_8, \dots, n_{15}$ in terms of the first six independent cubic graphs plus the three quartic graphs,

$$n_7 = n_2 - n_4, \quad n_8 = -n_3 + n_5, \quad n_9 = n_3 - n_5 + n_6, \tag{6.26}$$

$$n_{10} = -n_1 + n_3 + n_4 - n_5 + n_6 - (s_{21} - s_{31})n_{16}, \tag{6.27}$$

$$n_{11} = n_2 - n_5 - (s_{34} - s_{24})n_{17}, \quad n_{12} = n_1 - n_3, \tag{6.28}$$

$$n_{13} = n_1 + n_2 - n_3 - n_4 - n_6 - (s_{34} - s_{24})n_{17} + (s_{21} - s_{31})n_{16}, \tag{6.29}$$

$$n_{14} = -n_2 + n_4 + n_6 - (s_{35} - s_{25})n_{18}, \quad n_{15} = n_1 - n_4 + (s_{21} - s_{31})n_{16}. \tag{6.30}$$

Furthermore we note that all three quartic graphs actually contribute the same value,

$$n_{18} = n_{17} = n_{16} = (\epsilon_2 \cdot \epsilon_3) \times \left(\frac{-1}{2} \right) f^{a_1 a_4 a_5}. \tag{6.31}$$

Bearing all these in mind we calculate the five-point numerator $n(12_g 3_g 45)$ from KLT relation by summing over KK basis and get

$$n(12_g 3_g 45) = \sum_{\sigma \in S_3} \mathcal{S}[234|\sigma] J^{\text{YMs}}(1, \sigma, 5) \tag{6.32}$$

$$= n_1 + s_{12} n_{16} = \text{diagram 1} + s_{12} \text{diagram 2}.$$

All other numerators follow the same derivation, and we obtain

$$n(12_g 43_g 5) = \text{Diagram 1} + s_{21} \text{Diagram 2}, \quad (6.33)$$

$$n(13_g 2_g 45) = \text{Diagram 3} + s_{31} \text{Diagram 4}, \quad (6.34)$$

$$n(13_g 42_g 5) = \text{Diagram 5} + s_{31} \text{Diagram 6}, \quad (6.35)$$

$$n(142_g 3_g 5) = \text{Diagram 7} + (s_{21} + s_{24}) \text{Diagram 8}, \quad (6.36)$$

$$n(143_g 2_g 5) = \text{Diagram 9} + (s_{31} + s_{34}) \text{Diagram 10}. \quad (6.37)$$

Plugging the above results into DDM expression yields the two graviton EYM amplitude at five points,

$$\begin{aligned} A_{3,2}^{\text{EYM}}(1, 4, 5; h_2, h_3) &= \sqrt{2}^3 i \left((\epsilon_2 \cdot X_2)(\epsilon_3 \cdot X_3) - \frac{1}{4}(\epsilon_2 \cdot \epsilon_3)s_{21} \right) A_5^{\text{YM}}(1, 2, 3, 4, 5) \\ &+ \sqrt{2}^3 i \left((\epsilon_2 \cdot X_2)(\epsilon_3 \cdot X_3) - \frac{1}{4}(\epsilon_2 \cdot \epsilon_3)s_{21} \right) A_5^{\text{YM}}(1, 2, 4, 3, 5) + \dots \end{aligned} \quad (6.38)$$

6.4 The five and higher point amplitude involving two gravitons

Having witness that KLT relation successfully explains the new EYM amplitude expression for two graviton scattering at four and five points, perhaps it is not much of a surprise that the explanation generalizes to higher points. Indeed, one can actually read off the n -point two gluon numerator, and the two graviton EYM amplitude is determined by the corresponding DDM expression. We shall use the algorithm introduced originally for the pure scalar scenario in [71] to systematically calculate the numerator (i.e., to systematically sum over KK basis). As we shall see, in the case when only two gluons (p, q) are involved, the numerators remain fairly simple,

$$\begin{aligned} n(12 \cdots i \ p_g \cdots j \ q_g \cdots n) &= \text{Diagram 11} + 2(p \cdot Y_p) \text{Diagram 12} \\ &= \sqrt{2}^{n-2} (-1)^{n+1} i \left((\epsilon_p \cdot x_p)(\epsilon_q \cdot x_q) - \frac{1}{2}(\epsilon_p \cdot \epsilon_q)(p \cdot Y_p) \right). \end{aligned} \quad (6.39)$$

