

On gauge amplitudes first appearing at two loops

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ABSTRACT: We study scattering amplitudes in massless non-abelian gauge theory where all outgoing gluons have positive helicity. It has been argued recently by Costello that for a particular fermion representation (8 fundamentals plus one antisymmetric-tensor representation in $SU(N)$) the one-loop amplitudes vanish identically. We show that this vanishing leads to previously-observed identities among one-loop color-ordered partial amplitudes. We then turn to two loops, where Costello has computed the all-plus amplitudes for this theory, as rational functions of the kinematics for any number of gluons using the celestial chiral algebra (CCA) bootstrap. We show that in dimensional regularization, these two-loop amplitudes are not rational, and they are not even finite as $\epsilon \rightarrow 0$. However, the finite remainder for four gluons agrees with the formula by Costello. In addition, we provide a mass regulator for the infrared-divergent loop integrals; with this regulator, the CCA bootstrap formula is recovered exactly. Finally, we use the CCA bootstrap to compute the double-trace terms in the theory at two loops for an arbitrary number of gluons.

Dedicated to the memory of Stefano Catani

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1 Introduction

The study of scattering amplitudes has seen great advances in recent years. On the more applied side, computing higher-point and higher-loop amplitudes in the Standard Model has allowed for more precise comparisons to data collected at particle colliders (see e.g. refs. [1, 2] and references therein). On the more formal side, amplitudes are fascinating theoretical objects in their own right. They provide insight into the behavior and symmetries of a theory, as well as exhibiting previously unforeseen mathematical structures. Having explicit

analytic expressions for amplitudes is paramount for finding such structures, and for better understanding aspects of quantum field theory.

Often, direct calculation of amplitudes by evaluating Feynman diagrams can be bypassed for more computationally efficient methods. In particular, a general understanding of the singular behavior of amplitudes can allow them to be “bootstrapped” to higher orders in perturbation theory, or for a greater number of scattering particles. This program has had remarkable success in $\mathcal{N} = 4$ supersymmetric Yang-Mills in the planar limit (see e.g. refs. [3, 4] and references therein).

Amplitudes in ordinary, non-supersymmetric Yang-Mills (YM) theory remain more challenging. There have been remarkable recent advances in computing the full-color all-helicity massless QCD amplitudes for $2 \rightarrow 3$ scattering at two loops [5–7] and for $2 \rightarrow 2$ scattering at three loops [8–10]. These amplitudes have a rather intricate analytic structure, and pushing directly to one more loop or one more leg may be difficult.

Another avenue for progress, which we will pursue here, is to investigate the simplest possible helicity configuration, called “all-plus”, when all n outgoing gluons have the same positive helicity. Such amplitudes vanish for any n in any supersymmetric massless gauge theory [11–13], and therefore they vanish at tree level in YM theory. At one loop, in any massless gauge theory, their unitarity cuts vanish in four dimensions, and they are infrared (IR) and ultraviolet (UV) finite, rational functions of the spinor products of the external momenta, which are known for an arbitrary number of gluons [14, 15].

Self-dual Yang-Mills theory (sdYM) [16] involves path integrals over only self-dual gauge field configurations. Classically, sdYM is integrable [17–19]. For free plane waves, such configurations include only the positive-helicity gluons. Interactions between plane waves include a $(-++)$ vertex [20, 21], but not the parity conjugate $(+--)$ vertex. At tree level, one can build the one-minus amplitude $(-++\cdots+)$ by sewing together $(-++)$ vertices, but this vanishes on shell. At loop level, the same sewing leads to the one-loop all-plus amplitudes [22, 23], which validates the suggestion that the non-vanishing of these amplitudes can be considered an anomaly in the conservation of the currents associated with integrability of sdYM [24, 25].

At two loops, the connection to sdYM becomes less clear. Two-loop all-plus gauge theory amplitudes were first computed for four gluons using generalized unitarity [26, 27]. For five external gluons, the leading-color terms were computed first numerically [28], and later analytically [29, 30]. The nonplanar integrands in the pure-glue theory were found in ref. [31], and the complete nonplanar results are available in refs. [5, 7]. For $n > 5$, the polylogarithmic part of the leading-color result was proposed for arbitrarily many gluons in ref. [32], and the rational part was computed using an augmented recursion relation for $n = 6$ [33] and $n = 7$ [34]. (The planar $n = 6$ integrand was presented in ref. [35].) Full-color results for $n = 6$ in pure gauge theory were given in ref. [36]. The all- n result for a particular color structure has been conjectured in ref. [37], and checked numerically for $n = 8$ and 9 in refs. [38, 39] (where the $n < 8$ rational results were also checked). Many of these results rely on D -dimensional generalized unitarity for the construction of integrands, although the

polylogarithmic results in refs. [30, 32, 40] carry out the cuts four-dimensionally, and the rational parts in refs. [30, 33, 34, 36, 37, 40] are constructed recursively.

The connection between twistors, string theory, and tree-level gluon scattering amplitudes of (mostly) positive helicity goes back to Nair [41], Witten [42], the MHV rules of Cachazo, Svrček and Witten [43], and the derivation of these rules from the YM action by Mason [44]. They have also been derived from a twistor action [45]. These works clarify the relations between sdYM and tree level amplitudes. The MHV rules were applied to compute tree-level form factors of operators composed of anti-self-dual field strengths, e.g. $\text{tr}(F_{\text{ASD}}^2)$ [46]. The all-plus and one-minus form factors for this operator were computed at one loop in a non-supersymmetric $SU(N)$ theory in ref. [47].

Recently, a novel bootstrap method for amplitudes in special theories has been suggested in ref. [48]. It stems from a combination of ideas from celestial holography, twisted holography, and twistor theory. In some sense, it is a loop level generalization of the earlier tree-level work [44, 45]. In this method, the cancellation of an anomaly in a theory that lives in twistor space allows for the existence of a chiral algebra, the elements of which are in bijection with the states of the theory. The correlators of the chiral algebra correspond to form factors of the theory. The operator product expansions (OPEs) between the elements of the chiral algebra are used to constrain the pole-structure of correlators, the residues of these poles being lower-loop or lower-point correlators. In this way, one can bootstrap the form factors of these theories.

In ref. [49], this *celestial chiral algebra (CCA) bootstrap* was used to compute a two-loop n -gluon all-plus-helicity form factor in sdYM with Weyl fermions transforming in the representation

$$R_0 \equiv 8F \oplus 8\bar{F} \oplus \wedge^2 F \oplus \wedge^2 \bar{F} \quad (1.1)$$

of the Lie algebra of $SU(N)$. Here F is the fundamental representation, and $\wedge^2 F$ is the antisymmetric tensor representation. In terms of Dirac fermions, the representation has 8 fundamentals (quarks) plus one antisymmetric tensor. It solves the anomaly cancellation condition from the six-dimensional twistor-space theory [48],

$$\text{tr}_{R_0}(X^4) = \text{tr}_G(X^4), \quad (1.2)$$

for any generator X of the $SU(N)$ Lie algebra, where G denotes the adjoint representation. The form factor is for an operator $\frac{1}{2}\text{tr}(B \wedge B)$, involving an adjoint-valued, antisymmetric, anti-self-dual tensor field $B_{\mu\nu}$, which is used to enforce self-duality of the gauge field.

The sdYM form factor computed in ref. [49] should reproduce scattering amplitudes in YM for arbitrary n . Due to the anomaly cancellation condition, the one-loop amplitude should vanish in this theory. As we will see, this condition implies identities among the QCD all-plus partial amplitudes. The identities include the “three-photon vanishing” relations first noticed in ref. [15]. A more general set of linear relations was found in ref. [50]; we will show that these relations are all explained by the vanishing of the one-loop all-plus amplitude for representation R_0 .

The relevant two-loop sdYM form factor was computed for all n in ref. [49]. The four-point result is

$$\begin{aligned} \mathcal{A}_{4,\text{sdYM}}^{\text{2-loop}} = & \frac{g^6}{(4\pi)^4} \rho \left[\left(12N - 4 \frac{s^2 + 4st + t^2}{st} - \frac{24}{N} \right) (\text{tr}(1234) + \text{tr}(1432)) \right. \\ & \left. + \left(24 + \frac{24}{N} \right) \text{tr}(12)\text{tr}(34) \right] + \mathcal{C}(234), \end{aligned} \quad (1.3)$$

where

$$\rho = i \frac{[12][34]}{\langle 12 \rangle \langle 34 \rangle}, \quad (1.4)$$

and $s = (k_1 + k_2)^2$ and $t = (k_2 + k_3)^2$ are the four-point Mandelstam variables. We use the shorthand notation

$$\text{tr}_R(ij \cdots k) = \text{tr}_R(t^{a_i} t^{a_j} \cdots t^{a_k}), \quad (1.5)$$

which is the trace over the generators t^a of the Lie algebra of $SU(N)$ in an arbitrary representation R . Throughout this paper, traces without a subscript, as in eq. (1.3), will mean the trace over fundamental-representation generators. The “ $+\mathcal{C}(234)$ ” instructs one to add the two non-trivial cyclic permutations of $(2, 3, 4)$ acting on the previous expression.