A brief review of the algorithm for numerators in the scalar scenario: for the purpose of being self-contained, we briefly review the algorithm used by the authors in [71] and [61] to calculate numerators. The idea is to divide the full S_{n-2} permutation sum appears in the numerator-current relation $n(1 \alpha n) = \sum_{\beta \in S_{n-2}} \mathcal{S}[\alpha^T | \beta] J^{YMs}(1, \beta, n)$ into BCJ sums, and proceed repeatedly if the Fundamental BCJ relation between currents admits further simplifications. For example, it was shown in [71] that the Fundamental BCJ relation between ϕ^3 currents yields another current, with the leg running through all insertions in the BCJ sum fixed at the off-shell continued line,

$$s_{21} \begin{array}{c} n \\ | \\ \bigcirc \\ / \backslash \\ 1 \quad 2 \quad 3 \quad \dots \quad n-1 \end{array} + (s_{21} + s_{31}) \begin{array}{c} n \\ | \\ \bigcirc \\ / \backslash \\ 1 \quad 3 \quad 2 \quad \dots \quad n-1 \end{array} + \dots = k_n^2 \begin{array}{c} n \\ | \\ \text{---} 2 \\ | \\ \bigcirc \\ / \backslash \\ 1 \quad 3 \quad \dots \quad n-1 \end{array}, \quad (6.40)$$

so that if we divide the full permutation sum S_3 in the five-point numerator calculation into BCJ sums, after substituting these summations using Fundamental BCJ relation (6.40), the collected result is yet another BCJ sum, but only performed over permutations of the legs of fewer-point sub-currents,

$$\begin{aligned} \sum_{\beta \in S_3} \mathcal{S}[432 | \beta_2 \beta_3 \beta_4] J^{\phi^3}(1, \beta_2, \beta_3, \beta_4, 5) &= s_{21} s_{31} \left(s_{41} J^{\phi^3}(14325) + (s_{41} + s_{43}) J^{\phi^3}(13425) + \dots \right) \\ &\quad + s_{21} (s_{31} + s_{32}) \left(s_{41} J^{\phi^3}(14235) + (s_{41} + s_{42}) J^{\phi^3}(12435) + \dots \right) \\ &= k_5^2 s_{21} \left(s_{31} \begin{array}{c} 5 \\ | \\ \text{---} 4 \\ | \\ \bigcirc \\ / \backslash \\ 1 \quad 3 \quad 2 \end{array} + (s_{31} + s_{32}) \begin{array}{c} 5 \\ | \\ \text{---} 4 \\ | \\ \bigcirc \\ / \backslash \\ 1 \quad 2 \quad 3 \end{array} \right), \end{aligned} \quad (6.41)$$

where we used (6.40) to replace the first and the second line of the equation above with the two graphs in (6.41). The result is another BCJ sum over currents. Repeat the substitution using Fundamental BCJ relation, and we obtain the numerator

$$k_{1234}^2 k_{123}^2 k_{12}^2 \begin{array}{c} 5 \\ | \\ \text{---} 4 \\ | \\ \text{---} 3 \\ | \\ \text{---} 2 \\ | \\ 1 \end{array}. \quad (6.42)$$

The five-point scalar Yang-Mills numerators involving two gluons. The calculation explained above only complicates slightly when few gluons are present. As far as single trace contributions are concerned, all amplitudes are consisted of Jacobi satisfying cubic graphs when only one gluon participates the scattering, and the same algorithm applies. It is straightforward to see that the numerator is given by $n(12 \dots p_g \dots n) = f^{1,2,*} f^{*,3,*} \dots f^{*,n-1,n} \epsilon_p \cdot x_p$, which when plugged into the summing expression readily reproduces the new EYM formula. In other words, (6.4) can also be understood from this point of view.

Things will become a little bit more complicated when two and more gluons are involved, since quartic vertices start to come into play, although they still remain quite manageable, in the sense that the modified Fundamental BCJ relations brought by the quartic term also permit repeated use of the relation when we carry out the summation. Explicitly, at five points the two-gluon Fundamental BCJ relations are modified as

$$s_{21}J^{\text{YMs}}(12_g3_g45) + s_{2,13}J^{\text{YMs}}(13_g2_g45) + s_{2,134}J^{\text{YMs}}(13_g42_g5) = k_5^2 \text{ (diagram)} , \quad (6.43)$$

$$s_{21}J^{\text{YMs}}(12_g34_g5) + s_{2,13}J^{\text{YMs}}(132_g4_g5) + s_{2,134}J^{\text{YMs}}(134_g2_g5) = k_5^2 \left(\text{diagram 1} + \text{diagram 2} \right),$$

$$\vdots \quad (6.44)$$

The rules to modification is as follows. Generically one only needs to replace the appropriate scalar by gluon lines in the original Fundamental BCJ relation between currents (6.40), and the right hand side of the equation is a current with the running leg fixed at the off-shell line. The only exception is when the running leg is gluonic, also that either leg 1 or leg $n-1$ (legs adjacent to the off-shell line) is a gluon line. In these cases an additional current needs to be added, where a quartic vertex resides on the off-shell line connects the two gluons.

We leave the details of a proof to these relations at five-point to appendix B because of its complicated nature. The principles are however not much different from the pure scalar scenario and is conceptually straightforward. Basically we cancel graphs related by Jacobi identities among Berends-Giele decomposed five-point current in the BCJ sum. The result after cancelation is then collected and identified to be the Berends-Giele decomposition of the right hand side of the equation. The proof for generic n points follows rather trivially from the structure of the proof, since adding more scalar lines into sub-currents at peripherals does not change Jacobi identities.

Assuming the Fundamental BCJ relations above, it is not difficult to see that the numerator is genuinely given by the formula (6.39) we claimed earlier. Consider for example the derivation that leads to numerator $n(123_g4_g5)$,

$$n(123_g4_g5) = s_{21}s_{31} \left(s_{41}J^{\text{YMs}}(14_g3_g25) + (s_{41} + s_{43})J^{\text{YMs}}(13_g4_g25) + \dots \right) \quad (6.45)$$

$$+ s_{21}(s_{31} + s_{32}) \left(s_{41}J^{\text{YMs}}(14_g23_g5) + (s_{41} + s_{42})J^{\text{YMs}}(124_g3_g5) + \dots \right)$$

$$= k_5^2 s_{21} \left(s_{31} \text{ (diagram 1)} + (s_{31} + s_{32}) \left(\text{diagram 2} + \text{diagram 3} \right) \right).$$

As was explained earlier we obtain the numerator by first dividing the full S_{n-2} permutation sum appears in the KLT inspired prescription (6.2) into BCJ sums, and then use the Fundamental BCJ relation between currents to fix the $n-2$ legs one by one in descending order. For the most part, this procedure is not different from the derivation of a pure scalar numerator, and the result does contain a cubic half ladder graph. The only modification occurs whenever the leg we attempt to fix is gluonic, in which case an additional graph is included, where a quartic vertex connecting both gluon lines emerges. The derivation afterwards again follows that of a pure scalar numerator. In the $n(123_g 4_g 5)$ example this leads to

$$n(123_g 4_g 5) = k_{1234}^2 k_{123}^2 k_{12}^2 \text{ (cubic half ladder) } + k_{1234}^2 k_{12}^2 (s_{31} + s_{32}) \text{ (quartic vertex) } . \quad (6.46)$$