In this paper, we wish to investigate the relation between the sdYM form factor given in eq. (1.3) and all-plus amplitudes in ordinary YM. The two-loop all-plus four-point amplitude in QCD was computed in dimensional regularization in refs. [26, 27]. Here we will replace the fermion loops for QCD (i.e. for fermions in the fundamental (+ antifundamental) representation only) with fermion loops in the representation R_0 in eq. (1.1). Then we can directly compare the form factor in sdYM to the two-loop amplitude in YM. The double-trace term is not provided in ref. [49], so we compute it in Appendix B. Our results agree *only after* UV renormalization and after subtracting off the universal two-loop IR divergences given by Catani [51]. This statement does not disprove eq. (1.3); rather, the discrepancy most likely arises from the fact that the CCA bootstrap technique keeps all momenta four-dimensional, in contrast to dimensional regularization. We resolve the discrepancy by using a different IR regularization scheme, namely a mass regularization of the loop integrands. With this scheme, the two-loop four-point sdYM form factor equals the YM amplitude, and we suppose that the same will be true for $n > 4$. We also argue that the n -gluon sdYM result gives the finite remainder of the YM amplitude in dimensional regularization. This result could provide a check of higher-point two-loop all-plus helicity amplitudes, once all the fermionic and subleading-color terms become available.

2 An overview of the CCA bootstrap

In this section, we provide a non-rigorous overview of a method used to bootstrap certain two-loop amplitudes [49]. We will refer to this method as the *celestial chiral algebra (CCA) bootstrap*. Positive- and negative-helicity states of sdYM on twistor space are in one-to-one correspondence with local operators in an (extended) chiral algebra. The conformal blocks of

this algebra are the local operators in the self-dual theory. Therefore, correlation functions of the chiral algebra in a given conformal block correspond to form factors of the gauge theory. Moreover, the OPEs in the algebra are collinear limits of states in the field theory. This suggests that one can use the chiral algebra to “bootstrap” form factors of sdYM by using the analytic properties of the OPEs.

A requirement for the existence of a chiral algebra is the associativity of its OPEs. Associativity fails at the first loop correction for pure gauge theory, due to a gauge anomaly arising from the all-plus helicity amplitude on twistor space. In order to remedy this, a fourth-order scalar field that couples to the Yang-Mills topological term was introduced in refs. [48, 52, 53]. However, the mechanism can only cancel double-trace contributions, and so it is necessary for the gauge group to not have an independent quartic Casimir structure. Alternatively, the anomaly can be cured by introducing fermions in special representations of the gauge group [49]. In particular, the requirement is that the quartic Casimir in the adjoint representation is exactly that in the (real) representation R

$$\text{tr}_G(X^4) = \text{tr}_R(X^4). \quad (2.1)$$

For $SU(N)$ gauge theory, one such example of this type of representation is R_0 given in eq. (1.1).

With this choice of matter representation, the one-loop OPEs are associative. Therefore, the chiral algebra exists for this theory and can be used to compute form factors. In fact, associativity constrains all form factors of self-dual Yang-Mills (plus matter) to be rational functions, with poles only in the spinor products $\langle ij \rangle$. The chiral algebra OPEs determine all possible poles in the form factor, and the residues of these poles are chiral algebra correlators that have fewer external states or are at lower loop order. In this way, one can determine the n -point form factors inductively.

The form factor of most interest is the one with the operator

$$\frac{1}{2}\text{tr}(B \wedge B), \quad (2.2)$$

inserted at the origin,¹ where B is the adjoint-valued anti-self-dual two-form appearing in the sdYM Lagrangian [21],

$$\mathcal{L}_{\text{sdYM}} = \text{tr}(B \wedge F). \quad (2.3)$$

Deforming the self-dual Lagrangian by $\frac{1}{2}g^2\text{tr}(B \wedge B)$ and integrating out B yields the regular Yang-Mills Lagrangian, up to a topological term which does not affect the perturbation theory. So form factors of self-dual Yang-Mills with the operator $\frac{1}{2}\text{tr}(B \wedge B)$ inserted at the origin are amplitudes of ordinary Yang-Mills theory.

Using the CCA bootstrap, massless QCD amplitudes with matter in the representation (1.1) were computed at tree level [48], one loop [53], and two loops [49] for the two-minus,

¹We mean the origin in position space x . The x -dependence of the correlator is $\propto \exp(i \sum_{j=1}^n k_j \cdot x)$ where k_j are the gluon momenta.

one-minus, and all-plus helicity configurations, respectively. The two-loop all-plus four-point sdYM form factor is¹

$$\mathcal{A}_{4,\text{sdYM}}^{\text{2-loop}} = g^6 \left[A_{4;1,\text{sdYM}}^{\text{2-loop}} (\text{tr}(1234) + \text{tr}(1432)) + A_{4;3,\text{sdYM}}^{\text{2-loop}} \text{tr}(12)\text{tr}(34) \right] + \mathcal{C}(234), \quad (2.4)$$

where

$$\begin{aligned} A_{4;1,\text{sdYM}}^{\text{2-loop}} = & \frac{i}{(4\pi)^4} \left[(6N - 4 - 8N^{-1}) \left(\frac{[12][34]}{\langle 12 \rangle \langle 34 \rangle} + \frac{[14][23]}{\langle 14 \rangle \langle 23 \rangle} \right) - (4 + 8N^{-1}) \frac{[13][24]}{\langle 13 \rangle \langle 24 \rangle} \right. \\ & \left. - 2 \frac{[12][34]}{\langle 12 \rangle \langle 34 \rangle} \frac{\langle 13 \rangle \langle 24 \rangle + \langle 14 \rangle \langle 23 \rangle}{\langle 12 \rangle \langle 34 \rangle} - 2 \frac{[14][23]}{\langle 14 \rangle \langle 23 \rangle} \frac{\langle 13 \rangle \langle 24 \rangle + \langle 12 \rangle \langle 34 \rangle}{\langle 14 \rangle \langle 23 \rangle} \right] \end{aligned} \quad (2.5)$$

and

$$A_{4;3,\text{sdYM}}^{\text{2-loop}} = \frac{8i}{(4\pi)^4} (1 + N^{-1}) \left(\frac{[12][34]}{\langle 12 \rangle \langle 34 \rangle} + \frac{[13][24]}{\langle 13 \rangle \langle 24 \rangle} + \frac{[14][23]}{\langle 14 \rangle \langle 23 \rangle} \right). \quad (2.6)$$

This expression can be simplified using the Schouten spinor identity and four-point momentum conservation, which includes the result that ρ is totally symmetric,²

$$\frac{\rho}{i} = \frac{[12][34]}{\langle 12 \rangle \langle 34 \rangle} = \frac{[13][24]}{\langle 13 \rangle \langle 24 \rangle} = \frac{[14][23]}{\langle 14 \rangle \langle 23 \rangle}. \quad (2.7)$$

Then eqs. (2.5) and (2.6) collapse to eq. (1.3). However, when computing n -point form factors based on lower-point ones, one must remember *not* to use lower-point momentum conservation to simplify the lower-point form factors, as it is the sum of the n gluon momenta that is conserved, not a subset of them.

With this in mind, the n -point color-ordered amplitude is constructed recursively, based on eqs. (2.5) and (2.6), and is given by

$$\begin{aligned} \mathcal{A}_{n,\text{sdYM}}^{\text{2-loop}} = & g^{n+2} \left[\sum_{\sigma \in S_n / \mathbb{Z}_n} \text{tr}(\sigma_1 \cdots \sigma_n) \right. \\ & \times \sum_{1 \leq i < j < k < l \leq n} A_{4;1,\text{sdYM}}^{\text{2-loop}}(\sigma_i, \sigma_j, \sigma_k, \sigma_l) \frac{\langle \sigma_i \sigma_j \rangle \langle \sigma_j \sigma_k \rangle \langle \sigma_k \sigma_l \rangle \langle \sigma_l \sigma_i \rangle}{\langle \sigma_1 \sigma_2 \rangle \langle \sigma_2 \sigma_3 \rangle \cdots \langle \sigma_n \sigma_1 \rangle} \\ & \left. + \sum_{c=3}^{\lfloor n/2 \rfloor + 1} \sum_{\sigma \in S_n / S_{n;c}} \text{tr}(\sigma_1 \cdots \sigma_{c-1}) \text{tr}(\sigma_c \cdots \sigma_n) \sum_{1 \leq i < j < k < l \leq n} A_{n;c,\text{sdYM}}^{\text{2-loop}}(\sigma_i, \sigma_j, \sigma_k, \sigma_l) \right], \end{aligned} \quad (2.8)$$

¹The double-trace term was not provided in ref. [49]. However, Appendix B of ref. [49] outlines the computation of the color factors, so that one can keep track of the double-trace terms if desired relatively easily; see Appendix B.

²Our overall normalization of form factors and amplitudes differs from ref. [49] by a factor of i .

where $S_{n;c}$ is the subgroup of S_n consisting of permutations that keep the double-trace structure $\text{tr}(1, \dots, c-1)\text{tr}(c, \dots, n)$ invariant. $A_{n,c,\text{sdYM}}^{\text{2-loop}}(i, j, k, l)$ is the kinematic factor that multiplies this double-trace structure for the form factor with energy-level-1 insertions at i, j, k, l (as explained in Appendix B). It is defined as

$$A_{n,c,\text{sdYM}}^{\text{2-loop}}(i, j, k, l) = \frac{A_{4;3,\text{sdYM}}^{\text{2-loop}}(i, j, k, l)\langle ij \rangle^2 \langle kl \rangle^2}{\langle 12 \rangle \langle 23 \rangle \dots \langle c-1, 1 \rangle \langle c, c+1 \rangle \langle c+1, c+2 \rangle \dots \langle n, c \rangle} \quad (2.9)$$

for $1 \leq i < j \leq c-1$ and $c \leq k < l \leq n$, and it is zero otherwise. In Appendix B, we prove eq. (2.9) using the CCA bootstrap.

Note that for fermionic matter in R_0 there is no triple trace contribution, which would be present generically. The triple-trace cancellation is a consequence of the recursive construction, and its absence for $n = 4$ since $\text{tr}(t^a) = 0$ in $SU(N)$.

We wish to check eqs. (2.5)–(2.9) in the simplest case, $n = 4$, via an alternative method. We will use the fact that the two-loop four-gluon amplitudes were computed in QCD in dimensional regularization [26, 27] in a color-decomposed form which makes it straightforward to modify the fermion representation to R_0 .

Before doing the two-loop color algebra, we first warm up by computing the one-loop all-plus n -point amplitude, which vanishes (non-trivially) in this theory due to the anomaly cancellation (1.2).

3 The One-loop Amplitude

Here, we compute the one-loop all-plus n -point amplitude for massless QCD with matter in the representation (1.1). Color-decomposition plays a crucial role in this computation. We begin by reviewing the color-decomposition of one-loop n -gluon amplitudes in QCD for gauge group $SU(N)$ with matter in the representation $N_F(F \oplus \bar{F})$, where N_F is the number of quark flavors.

3.1 One-loop in QCD

The one-loop n -gluon QCD amplitude can be color-decomposed as [54]

$$\begin{aligned} \mathcal{A}_{n,\text{QCD}}^{\text{1-loop}} = & g^n \left[N \sum_{\sigma \in S_n / \mathbb{Z}_n} \text{tr}(\sigma_1 \dots \sigma_n) A_n^{[1]}(\sigma_1, \dots, \sigma_n) \right. \\ & + \sum_{c=3}^{\lfloor n/2 \rfloor + 1} \sum_{\sigma \in S_n / S_{n;c}} \text{tr}(\sigma_1 \dots \sigma_{c-1}) \text{tr}(\sigma_c \dots \sigma_n) A_{n;c}(\sigma_1, \dots, \sigma_n) \\ & \left. + N_F \sum_{\sigma \in S_n / \mathbb{Z}_n} \text{tr}(\sigma_1 \dots \sigma_n) A_n^{[1/2]}(\sigma_1, \dots, \sigma_n) \right], \end{aligned} \quad (3.1)$$

where the $A_{n;c}$ are the subamplitudes. The superscript $[j]$ denotes the spin of the particle circulating in the loop, $j = 1/2$ or 1 . The subamplitudes $A_n^{[j]}$ are color-ordered.

The subleading subamplitudes $A_{n;c}$ are obtained from the leading ones $A_n^{[1]}$ through the permutation sum [55, 56]

$$A_{n;c}(\alpha, \beta) = (-1)^{|\beta|} \sum_{\sigma \in \alpha \sqcup \beta^T} A_n^{[1]}(\sigma_1, \dots, \sigma_n), \quad (3.2)$$

where $\alpha = (1, 2, \dots, c-1)$ and $\beta = (c, c+1, \dots, n)$ are cyclicly ordered lists, and $\beta^T = (n, \dots, c+1, c)$ is the reverse ordering, with the understanding that α and β^T are actually equivalence classes under cyclic permutations of their arguments, i.e.

$$\alpha = \{(1, 2, \dots, c-1), (2, \dots, c-1, 1), \dots, (c-1, 1, \dots, c-2)\}, \quad (3.3)$$

$$\beta^T = \{(n, n-1, \dots, c), (n-1, \dots, c, n), \dots, (c, n, \dots, c+1)\}. \quad (3.4)$$

The symbol $\alpha \sqcup \beta^T$ denotes the cyclic shuffle product, which is the set of all permutations up to cycles of $\{1, 2, \dots, n\}$ that preserve the cyclic ordering of α and β^T , while allowing all possible relative orderings of the elements of α with respect to the elements of β^T . For example, letting $\alpha = (1, 2, 3)$ and $\beta = (4, 5)$, we have

$$\begin{aligned} \alpha \sqcup \beta^T = & \{(1, 2, 3, 4, 5), (1, 2, 4, 3, 5), (1, 4, 2, 3, 5), (1, 2, 4, 5, 3), (1, 4, 2, 5, 3), (1, 4, 5, 2, 3), \\ & (1, 2, 3, 5, 4), (1, 2, 5, 3, 4), (1, 5, 2, 3, 4), (1, 2, 5, 4, 3), (1, 5, 2, 4, 3), (1, 5, 4, 2, 3)\}. \end{aligned} \quad (3.5)$$

Again, it is understood that the lists within this set are equivalence classes under cyclic permutations of their arguments.

Another color decomposition also exists for the gluon (adjoint) contribution, in terms of traces over generators in the adjoint representation of $SU(N)$ [56]

$$\mathcal{A}_{n, \text{QCD}}^{\text{1-loop}} = \frac{g^n}{2} \sum_{\sigma \in S_n / \mathbb{Z}_n} \left[\text{tr}_G(\sigma_1 \dots \sigma_n) A_n^{[1]}(\sigma_1, \dots, \sigma_n) + 2N_F \text{tr}(\sigma_1 \dots \sigma_n) A_n^{[1/2]}(\sigma_1, \dots, \sigma_n) \right]. \quad (3.6)$$

The factor of 1/2 accounts for a reflection identity $\text{tr}_G(i_n i_{n-1} \dots i_1) = (-1)^n \text{tr}_G(i_1 i_2 \dots i_n)$, which implies a reflection identity on the color-ordered subamplitude $A_n^{[1]}$ (which also holds for $A_n^{[1/2]}$):

$$A_n^{[j]}(n, n-1, \dots, 1) = (-1)^n A_n^{[j]}(1, 2, \dots, n). \quad (3.7)$$

The sum in eq. (3.6) includes σ^T for all $\sigma \in S_n / \mathbb{Z}_n$, so the factor of 1/2 is needed.

The equivalence of eqs. (3.1) and (3.2) with eq. (3.6) can be seen by representing the adjoint representation G in terms of fundamental representations, $G \oplus 1 \cong F \otimes \bar{F}$. Evaluating the $F \otimes \bar{F}$ traces we have,

$$\begin{aligned} \text{tr}_G(1 \dots n) &= \text{tr}_{F \otimes \bar{F}}(1 \dots n) = \sum_{I \subset (1, \dots, n)} \text{tr}(I) \text{tr}_{\bar{F}}(I^c) \\ &= N \text{tr}(1 \dots n) + (-1)^n N \text{tr}(n \dots 1) \\ &\quad + \sum_{\emptyset \neq I \subsetneq (1, \dots, n)} (-1)^{|I^c|} \text{tr}(I) \text{tr}((I^c)^T), \end{aligned} \quad (3.8)$$

where I^c is the complement of the sublist I . The notation $I \subset (1, \dots, n)$ means that I is a sublist of $(1, \dots, n)$ with respect to which I is ordered. (In $SU(N)$, $\text{tr}(t^a) = 0$, so one can drop the cases with $|I| = 1$ and $|I| = n - 1$.) This relation has a nice diagrammatic representation in terms of color graphs using the double-line notation, as shown in fig. 1. As a reminder, in the double-line notation the rule is to sum all 2^n ways of attaching the n external lines to either the inner or outer ring of the annulus, with a minus sign for each attachment to the inner (\bar{F}) ring.

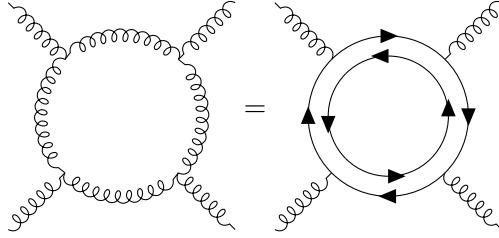


Figure 1: Graphical representation of the $SU(N)$ identity $G \oplus 1 \cong F \otimes \bar{F}$. The diagram on the right is evaluated by summing over all 2^n ways of attaching n external legs to either ring of the annulus, with a minus sign for each attachment to the inner (\bar{F}) ring.

When all external gluons have positive helicities, the color-ordered subamplitudes are finite, rational functions of spinor products $\langle ij \rangle$ and $[ij]$ given by [14, 15]

$$A_n^{[1]}(1, 2, \dots, n) = -\frac{i}{48\pi^2} \sum_{1 \leq i_1 < i_2 < i_3 < i_4 \leq n} \frac{\langle i_1 i_2 \rangle [i_2 i_3] \langle i_3 i_4 \rangle [i_4 i_1]}{\langle 12 \rangle \langle 23 \rangle \dots \langle n1 \rangle}, \quad (3.9)$$

$$A_n^{[1/2]}(1, 2, \dots, n) = -A_n^{[1]}(1, 2, \dots, n), \quad (3.10)$$

where we have taken $N_p = 2$ for $A_n^{[1]}$, where N_p is the number of bosonic states minus fermionic states. Eq. (3.10) is a supersymmetry Ward identity (SWI) [11–13] which holds in $D = 4$. At two loops, we will need to use dimensional regularization in $D = 4 - 2\epsilon$ spacetime dimensions, and we will need the one-loop result for $n = 4$ to higher orders in ϵ . For this purpose, a formula for the subamplitudes in terms of a dimensionally-regulated box integral is given in section 5.

3.2 Including Matter in $8F \oplus 8\bar{F} \oplus \wedge^2 F \oplus \wedge^2 \bar{F}$

According to ref. [49], including matter in the representation (1.1) should nullify the one-loop all-plus amplitude. This vanishing implies linear relations among the subamplitudes, which we wish to elucidate. To do so, we need to compute traces over the antisymmetric tensor representation in terms of traces over fundamental representation generators.