Note that the Mandelstam variables associated with the quartic graph was furnished by momentum kernel. Careful inspection of the derivation that leads to (6.45) shows that they should contain the inner products between gluon line carrying the smaller label and all the scalar lines which precede it. As another illustration we consider $n(12_g 34_g 5)$,

$$n(12_g 34_g 5) = k_5^2 s_{21} \left(s_{31} \left(\text{diagram 1} + \text{diagram 2} \right) + (s_{31} + s_{32}) \text{diagram 3} \right) . \quad (6.47)$$

A repeated use of the Fundamental BCJ relation yields

$$n(12_g 34_g 5) = k_{1234}^2 k_{123}^2 k_{12}^2 \text{ (cubic half ladder) } + k_{1234}^2 k_{13}^2 s_{21} \text{ (quartic vertex) } . \quad (6.48)$$

As a verification, note that applying the same rules to derive numerators with all possible combinations of gluon positions yields the same results as those listed from equation (6.32) to (6.37) previously obtained exclusively for five points.

7 Conclusion

In this paper, we studied the newly discovered EYM amplitude relation by gauge invariance principle, the BCFW recursion relation as well as the KLT relation respectively. It turns out that the problem of EYM amplitude expansion is also closely related to the problem of computing BCJ numerators and the boundary contribution of BCFW terms.

The major context of this paper is devoted to the principle of gauge invariance applied to the determination of EYM amplitude relations. We propose a constructive algorithm by expanding any EYM amplitude $A_{n,m}^{\text{EYM}}$ as a linear sum of $A_{n+i,m-i}^{\text{EYM}}$ for $i = 1, 2, \dots, m$

with given expansion coefficients, and the contributing terms of $A_{n+i,m-i}^{\text{EYM}}$ are determined by $A_{n+i-1,m-i+1}^{\text{EYM}}$. This means that any contributing terms can be recursively determined by the very first one $A_{n+1,m-1}^{\text{EYM}}$, while keeping the gauge invariance in each step. This leads to a compact formula (3.39) for general EYM amplitude relations with arbitrary number of gravitons. Realizing that the expansion of Einstein-Yang-Mills amplitude into Yang-Mills amplitudes shares the same kinematic coefficient as the expansion of Yang-Mills-scalar amplitude into cubic-scalar amplitudes, we copy the EYM amplitude relation to YMs amplitude relation, and generalize the later one to the expansion of pure Yang-Mills amplitude into cubic-scalar amplitudes by the help of Pfaffian expansion. With the Yang-Mills amplitude expanded recursively into the cubic graphs, we further outline the strategy of rewriting the scalar amplitudes into KK basis, manifesting the color-kinematics duality and computing the BCJ numerators of Yang-Mills amplitude.

We also study the EYM amplitude relations in the S-matrix framework, and present the proof of EYM amplitude relations with two gravitons by BCFW recursion relations. In this case, any choice of deformed momenta is not possible to avoid the boundary contributions, so we need to compare the contributions of both sides in the relations from finite poles and also the boundary. The matching of both contributions also constraints the possible form of the non-trivial relations. Besides, we examine the problem again from the perspective of KLT relations. The expansion coefficients of EYM amplitude relations are identical to the BCJ numerators of DDM basis, and by computing the BCJ relations for currents we confirm the validation of EYM amplitude relations.

Following our results, there are many interesting directions to explore further. In our paper, one of the most important results is the recursive construction (3.39) of EYM amplitude relation. We have claimed this expression by a few explicit examples plus the guidance of gauge invariance principle. For the confirmation of the claim, a rigorous derivation by other methods is favorable. In an upcoming paper, we would explore the recursive construction directly from operations on the CHY-integrand level. Furthermore, we believe that, such recursive pattern can also find its hints in the BCFW recursion relation or KLT relation investigation of EYM amplitude expansion, which worth to work on with.

Another possible work would be that, in our recursive construction, the gauge invariance is manifest for all gravitons at each step except the first one that started the recursive algorithm. As shown in [45, 47–49], for Yang-Mills theory, the requirement of gauge invariance for $(n-1)$ points is sufficient to guarantee the correctness of the full amplitude. This observation seems to be also true in the EYM theory, thus finding an explicit proof along the same line as in [47–49] would be a thing worth to do.