For this computation, we can simply replace the fermion loops in the fundamental representation that appear in the one-loop color graphs with loops in the representation (1.1). This

replacement is permitted for the following reason. Every Feynman diagram can be written as the product of a color factor and a kinematic factor. The Jacobi identity on the color factors can be used to remove color graphs with nontrivial trees attached to the loop [56], and thereby rewrite the matter contribution as a sum of permutations of the “ring” color diagram in fig. 2. Because the Jacobi identity is independent of the choice of representation of the fermion loop, we arrive at the same sum over color diagrams, with the same choice of fermion representation with which we began, without affecting the final kinematic factors. That is to say, $A_n^{[j]}$ depends solely on the spin of the particle propagating in the loop, not the representation of the Lie algebra in which it resides.

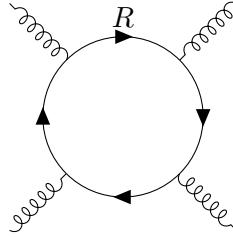


Figure 2: The one-loop color diagram for matter in an arbitrary representation R of $SU(N)$.

In other words, the contribution from matter in the representation (1.1) to the one-loop amplitude is

$$g^n \sum_{\sigma \in S_n / \mathbb{Z}_n} \text{tr}_{R_0}(\sigma_1 \cdots \sigma_n) A_n^{[1/2]}(\sigma_1, \dots, \sigma_n). \quad (3.11)$$

The color diagram $\text{tr}_{R_0}(\sigma_1 \cdots \sigma_n)$ associated to $A_n^{[1/2]}$ for this specific choice of representation is shown in fig. 3. The rectangle covering the lines appearing in the diagrams denotes antisymmetrization of those lines, as depicted in fig. 4. The trace over R_0 in terms of traces over the fundamental is worked out in Appendix A, and is

$$\begin{aligned} \text{tr}_{R_0}(t^{a_1} \cdots t^{a_n}) &= 8\text{tr}(1 \cdots n) + 8\text{tr}_{\bar{F}}(1 \cdots n) + \text{tr}_{\wedge^2 F}(1 \cdots n) + \text{tr}_{\wedge^2 \bar{F}}(1 \cdots n) \\ &= 8\text{tr}(1 \cdots n) + (-1)^n 8\text{tr}(n \cdots 1) + N\text{tr}(1 \cdots n) + (-1)^n N\text{tr}(n \cdots 1) \\ &\quad - \frac{1}{2} \sum_{I \subset (1, \dots, n)} [\text{tr}(I \cdot I^c) + (-1)^n \text{tr}((I \cdot I^c)^T)] \\ &\quad + \frac{1}{2} \sum_{\emptyset \neq I \subsetneq (1, \dots, n)} [\text{tr}(I)\text{tr}(I^c) + (-1)^n \text{tr}(I^T)\text{tr}((I^c)^T)], \end{aligned} \quad (3.12)$$

where $I \cdot I^c$ means to concatenate the lists I and I^c .

Combining the decomposition (3.8) of the adjoint pure-gluon contribution with the R_0

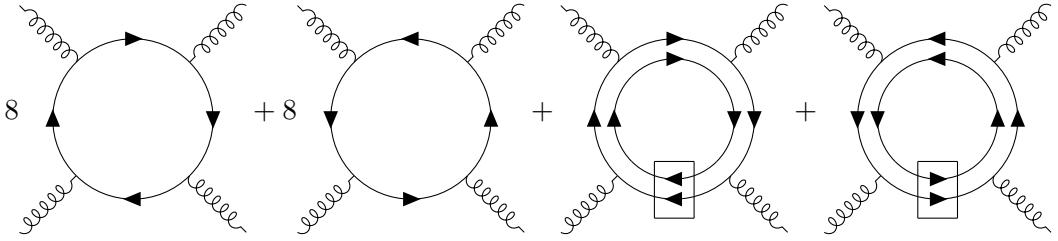


Figure 3: The one-loop color diagram for matter in the representation $R_0 = 8F \oplus \bar{F} \oplus \wedge^2 F \oplus \wedge^2 \bar{F}$.

$$\begin{array}{c} \text{---} \xrightarrow{\quad} \text{---} \xrightarrow{\quad} \\ \text{---} \xrightarrow{\quad} \text{---} \xrightarrow{\quad} \end{array} = \frac{1}{2} \left(\begin{array}{c} \text{---} \xrightarrow{\quad} \text{---} \xrightarrow{\quad} \\ \text{---} \xrightarrow{\quad} \text{---} \xrightarrow{\quad} \end{array} - \begin{array}{c} \text{---} \xrightarrow{\quad} \text{---} \xrightarrow{\quad} \\ \text{---} \xrightarrow{\quad} \text{---} \xrightarrow{\quad} \end{array} \right)$$

Figure 4: Graphical representation of the antisymmetric tensor product of the fundamental representation in terms of two fundamental lines.

matter contribution (3.12) yields

$$\begin{aligned} & \text{tr}_G(1 \cdots n) A_n^{[1]}(1, \dots, n) + \text{tr}_{R_0}(1 \cdots n) A_n^{[1/2]}(1, \dots, n) \\ &= -8 \text{tr}(1 \cdots n) A_n^{[1]}(1, \dots, n) - 8 \text{tr}(n \cdots 1) A_n^{[1]}(n, \dots, 1) \\ &+ \frac{1}{2} \sum_{I \subset (1, \dots, n)} [\text{tr}(I \cdot I^c) A_n^{[1]}(1, \dots, n) + \text{tr}((I \cdot I^c)^T) A_n^{[1]}(n, \dots, 1)] \\ &+ \frac{1}{2} \sum_{\emptyset \neq I \subsetneq (1, \dots, n)} [2\text{tr}(I)\text{tr}((I^c)^T) - \text{tr}(I)\text{tr}(I^c) - \text{tr}(I^T)\text{tr}((I^c)^T)] A_n^{[1]}(1, \dots, n), \end{aligned} \quad (3.13)$$

where we have used the SWI (3.10) and the reflection identity (3.7) obeyed by the subamplitude. The full amplitude is then given by the sum over all permutations on n letters, modulo permutations related by cycles and reflections.

We define the subamplitude $A_n^{R_0}(1, \dots, n)$ to be the kinematic factor multiplying the single-trace color factor $\text{tr}(1, \dots, n)$ in eq. (3.13). It is given by

$$A_n^{R_0}(1, \dots, n) = -8A_n^{[1]}(1, \dots, n) + \sum_{k=1}^n \sum_{\sigma \in \alpha_k \sqcup \beta_k} A_n^{[1]}(1, \sigma), \quad (3.14)$$

where $\alpha_k = (2, \dots, k)$ and $\beta_k = (k+1, \dots, n)$. The first term comes from the trace over eight copies of the fundamental. The remaining terms come from the exchange term in the trace

over the antisymmetric tensor representation,

$$\frac{1}{2} \text{tr}_{F \otimes F}(1 \cdots n P) = \frac{1}{2} \sum_{I \subset (1, \dots, n)} \text{tr}(I \cdot I^c), \quad (3.15)$$

where P is the permutation operator that exchanges the two F representations. In particular, the sum over k appears since the list $(1, \dots, k) = (1, \alpha_k)$ appears in the sum in eq. (3.15) for all $1 \leq k \leq n$. In Appendix C, we show that the subamplitude $A_n^{R_0}(1, \dots, n)$ is given by eq. (3.14).

Since the full amplitude vanishes for the fermion representation R_0 and the traces over the generators are linearly independent in $SU(N)$ (up to dihedral symmetries), eq. (3.14) must also vanish:

$$0 = -8A_n^{[1]}(1, \dots, n) + \sum_{k=1}^n \sum_{\sigma \in \alpha_k \sqcup \beta_k} A_n^{[1]}(1, \sigma). \quad (3.16)$$

Remarkably, these relations are exactly the same all-plus relations conjectured in ref. [50]. Ref. [50] based their formula³ on a decomposition into kinematic diagrams containing a single totally symmetric quartic vertex, and the remaining vertices are all cubic and totally anti-symmetric. If one accepts that the twistor-space anomaly cancellation implies the vanishing of the one-loop all-plus amplitude, then one obtains a proof of this conjecture. In a forthcoming paper [57], we analyze these all-plus relations, relations among one-loop one-minus amplitudes, as well as their connections to the twistor-space anomaly cancellation mechanism that uses a fourth-order pseudoscalar [48, 52, 53].

We can verify eq. (3.16) for the case $n = 4$. The $n = 4$ all-plus partial amplitude is

$$A_4^{[1]}(1, 2, 3, 4) = -\frac{i}{48\pi^2} \frac{[23][41]}{\langle 23 \rangle \langle 41 \rangle} = -\frac{\rho}{48\pi^2}. \quad (3.17)$$

This expression is totally symmetric, as shown in eq. (2.7). For general n , the number of terms appearing in the sum over k in eq. (3.16) is

$$\sum_{k=1}^n \binom{n-1}{k-1} = 2^{n-1}, \quad (3.18)$$

counting multiplicities. So, for $n = 4$, there are $2^3 = 8$ terms, all of which are equal, thanks to the total symmetry of the four-point subamplitude. These eight copies come with the opposite sign of the 8 terms not in the sum over k , resulting in a total of zero.

Because of the total kinematic symmetry of eq. (3.17), the above verification of eq. (3.16) for $n = 4$ is equivalent to checking the anomaly cancellation condition (1.2); both involve the same symmetrized trace over four generators in the appropriate representations.

³Note that the boundary terms $k = 1$ and $k = n$ have an empty set for α_k and for β_k , respectively, so they each just give $A_n^{[1]}(1, \dots, n)$. Removing them from the sum over k puts the formula into the precise form in ref. [50].

For $n > 4$, eq. (3.16) is not so easily verified from the explicit formula (3.9). We have checked [57] that it holds for $n \leq 11$ by replacing all spinor brackets with $3n - 10$ independent momentum-invariants, using a momentum-twistor-based parametrization [28, 58].

So far we have discussed the consequence of the all-plus vanishing for R_0 via the coefficient of the single trace $\text{tr}(1 \cdots n)$. However, eq. (3.13) also has a double-trace contribution, which must vanish as well. The relations among color-ordered amplitudes that follow from this vanishing imply the the vanishing of amplitudes with three photons and $(n-3)$ gluons observed previously [15]. We will discuss these double-trace relations in a forthcoming paper [57].

The vanishing of the one-loop amplitude in the R_0 theory suggests that the two-loop amplitude should be finite and rational; indeed, such behavior is found via the CCA bootstrap [49]. However, we will see that eq. (3.16) only holds at order ϵ^0 in dimensional regularization; it fails at higher orders in ϵ , for the case $n = 4$ (see section 5). Consequently, the IR structure of the dimensionally-regulated two-loop result is more intricate, and not even finite as $\epsilon \rightarrow 0$.

4 The 2-loop 4-gluon amplitude

We now turn to the computation of the two-loop all-plus four-gluon amplitude for fermions in the representation R_0 .

Our starting point is the two-loop four-gluon amplitude in QCD, which is given in ref. [59] as

$$\mathcal{A}_{4,\text{QCD}}^{\text{2-loop}} = \mathcal{A}_G^{\text{adj}} + \mathcal{A}_F^{\text{fund}}, \quad (4.1)$$

where $\mathcal{A}_G^{\text{adj}}$ is the adjoint gluon contribution and $\mathcal{A}_F^{\text{fund}}$ is the fundamental matter contribution. Each particle contribution above can be decomposed into a sum of “parent” diagrams,

$$\mathcal{A}_X^{\text{rep}} = g^6 \sum_{D_i} \left[(C_{\text{rep}})_{1234}^{D_i} A_{X1234}^{D_i} + (C_{\text{rep}})_{3421}^{D_i} A_{X3421}^{D_i} \right] + \mathcal{C}(234), \quad (4.2)$$

where each D_i corresponds to a parent diagram. The subscript $X \in \{G, F\}$ denotes either the pure-gluon contribution G , or a fermion F propagating in at least one of the two loops in the diagrams. The quantities C_{rep} denote the color factors associated to the kinematic factors A_X , with “rep” signifying the gauge group representation in which particle X resides. The F parent diagrams span the space of all independent four-gluon color-factors with a fermion-loop contribution and a non-vanishing kinematic factor. This result can be shown by applying the Jacobi identity suitably to color diagrams containing triangle subdiagrams.

We want to compute the two-loop four-gluon amplitude with matter in the representation R_0 ,

$$\mathcal{A}_4^{\text{2-loop}} = \mathcal{A}_G^{\text{adj}} + \mathcal{A}_F^{R_0}. \quad (4.3)$$

4.1 Pure gauge contribution

The color decomposition of the pure Yang-Mills two-loop four-point amplitude is [26, 59]

$$\mathcal{A}_G^{\text{adj}} = g^6 \left(C_{1234}^P A_{G1234}^P + C_{3421}^P A_{G3421}^P + C_{1234}^{NP} A_{G1234}^{NP} + C_{3421}^{NP} A_{G3421}^{NP} \right) + \mathcal{C}(234), \quad (4.4)$$

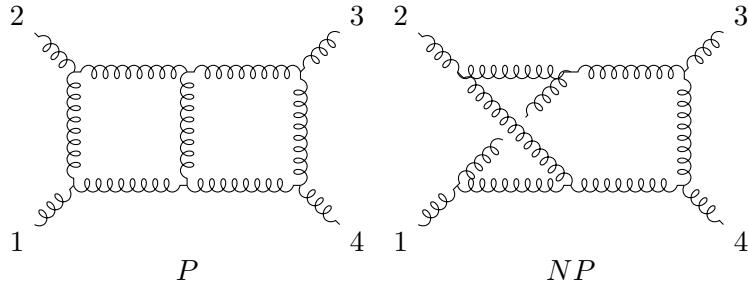


Figure 5: The planar (P) and non-planar (NP) parent color diagrams for the pure-gauge two-loop amplitude.

where C_{1234}^P and C_{1234}^{NP} are color factors given by the planar and non-planar parent diagrams in fig. 5. They are computed by dressing each vertex and each propagator with the diagrammatic rules given in eq. (A.3).

The color factors evaluate to

$$C_{1234}^P = (N^2 + 2)[\text{tr}(1234) + \text{tr}(1432)] + 2[\text{tr}(1243) + \text{tr}(1342)] - 4[\text{tr}(1324) + \text{tr}(1423)] + 6N\text{tr}(12)\text{tr}(34), \quad (4.5)$$

$$C_{1234}^{NP} = 2[\text{tr}(1234) + \text{tr}(1432) + \text{tr}(1243) + \text{tr}(1342)] - 4[\text{tr}(1324) + \text{tr}(1423)] + 2N[2\text{tr}(12)\text{tr}(34) - \text{tr}(13)\text{tr}(24) - \text{tr}(14)\text{tr}(23)]. \quad (4.6)$$

These color factors have the following symmetries, which will prove useful in section 5:

$$C_{1234}^P = C_{3412}^P = C_{2143}^P = C_{4321}^P, \\ C_{1234}^{NP} = C_{2134}^{NP} = C_{1243}^{NP} = C_{2143}^{NP}. \quad (4.7)$$

The planar and non-planar primitive amplitudes are given by

$$A_{G1234}^P = \rho \left\{ s(D_s - 2)\mathcal{I}_4^P \left[\lambda_p^2 \lambda_{p+q}^2 + \lambda_q^2 \lambda_{p+q}^2 \right] (s, t) + \frac{(D_s - 2)^2}{s} \mathcal{I}_4^{\text{bow-tie}} \left[\lambda_p^2 \lambda_q^2 ((p+q)^2 + s) \right] (s, t) \right\}, \\ A_{G1234}^{NP} = \rho s(D_s - 2)\mathcal{I}_4^{NP} \left[\lambda_p^2 \lambda_q^2 + \lambda_p^2 \lambda_{p+q}^2 + \lambda_q^2 \lambda_{p+q}^2 \right], \quad (4.8)$$

where we have only included non-vanishing terms at $\mathcal{O}(\epsilon^0)$ in the integral. The three two-loop momentum integrals that appear above are the planar double box integral \mathcal{I}_4^P , the non-planar double box integral \mathcal{I}_4^{NP} , and the bow-tie integral $\mathcal{I}_4^{\text{bow-tie}}$. They are shown in fig. 6 and are defined by,

$$\mathcal{I}_4^P[\mathcal{P}(\lambda_i, p, q, k_i)](s, t) = \int \frac{d^D p}{(2\pi)^D} \frac{d^D q}{(2\pi)^D} \frac{\mathcal{P}(\lambda_i, p, q, k_i)}{p^2 q^2 (p+q)^2 (p-k_1)^2 (p-k_1-k_2)^2 (q-k_4)^2 (q-k_3-k_4)^2}, \quad (4.9)$$

$$\begin{aligned} \mathcal{I}_4^{NP}[\mathcal{P}(\lambda_i, p, q, k_i)](s, t) \\ = \int \frac{d^D p}{(2\pi)^D} \frac{d^D q}{(2\pi)^D} \frac{\mathcal{P}(\lambda_i, p, q, k_i)}{p^2 q^2 (p+q)^2 (p-k_1)^2 (q-k_2)^2 (p+q+k_3)^2 (p+q+k_3+k_4)^2}, \end{aligned} \quad (4.10)$$

and

$$\begin{aligned} \mathcal{I}_4^{\text{bow-tie}}[\mathcal{P}(\lambda_i, p, q, k_i)](s, t) \\ = \int \frac{d^D p}{(2\pi)^D} \frac{d^D q}{(2\pi)^D} \frac{\mathcal{P}(\lambda_i, p, q, k_i)}{p^2 q^2 (p-k_1)^2 (p-k_1-k_2)^2 (q-k_4)^2 (q-k_3-k_4)^2}, \end{aligned} \quad (4.11)$$

where the k_i are the external momenta. The numerator factor $\mathcal{P}(\lambda_i, p, q, k_i)$ is a polynomial in the external and loop momenta. The vectors λ_p and λ_q represent the (-2ϵ) -dimensional components of the loop momenta p and q . We use the notation $\lambda_i^2 = \lambda_i \cdot \lambda_i \geq 0$ and $\lambda_{p+q}^2 = (\lambda_p + \lambda_q)^2 = \lambda_p^2 + \lambda_q^2 + 2\lambda_p \cdot \lambda_q$. The explicit values of these integrals, as a series in ϵ and expressed in terms of polylogarithms, are given in appendix A of ref. [26]. We provide the bow-tie integrals in eq. (4.23) and the remaining ones in appendix D of this manuscript. The symmetries obeyed by the color factors (4.7) carry over to the primitive amplitudes (4.8).