A most interesting and important future direction would be the systematic study of the CHY-integrand expansion. In section 2, we have laid down the general framework for the expansion, while in the whole paper we are focus only on the expansion of (reduced) Pfaffian. However, many CHY-integrands, such as $(\text{Pf}'(A))^2$ can be obtained from Pfaffian with proper reduction. Thus our results could be easily generalized to many other theories. Especially by similar calculations, we can check if the soft theorem can be used to uniquely determine the amplitude for some theories, such as NLSM as advertised in [47–49].

Finally, as a byproduct of the EYM expansion, we have outlined the strategy of computing BCJ numerators⁴ from the expansion relation for general EYM amplitudes. The four-point example shows the procedure of computing the BCJ numerators as polynomial of $(\epsilon \cdot \epsilon)$, $(\epsilon \cdot k)$ and $(k \cdot k)$, constructed neatly from the expansion coefficients of EYM amplitudes into Yang-Mills amplitudes. This construction, when generalized to loop-level, would fascinate many important calculations involving gravitons.

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A Scalar Yang-Mills Feynman rules

For reference purposes we list below the color-ordered Feynman rules for constructing scalar Yang-Mills amplitudes [72]. The scalars and gluons are understood to be represented by straight lines and wavy lines respectively,

$$\begin{array}{c} \text{1 } \mu \\ \text{2 } \nu \end{array} \begin{array}{c} \text{wavy line} \\ \text{wavy line} \end{array} \begin{array}{c} \text{3 } \rho \\ \text{4 } \sigma \end{array} = \frac{i}{\sqrt{2}} \eta^{\mu\nu} (k_1 - k_2)^\rho + \text{cyclic}, \quad \begin{array}{c} \text{1 } \mu \\ \text{2 } \nu \end{array} \begin{array}{c} \text{wavy line} \\ \text{wavy line} \end{array} \begin{array}{c} \text{3 } \rho \\ \text{4 } \sigma \end{array} = i \eta^{\mu\rho} \eta^{\nu\sigma} - \frac{i}{2} (\eta^{\mu\nu} \eta^{\rho\sigma} + \eta^{\mu\sigma} \eta^{\nu\rho}), \quad (\text{A.1})$$

$$\begin{array}{c} \text{a} \\ \text{b} \end{array} \begin{array}{c} \text{straight line} \\ \text{straight line} \end{array} \begin{array}{c} \text{c} \\ \text{d} \end{array} = \sqrt{2} f^{abc}, \quad \begin{array}{c} \text{1 a} \\ \text{2 b} \end{array} \begin{array}{c} \text{straight line} \\ \text{straight line} \end{array} \begin{array}{c} \text{wavy line} \\ \text{wavy line} \end{array} \begin{array}{c} \mu \\ \nu \end{array} = -\frac{i}{\sqrt{2}} \delta^{ab} (k_1 - k_2)^\mu, \quad (\text{A.2})$$

$$\begin{array}{c} \text{a} \\ \text{b} \end{array} \begin{array}{c} \text{straight line} \\ \text{straight line} \end{array} \begin{array}{c} \text{wavy line} \\ \text{wavy line} \end{array} \begin{array}{c} \nu \\ \mu \end{array} = \frac{i}{2} \delta^{ab} \eta^{\mu\nu}, \quad \begin{array}{c} \text{a} \\ \text{b} \end{array} \begin{array}{c} \text{straight line} \\ \text{straight line} \end{array} \begin{array}{c} \text{wavy line} \\ \text{wavy line} \end{array} \begin{array}{c} \nu \\ \mu \end{array} = -i \delta^{ab} \eta^{\mu\nu}. \quad (\text{A.3})$$

B Graphical proof of the two-gluon fundamental BCJ relation between currents

As a demonstration of the general idea, in this appendix we prove two of the Fundamental BCJ relations at five points involving two gluons, equations (6.43) and (6.44), following the

⁴The polynomial expression of BCJ numerator of (reduced) Pfaffian has been applied to the proof of vanishing double poles in a recent work [76].

method used in [71] (which was also briefly outlined earlier in section 6.4). We shall neglect repeating a similar proof for generic n points, as it can be readily derived by induction and by attaching more external legs on the sub-currents represented by blank circles in the graphs below.