4.2 Matter Contribution

In order to compute the color factors for the fermionic matter contribution in the representation R_0 , one can simply replace the fundamental loops appearing in the parent diagrams with a loop in R_0 . This replacement is allowed, because one can rewrite any color diagram in terms of parent diagrams using only Jacobi identities, which are independent of the fermion representation. We denote the color factor given by a diagram D_i with matter representation R_0 by $R_{1234}^{D_i}$. The color decomposition for the amplitude is then

$$\mathcal{A}_F^{R_0} = g^6 \sum_{D_i} \left(R_{1234}^{D_i} A_{F1234}^{D_i} + R_{3421}^{D_i} A_{F3421}^{D_i} \right) + \mathcal{C}(234), \quad (4.12)$$

where the seven parent diagrams D_i are given in fig. 7. The full color factor R^{D_i} also has the addition of the same diagram but with the matter representation arrows pointing in the

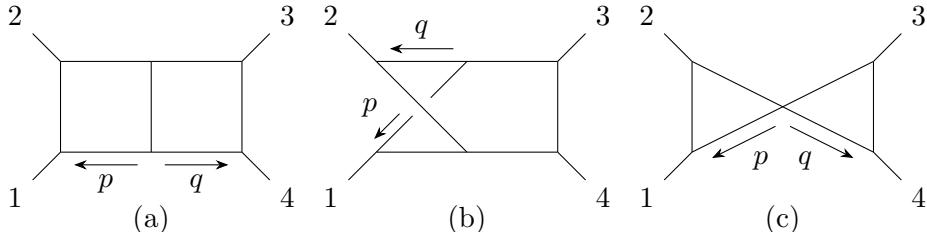


Figure 6: The three scalar integral topologies appearing in the two-loop all-plus amplitude, with the loop-momentum routings displayed: (a) the planar double box; (b) the non-planar double box; (c) the bow-tie.

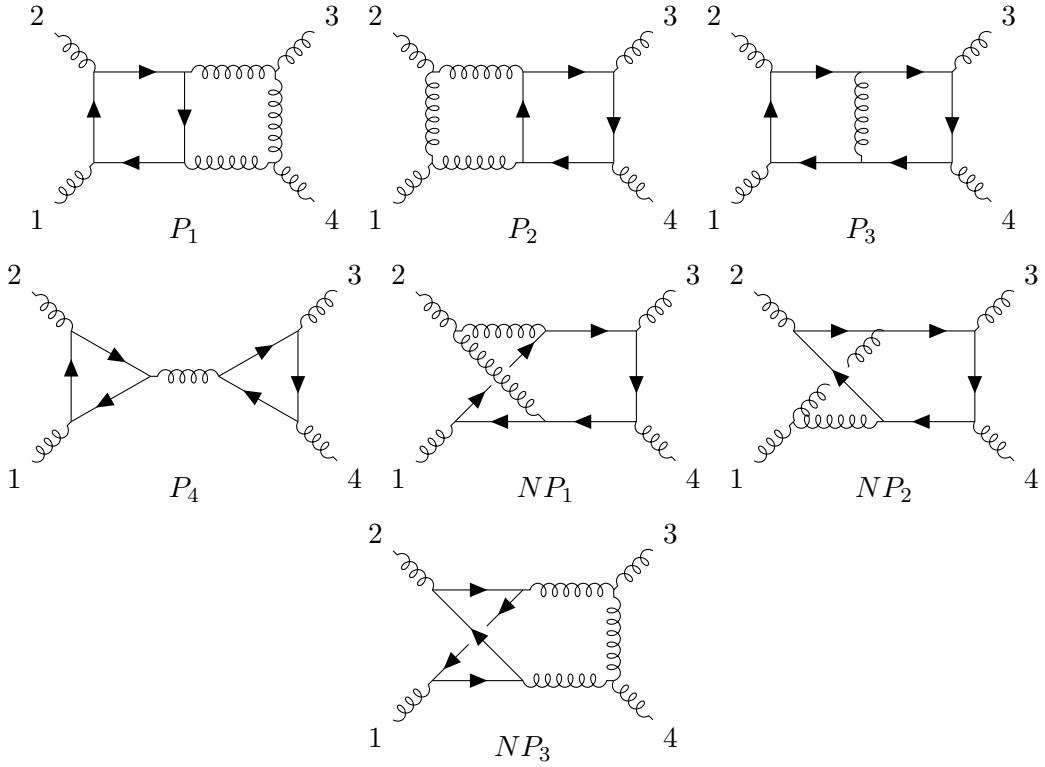


Figure 7: Parent diagrams for the fermion loop R_0 contributions.

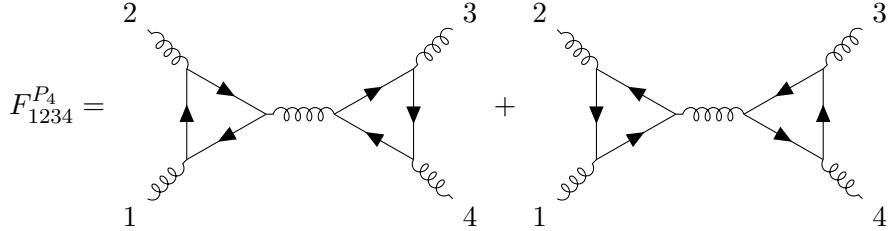


Figure 8: The total contribution to F_{1234}^{P4} . Notice that the terms $\text{tr}_F(12c)\text{tr}_{\bar{F}}(c34)$ and $\text{tr}_{\bar{F}}(12c)\text{tr}_F(c34)$ with partially-reversed arrows do not contribute to its value.

opposite direction. The color factors are then evaluated in terms of traces in the fundamental with no contracted indices, using the rules given in eq. (A.3).

There is an exception to the evaluation procedure for R_{1234}^{P4} , since we follow the conventions of ref. [59]. In that reference, the color factors were evaluated by adding to the diagram P_4 the contribution of the anti-fundamental representation only, i.e. they reverse the direction of the two arrows simultaneously. In particular, the full diagrammatic color factor for F_{1234}^{P4} is in fig. 8. Notice that the $F \times \bar{F}$ and $\bar{F} \times F$ cross terms are not to be included;

their contributions are already included in the definition of the kinematic factor $A_{F1234}^{P_4}$. We must account for this convention by not including any terms of the form $F \times \bar{F}$, $F \times \wedge^2 \bar{F}$, $\wedge^2 F \times \wedge^2 \bar{F}$, and their conjugates in $R_{1234}^{P_4}$. Thus, $R_{1234}^{P_4}$ is given by

$$\begin{aligned} R_{1234}^{P_4} = & 8^2 \text{tr}_F(12c) \text{tr}_F(c34) + 8 \text{tr}_F(12c) \text{tr}_{\wedge^2 F}(c34) \\ & + 8 \text{tr}_{\wedge^2 F}(12c) \text{tr}_F(c34) + \text{tr}_{\wedge^2 F}(12c) \text{tr}_{\wedge^2 F}(c34) \\ & + \text{conjugate.} \end{aligned} \quad (4.13)$$

With some help from trace identities provided in Appendix A, the results are

$$\begin{aligned} R_{1234}^{P_1} = & (N^2 + 4N + 2) [\text{tr}(1234) + \text{tr}(1432)] \\ & + (-2N + 2) [\text{tr}(1243) + \text{tr}(1342)] - 4 [\text{tr}(1324) + \text{tr}(1423)] \\ & + (6N + 4) \text{tr}(12) \text{tr}(34) + 4 [\text{tr}(13) \text{tr}(24) + \text{tr}(14) \text{tr}(23)], \end{aligned} \quad (4.14)$$

$$R_{1234}^{P_2} = R_{1234}^{P_1}, \quad (4.15)$$

$$\begin{aligned} R_{1234}^{P_3} = & (N^2 - 6N + 6 + 8N^{-1}) [\text{tr}(1234) + \text{tr}(1432)] \\ & + (-2N + 6 + 8N^{-1}) [\text{tr}(1243) + \text{tr}(1342)] + 8N^{-1} [\text{tr}(1324) + \text{tr}(1423)] \\ & + (6N - 8N^{-1}) \text{tr}(12) \text{tr}(34) - 8N^{-1} [\text{tr}(13) \text{tr}(24) + \text{tr}(14) \text{tr}(23)], \end{aligned} \quad (4.16)$$

$$\begin{aligned} R_{1234}^{P_4} = & (N^2 + 10N + 26) [\text{tr}(1234) + \text{tr}(1432)] + (-2N - 10) [\text{tr}(1243) + \text{tr}(1342)] \\ & + (-2N - 16 - 32N^{-1}) \text{tr}(12) \text{tr}(34), \end{aligned} \quad (4.17)$$

$$\begin{aligned} R_{1234}^{NP_1} = & 2 [\text{tr}(1234) + \text{tr}(1432) + \text{tr}(1243) + \text{tr}(1342)] \\ & + (2N - 4) [\text{tr}(1324) + \text{tr}(1423)] \\ & + (4N + 4) \text{tr}(12) \text{tr}(34) + (-2N + 4) [\text{tr}(13) \text{tr}(24) + \text{tr}(14) \text{tr}(23)], \end{aligned} \quad (4.18)$$

$$R_{1234}^{NP_2} = R_{1234}^{NP_1}, \quad (4.19)$$

$$\begin{aligned} R_{1234}^{NP_3} = & (-2N + 2) [\text{tr}(1234) + \text{tr}(1432) + \text{tr}(1243) + \text{tr}(1342)] \\ & - 4 [\text{tr}(1324) + \text{tr}(1423)] \\ & + (4N - 8) \text{tr}(12) \text{tr}(34) + (-2N - 8) [\text{tr}(13) \text{tr}(24) + \text{tr}(14) \text{tr}(23)]. \end{aligned} \quad (4.20)$$

The color factors $R_{1234}^{P_1} = R_{1234}^{P_2}$ and $R_{1234}^{NP_3}$ also have the same symmetries as C^P and C^{NP} , respectively, in eq. (4.7):

$$\begin{aligned} R_{1234}^{P_1} = R_{3412}^{P_1} = R_{2143}^{P_1} = R_{4321}^{P_1}, \\ R_{1234}^{NP_3} = R_{2134}^{NP_3} = R_{1243}^{NP_3} = R_{2143}^{NP_3}. \end{aligned} \quad (4.21)$$

Again, this is evident directly from the diagrams by applying rotations and reflections to them, as well as using $R_{1234}^{P_1} = R_{1234}^{P_2}$.