Relations with no gluon adjacent to the off-shell leg. Consider first the configuration where the leg running over all possible insertions in the BCJ sum is a gluon, and the other gluon is non-adjacent to the off-shell leg. We would like to prove that

$$s_{21}J^{\text{YMs}}(12_g3_g45) + (s_{2,13})J^{\text{YMs}}(13_g2_g45) + (s_{2,134})J^{\text{YMs}}(13_g42_g5) = \text{Diagram} \quad . \quad (\text{B.1})$$

For this purpose we Berends-Giele decompose all three currents appear in the BCJ sum, yielding altogether nine graphs,

$$s_{21}J^{\text{YMs}}(12_g3_g45) = s_{21} \text{(a1)} + s_{21} \text{(a2)} + s_{21} \text{(a3)} \quad , \quad (\text{B.2})$$

$$s_{2,13}J^{\text{YMs}}(13_g2_g45) = s_{2,13} \text{(b1)} + s_{2,13} \text{(b2)} + s_{2,13} \text{(b3)} \quad , \quad (\text{B.3})$$

$$s_{2,134}J^{\text{YMs}}(13_g42_g5) = s_{2,134} \text{(c1)} + s_{2,134} \text{(c2)} + s_{2,134} \text{(c3)} \quad , \quad (\text{B.4})$$

and notice that, aside from (c1), rest of the graphs can be regrouped as BCJ sums of sub-currents. Indeed, graphs (a1) and (b1) together make up a BCJ sum of the sub-currents involving legs 1, 2 and 3,

$$s_{21} \text{(a1)} + s_{2,13} \text{(b1)} = k_{123}^2 \text{Diagram1} + k_{123}^2 \text{Diagram2} \quad , \quad (\text{B.5})$$

and graph (a2) is by itself a (trivial) BCJ sum of three point current. The combination of (b2) and (c2) is also a BCJ sum of the three point current, after eliminating part of the sum that carries an s_{21} using U(1) decoupling identity,

$$\begin{array}{c}
 \begin{array}{ccc}
 \begin{array}{c} 5 \\ | \\ \text{---} \circ \text{---} \circ \text{---} \\ | \quad | \quad | \quad | \\ 1 \quad 3 \quad 2 \quad 4 \end{array} & + s_{2,13} \begin{array}{c} 5 \\ | \\ \text{---} \circ \text{---} \circ \text{---} \\ | \quad | \quad | \quad | \\ 1 \quad 3 \quad 4 \quad 2 \end{array} & = s_{23} \begin{array}{c} 5 \\ | \\ \text{---} \circ \text{---} \circ \text{---} \\ | \quad | \quad | \quad | \\ 1 \quad 3 \quad 4 \quad 2 \end{array} , \\
 (b2) & (c2) &
 \end{array}
 \end{array} \quad (B.6)$$

and similarly (a3), (b3) and (c3) combine to give, up to terms vanishing under U(1) decoupling identity,

$$\begin{array}{c}
 \begin{array}{ccccc}
 \begin{array}{c} 5 \\ | \\ \text{---} \circ \text{---} \text{---} \\ | \quad | \quad | \\ 1 \quad 2 \quad 3 \quad 4 \end{array} & + s_{2,13} \begin{array}{c} 5 \\ | \\ \text{---} \circ \text{---} \text{---} \\ | \quad | \quad | \\ 1 \quad 3 \quad 2 \quad 4 \end{array} & + s_{2,134} \begin{array}{c} 5 \\ | \\ \text{---} \circ \text{---} \text{---} \\ | \quad | \quad | \\ 1 \quad 3 \quad 4 \quad 2 \end{array} & = k_{234}^2 \begin{array}{c} 5 \\ | \\ \text{---} \circ \text{---} \text{---} \\ | \quad | \quad | \\ 1 \quad 3 \quad 4 \quad 2 \end{array} & - k_{234}^2 \begin{array}{c} 5 \\ | \\ \text{---} \circ \text{---} \text{---} \\ | \quad | \quad | \\ 1 \quad 2 \quad 3 \quad 4 \end{array} . \\
 (a3) & (b3) & (c3) & &
 \end{array}
 \end{array} \quad (B.7)$$

In the equations above we have assumed the BCJ relations between currents at four points. As for the remaining graph (c1) that does not regrouped with the others into a BCJ sum of sub-currents, we rewrite the coefficient it carries using the kinematic identity $s_{2,134} = k_5^2 - s_{134}$ and then further Berends-Giele decompose the part that carries a factor s_{134} , giving

$$\begin{array}{c}
 \begin{array}{cccc}
 \begin{array}{c} 5 \\ | \\ \text{---} \circ \text{---} \text{---} \\ | \quad | \quad | \\ 1 \quad 3 \quad 4 \quad 2 \end{array} & = k_5^2 \begin{array}{c} 5 \\ | \\ \text{---} \circ \text{---} \text{---} \\ | \quad | \quad | \\ 1 \quad 3 \quad 4 \quad 2 \end{array} & - s_{134} \begin{array}{c} 5 \\ | \\ \text{---} \circ \text{---} \text{---} \\ | \quad | \quad | \\ 1 \quad 3 \quad 4 \quad 2 \end{array} & - s_{134} \begin{array}{c} 5 \\ | \\ \text{---} \circ \text{---} \text{---} \\ | \quad | \quad | \\ 1 \quad 3 \quad 4 \quad 2 \end{array} . \\
 (c1) & & &
 \end{array}
 \end{array} \quad (B.8)$$

Because of the regrouping and the application of lower point BCJ relation on sub-currents, the full BCJ sum (B.1) is now translated into the right hand side of equations (B.5), graph (a2), (B.6), (B.7) and (B.8) combined. To see that this combination is indeed identical to the right hand side of equation (B.1) we must show that all other graphs cancel, and this is true because of the Jacobi identities

$$\begin{array}{c}
 \begin{array}{ccc}
 \begin{array}{c} 5 \\ | \\ \text{---} \circ \text{---} \text{---} \\ | \quad | \quad | \\ 1 \quad 3 \quad 4 \quad 2 \end{array} & + s_{24} \begin{array}{c} 5 \\ | \\ \text{---} \circ \text{---} \text{---} \\ | \quad | \quad | \\ 1 \quad 3 \quad 4 \quad 2 \end{array} & - s_{134} \begin{array}{c} 5 \\ | \\ \text{---} \circ \text{---} \text{---} \\ | \quad | \quad | \\ 1 \quad 3 \quad 4 \quad 2 \end{array} = 0 , \\
 k_{123}^2 & &
 \end{array}
 \end{array} \quad (B.9)$$

and

$$s_{12} \text{ (triangle with wavy 2,3) } + k_{234}^2 \text{ (triangle with wavy 2,3) } - s_{134} \text{ (triangle with wavy 2,3) } = 0, \quad (\text{B.10})$$

and the fact that the following two graphs contribute the same, up to a relative minus sign,

$$k_{123}^2 \text{ (triangle with wavy 2,3) } - k_{234}^2 \text{ (triangle with wavy 2,3) } = \left(\frac{i}{2}\right) f^{a_1 a_4 a_5} \epsilon_2 \cdot \epsilon_3 - \left(\frac{i}{2}\right) f^{a_1 a_4 a_5} \epsilon_2 \cdot \epsilon_3 = 0, \quad (\text{B.11})$$

therefore finishing our proof.