The primitive amplitudes associated to each diagram D_i are given in ref. [59]; however many of the integrals that compose them vanish. Removing the integrals that vanish at $\mathcal{O}(\epsilon^0)$,

the primitive amplitudes are

$$\begin{aligned}
A_{F1234}^{P_1} &= \rho \left\{ s \mathcal{I}_4^P \left[-2\lambda_p^2 \lambda_{p+q}^2 \right] (s, t) \right. \\
&\quad \left. - 2 \frac{D_s - 2}{s} \mathcal{I}_4^{\text{bow-tie}} \left[\lambda_p^2 \lambda_q^2 ((p+q)^2 + s) \right] (s, t) \right\}, \\
A_{F1234}^{P_2} &= \rho \left\{ s \mathcal{I}_4^P \left[-2\lambda_q^2 \lambda_{p+q}^2 \right] (s, t) \right. \\
&\quad \left. - 2 \frac{D_s - 2}{s} \mathcal{I}_4^{\text{bow-tie}} \left[\lambda_p^2 \lambda_q^2 ((p+q)^2 + s) \right] (s, t) \right\}, \\
A_{F1234}^{P_3} &= \rho (D_s - 2) \mathcal{I}_4^{\text{bow-tie}} \left[\lambda_p^2 \lambda_q^2 \right] (s, t), \\
A_{F1234}^{P_4} &= \rho \frac{4}{s} \mathcal{I}_4^{\text{bow-tie}} \left[\lambda_p^2 \lambda_q^2 ((p+q)^2 + \frac{1}{2}s) \right] (s, t), \\
A_{F1234}^{NP_1} &= \rho s \mathcal{I}_4^{NP} \left[-2\lambda_p^2 \lambda_{p+q}^2 \right] (s, t), \\
A_{F1234}^{NP_2} &= \rho s \mathcal{I}_4^{NP} \left[-2\lambda_q^2 \lambda_{p+q}^2 \right] (s, t), \\
A_{F1234}^{NP_3} &= \rho s \mathcal{I}_4^{NP} \left[-2\lambda_p^2 \lambda_q^2 \right] (s, t).
\end{aligned} \tag{4.22}$$

The bow-tie integrals are quite simple, as they are products of one-loop triangle integrals, and are given by [26]

$$\begin{aligned}
\mathcal{I}_4^{\text{bow-tie}} [\lambda_p^2 \lambda_q^2] (s, t) &= -\frac{1}{4} \frac{1}{(4\pi)^4}, \\
\mathcal{I}_4^{\text{bow-tie}} [\lambda_p^2 \lambda_q^2 (p+q)^2] (s, t) &= -\frac{1}{36} \frac{1}{(4\pi)^4} (t - 4s).
\end{aligned} \tag{4.23}$$

We provide the results for the remaining integrals from ref. [26] in appendix D. The primitive amplitudes $A_{F1234}^{P_1}$, $A_{F1234}^{P_2}$, and $A_{F1234}^{NP_3}$ obey the same relations as their corresponding color factors in eq. (4.21). For later use, notice that these amplitudes are the only ones out of the matter contribution that contain $1/\epsilon$ poles.

4.3 The full amplitude

The two-loop four-gluon amplitude with fermionic matter in the representation R_0 is the sum of eqs. (4.12) and (4.4). Using the values of the color factors given above, we have

$$\begin{aligned}
\mathcal{A}_4^{\text{2-loop}} &= g^6 \sum_{\sigma \in S_4 / \mathbb{Z}_4} A_{4;1}^{\text{2-loop}} (\sigma(1, 2, 3, 4)) \text{tr}(\sigma(1, 2, 3, 4)) \\
&\quad + g^6 \sum_{\sigma \in S_4 / S_{4;3}} A_{4;3}^{\text{2-loop}} (\sigma(1, 2, 3, 4)) \text{tr}(\sigma(1, 2)) \text{tr}(\sigma(3, 4)),
\end{aligned} \tag{4.24}$$

where the $A_{4;c}^{\text{2-loop}}$, $c = 1, 3$ are the two-loop color-ordered subamplitudes. The $A_{4;c}$ contain various powers of N , so we separate them into these different powers as

$$A_{4;c}^{\text{2-loop}} = A_{4;c;2} N^2 + A_{4;c;1} N + A_{4;c;0} + A_{4;c;-1} N^{-1}. \tag{4.25}$$

Of course, the $A_{4;c;i}$ are linear combinations of the primitive amplitudes $A_{G1234}^{D_i}$ and $A_{F1234}^{D_i}$, which are given by

$$A_{4;1;2}(1, 2, 3, 4) = A_{G1234}^P + A_{G2341}^P + \sum_{i=1}^4 (A_{F1234}^{P_i} + A_{F2341}^{P_i}), \quad (4.26)$$

$$\begin{aligned} A_{4;1;1}(1, 2, 3, 4) = & 2A_{F1234}^Z + 2A_{F2341}^Z - 2A_{F1234}^{NP_3} - 2A_{F2341}^{NP_3} \\ & - 2A_{F3421}^{NP_3} - 2A_{F1423}^{NP_3} - 2 \sum_{i=1}^4 (A_{F3421}^{P_i} + A_{F1423}^{P_i}) \\ & + 2A_{F1342}^{NP_1} + 2A_{F1342}^{NP_2} + 2A_{F4231}^{NP_1} + 2A_{F4231}^{NP_2}, \end{aligned} \quad (4.27)$$

$$\begin{aligned} A_{4;1;0}(1, 2, 3, 4) = & 2A_{1234}^{\text{all}} + 2A_{3421}^{\text{all}} - 4A_{1342}^{\text{all}} - 4A_{4231}^{\text{all}} + 2A_{1423}^{\text{all}} + 2A_{2341}^{\text{all}} \\ & + 4(A_{F1234}^{P_3} + \text{perms}) \\ & + 24A_{F1234}^{P_4} - 12A_{F3421}^{P_4} + 4A_{F1342}^{P_4} \\ & + 4A_{F4231}^{P_4} - 12A_{F1423}^{P_4} + 24A_{F2341}^{P_4}, \end{aligned} \quad (4.28)$$

$$A_{4;1;-1}(1, 2, 3, 4) = 8(A_{F1234}^{P_3} + \text{perms}), \quad (4.29)$$

$$A_{4;3;2}(1, 2, 3, 4) = 0, \quad (4.30)$$

$$\begin{aligned} A_{4;3;1}(1, 2, 3, 4) = & 6A_{1234}^{\text{all}} + 6A_{3421}^{\text{all}} - 6A_{F1234}^{P_4} - 6A_{F3421}^{P_4} \\ & - 2(A_{G1234}^{NP} + \sum_{i=1}^3 A_{F1234}^{NP_i} + \text{perms}), \end{aligned} \quad (4.31)$$

$$\begin{aligned} A_{4;3;0}(1, 2, 3, 4) = & 4(A_{F1234}^{P_1} + A_{F1234}^{P_2} + A_{F1234}^{NP_1} + A_{F1234}^{NP_2} - 2A_{F1234}^{NP_3} + \text{perms}) \\ & - 16A_{F1234}^{P_4} - 16A_{F3421}^{P_4}, \end{aligned} \quad (4.32)$$

$$A_{4;3;-1}(1, 2, 3, 4) = -8(A_{F1234}^{P_3} + \text{perms}) - 32A_{F1234}^{P_4} - 32A_{F3421}^{P_4}, \quad (4.33)$$

where $A_{1234}^{\text{all}} = A_{G1234}^P + A_{G1234}^{NP} + \sum_{D_i} A_{F1234}^{D_i}$, the sum of all 9 primitive amplitudes, and

$$A_{F1234}^Z \equiv 2A_{F1234}^{P_1} + 2A_{F1234}^{P_2} - 3A_{F1234}^{P_3} + 5A_{F1234}^{P_4}. \quad (4.34)$$

The term “+perms” means to add all non-trivial permutations

$$(3, 4, 2, 1), (1, 3, 4, 2), (4, 2, 3, 1), (1, 4, 2, 3), (2, 3, 4, 1), \quad (4.35)$$

of the preceding terms inside the parentheses.

4.4 Dimensional regularization scheme

The primitive amplitudes are evaluated in refs. [26, 59] using dimensional regularization with the loop momentum being in $D = 4 - 2\epsilon > 4$ dimensions. The dimension of the “unobserved” internal gluonic states D_s is left explicit in their results, with $D_s \geq D$ in intermediate steps of their calculation. The unobserved states include virtual states in loops and virtual intermediate states in trees. Setting $D_s = D$ corresponds to the standard ’t Hooft-Veltman (HV) scheme. In the four-dimensional helicity (FDH) scheme, one would set $D_s = 4$.