Relations with one gluon adjacent to the off-shell leg. The proof when one gluon is adjacent to the off-shell leg follows exactly the same derivation, except that now we have a few additional quartic graphs. The relation we are aiming to prove is

$$s_{21} J^{\text{YMs}}(12_g 34_g 5) + s_{2,13} J^{\text{YMs}}(132_g 4_g 5) + s_{2,134} J^{\text{YMs}}(134_g 2_g 5) = k_5^2 \text{ (triangle with wavy 2,3) } + k_5^2 \text{ (triangle with wavy 2,3) }. \quad (\text{B.12})$$

Currents that appear in the BCJ sum Berends-Giele decompose as

$$s_{21} J^{\text{YMs}}(12_g 34_g 5) = s_{21} \text{ (a1) } + s_{21} \text{ (a2) } + s_{21} \text{ (a3) }, \quad (\text{B.13})$$

$$\begin{aligned} s_{2,13} J^{\text{YMs}}(132_g 4_g 5) &= s_{2,13} \text{ (b1) } + s_{2,13} \text{ (b2) } \\ &+ s_{2,13} \text{ (b3) } + s_{2,13} \text{ (b4) }, \end{aligned} \quad (\text{B.14})$$

$$\begin{aligned}
 s_{2,134} J^{\text{YMs}}(134_g 2_g 5) = & s_{2,134} \text{(c1)} + s_{2,134} \text{(c2)} \\
 & + s_{2,134} \text{(c3)} + s_{2,134} \text{(c4)} .
 \end{aligned}
 \tag{B.15}$$

Note the presence of two new quartic graphs $(b4)$ and $(c4)$. As in the previous example we regroup graphs into BCJ sums of sub-currents. Graphs $(a1)$ and $(b1)$ make up a BCJ sum of the sub-currents involving legs 1, 2 and 3,

$$\begin{aligned}
 s_{21} \text{(a1)} + s_{2,13} \text{(b1)} = & k_{123}^2 \text{(a1)} ,
 \end{aligned}
 \tag{B.16}$$

graph $(a2)$ forms a trivial BCJ sum of the three point current by itself, graphs $(b2)$ and $(c2)$ add up to another BCJ sum after eliminating terms using U(1) decoupling,

$$\begin{aligned}
 s_{21} \text{(b2)} + s_{2,13} \text{(c2)} = & s_{23} \text{(b2)} ,
 \end{aligned}
 \tag{B.17}$$

and similarly for the sum of graphs $(a3)$, $(b3)$ and $(c3)$,

$$\begin{aligned}
 s_{21} \text{(a3)} + s_{2,13} \text{(b3)} + s_{2,134} \text{(c3)} = & k_{234}^2 \text{(a3)} + k_{234}^2 \text{(a3)} .
 \end{aligned}
 \tag{B.18}$$

As for (c1), we Berends-Giele decompose it as in the previous example to give

$$s_{2,134} \text{ (c1) } = k_5^2 \text{ (b2) } - s_{134} \text{ (b4) } - s_{134} \text{ (c4) } . \quad (\text{B.19})$$

The full BCJ sum (B.12) is now translated into the right hand side of equation (B.16), graph (b2), (B.17), (B.18), (B.19) plus the additional graphs (b4) and (c4). To finish the proof we need to further translate these graphs into one of those on the right hand side of equation (B.12), and this is done by using Jacobi identities

$$k_{123}^2 \text{ (b4) } + s_{24} \text{ (b2) } - s_{123} \text{ (b4) } = (s_{4,13} - s_{2,13}) \text{ (b2) } , \quad (\text{B.20})$$

$$s_{21} \text{ (b4) } + k_{234}^2 \text{ (b2) } - s_{134} \text{ (b4) } = 0 , \quad (\text{B.21})$$

and the fact that the following two graphs contribute the same.

$$k_{234}^2 \text{ (b4) } = s_{13} \text{ (b2) } = \left(\frac{i}{2} \right) f^{a_1 a_3 a_5} \epsilon_2 \cdot \epsilon_4 . \quad (\text{B.22})$$

Collecting terms gives

$$\begin{aligned} & k_5^2 \text{ (b2) } + ((s_{4,13} - s_{2,13}) + s_{2,13} + s_{2,134} + s_{13}) \text{ (b2) } \\ &= k_5^2 \text{ (b2) } + k_5^2 \text{ (b2) } , \end{aligned}$$

which completes our proof.

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