The choice of D_s affects the compliance of the amplitudes with supersymmetry Ward identities (SWI) [11–13]. In particular, preserving the number of bosonic states relative to the fermionic states is necessary for preserving the SWI, and the choice $D_s = 4$ achieves this [59]. The SWI manifest themselves in terms of the primitive amplitudes as

$$\begin{aligned} A_{G1234}^P + \sum_{i=1}^4 A_{F1234}^{P_i} &= 0, \\ A_{G1234}^{NP} + \sum_{i=1}^3 A_{F1234}^{NP_i} &= 0 \end{aligned} \quad (4.36)$$

in the $\epsilon \rightarrow 0$ limit. These identities do not hold in the HV scheme. Applying the constraints in eq. (4.36) simplifies the $A_{4;c;i}$ considerably, and we get agreement with eq. (1.3) at order N^2 . Moreover, the choice $D_s = 4$ forces the one-loop partial amplitudes $A_n^{[1]}$ and $A_n^{[1/2]}$ to be equal with opposite signs to all orders in ϵ . For these reasons, we take $D_s = 4$ when evaluating the linear combinations of primitive amplitudes.

When eq. (4.36) is applied, the expressions for the $A_{4;c;i}$ in terms of the primitive amplitudes simplify to

$$A_{4;1;2}(1, 2, 3, 4) = 0, \quad (4.37)$$

$$\begin{aligned} A_{4;1;1}(1, 2, 3, 4) &= 2A_{F1234}^Z + 2A_{F2341}^Z - 2A_{F1234}^{NP_3} - 2A_{F2341}^{NP_3} \\ &\quad - 2A_{F3421}^{NP_3} - 2A_{F1423}^{NP_3} - 2 \sum_{i=1}^4 (A_{F3421}^{P_i} + A_{F1423}^{P_i}) \\ &\quad + 2A_{F1342}^{NP_1} + 2A_{F1342}^{NP_2} + 2A_{F4231}^{NP_1} + 2A_{F4231}^{NP_2}, \end{aligned} \quad (4.38)$$

$$A_{4;1;0}(1, 2, 3, 4) = 4(A_{F1234}^{P_3} + \text{perms}) + 36A_{F1234}^{P_4} + 36A_{F2341}^{P_4}, \quad (4.39)$$

$$A_{4;1;-1}(1, 2, 3, 4) = 8(A_{F1234}^{P_3} + \text{perms}), \quad (4.40)$$

$$A_{4;3;2}(1, 2, 3, 4) = 0, \quad (4.41)$$

$$A_{4;3;1}(1, 2, 3, 4) = 0, \quad (4.42)$$

$$A_{4;3;0}(1, 2, 3, 4) = 4(A_{F1234}^{P_1} + A_{F1234}^{P_2} + A_{F1234}^{NP_1} + A_{F1234}^{NP_2} - 2A_{F1234}^{NP_3} + \text{perms}), \quad (4.43)$$

$$A_{4;3;-1}(1, 2, 3, 4) = -8(A_{F1234}^{P_3} + \text{perms}), \quad (4.44)$$

where we also made use of the fact that $A_{F1234}^{P_4} = -A_{F3421}^{P_4}$, which follows from the reflection identity of the associated color factor, $F_{1234}^{P_4} = -F_{3421}^{P_4}$.

4.5 Evaluating the $A_{4;c;i}$

The vanishing of $A_{4;1;2}$, $A_{4;3;2}$, and $A_{4;3;1}$ agrees with eq. (1.3). Using the expressions given in eqs. (4.22) and (4.23), we see that $A_{4;1;0}$, $A_{4;1;-1}$, and $A_{4;3;-1}$ are finite and rational. They

evaluate to

$$A_{4;1;0}(1, 2, 3, 4) = -\frac{4\rho}{(4\pi)^4} \frac{s^2 + 4st + t^2}{st}, \quad (4.45)$$

$$A_{4;1;-1}(1, 2, 3, 4) = -\frac{24\rho}{(4\pi)^4}, \quad (4.46)$$

$$A_{4;3;-1}(1, 2, 3, 4) = \frac{24\rho}{(4\pi)^4}, \quad (4.47)$$

agreeing with eq. (1.3) at the corresponding powers of N .

The two remaining linear combinations of the primitive amplitudes, $A_{4;1;1}$ and $A_{4;3;0}$, do not simplify further using the SWI, and they explicitly contain non-finite and non-rational primitive amplitudes (see appendix D). Schematically, they are of the form

$$A_{4;1;1}(1, 2, 3, 4) = \frac{12\rho}{(4\pi)^4} + \frac{1}{\epsilon} \text{transcendental} + \text{transcendental} + \mathcal{O}(\epsilon), \quad (4.48)$$

and

$$A_{4;3;0}(1, 2, 3, 4) = \frac{24\rho}{(4\pi)^4} + \text{transcendental} + \mathcal{O}(\epsilon), \quad (4.49)$$

where transcendental refers to terms that (after multiplying by $(4\pi)^4$) contain products of \ln , Li_2 , and Li_3 , which have as their arguments $\pm t/s$, $1 + t/s$, and $t/(s + t)$ and which have rational coefficients in t/s .

These expressions clearly do not agree with eq. (1.3), because they have transcendental terms and/or $1/\epsilon$ poles, along with the rational terms shown explicitly, which do appear in eq. (1.3). This might at first seem to invalidate eq. (1.3). However, a comparison of the whole amplitude with the expected universal IR behavior of two-loop amplitudes given by [51] sheds light on the matter. We carry out this comparison next.

5 IR subtraction

In this section, we compare the IR behavior of eqs. (4.48) and (4.49) to that predicted on general principles. We follow closely the analysis in section 5 of ref. [26]. The principal issue is that the IR behavior of a two-loop amplitude in dimensional regularization involves $1/\epsilon^2$ poles multiplying the one-loop amplitude, so that higher order terms in ϵ are required. And while the one-loop amplitude in our case vanishes at $\mathcal{O}(\epsilon^0)$, it does *not* vanish at higher orders in ϵ , because the box integrals that enter it do not have the same symmetry properties beyond leading order in ϵ .

Catani provides a universal factorization formula for dimensionally regulated, UV-renormalized two-loop amplitudes [51]. In the color-space operator formalism, the renormalized two-loop n -point amplitude is given by

$$\begin{aligned} |\mathcal{M}_n^{(2)}(\mu^2; \{p\})\rangle_{\text{R.S.}} &= \mathbf{I}^{(1)}(\epsilon, \mu^2; \{p\})|\mathcal{M}_n^{(1)}(\mu^2; \{p\})\rangle_{\text{R.S.}} \\ &+ \mathbf{I}_{\text{R.S.}}^{(2)}(\epsilon, \mu^2; \{p\})|\mathcal{M}_n^{(0)}(\mu^2; \{p\})\rangle_{\text{R.S.}} + |\mathcal{M}_n^{(2),\text{fin}}(\mu^2; \{p\})\rangle_{\text{R.S.}}, \end{aligned} \quad (5.1)$$

where $|\mathcal{M}_n^{(L)}(\mu^2; \{p\})\rangle_{\text{R.S.}}$ is the vector in color space that represents the renormalized L -loop amplitude. The subscript R.S. signifies a dependence on the renormalization scheme, and μ is the renormalization mass scale. For notational simplicity, we set $\mu = 1$. The amplitudes are recovered by

$$\mathcal{A}_n(1^{a_1}, \dots, n^{a_n}) = \langle a_1, \dots, a_n | \mathcal{M}_n(p_1, \dots, p_n) \rangle, \quad (5.2)$$

where the a_i is the color index of the i -th external parton.

The operators $\mathbf{I}^{(1)}$ and $\mathbf{I}^{(2)}$ encode the IR divergences of \mathcal{A}_n . For all-plus helicity external gluons, the tree-level amplitude $\mathcal{M}_n^{(0)}(\mu^2; \{p\})$ vanishes, meaning that only $\mathbf{I}^{(1)}$ contributes to the divergences. This operator is given by

$$\mathbf{I}^{(1)}(\epsilon; \{p\}) = \frac{c_\Gamma}{2} \sum_{i=1}^n \sum_{j \neq i}^n \mathbf{T}_i \cdot \mathbf{T}_j \left[\frac{1}{\epsilon^2} \left(\frac{e^{-i\lambda_{ij}\pi}}{s_{ij}} \right)^\epsilon + 2 \frac{\gamma_i}{\mathbf{T}_i^2} \frac{1}{\epsilon} \right], \quad (5.3)$$

where $\lambda_{ij} = +1$ if i and j are both incoming or outgoing partons and $\lambda_{ij} = 0$ otherwise. The factor c_Γ is

$$c_\Gamma = \frac{1}{(4\pi)^{2-\epsilon}} \frac{\Gamma(1+\epsilon)\Gamma^2(1-\epsilon)}{\Gamma(1-2\epsilon)}. \quad (5.4)$$

The color charge $\mathbf{T}_i = \{T_i^a\}$ is a vector with respect to the generator label a and an $SU(N)$ matrix with respect to the color indices of the outgoing parton i . For the adjoint representation $T_{bc}^a = if^{bac}$, so $\mathbf{T}_i^2 = C_A = 2T_F N$.

For external gluons, $\gamma_i = b_0$, where b_0 is the one-loop β -function coefficient. For QCD with N_F quark flavors,

$$b_0^{\text{QCD}} = \frac{11C_A - 4T_F N_F}{6}, \quad (5.5)$$

and for fermions in the representation R_0 (see eq. (A.19)),

$$b_0^{R_0} = \frac{11C_A - 4T_F N_F - 4T_{\wedge^2 F} N_{\wedge^2 F}}{6} \Big|_{T_F=1, N_F=8, T_{\wedge^2 F}=N-2, N_{\wedge^2 F}=1} = 3N - 4. \quad (5.6)$$

Note that eq. (5.3) differs slightly from Catani's original formula. We have defined our structure constants such that they are greater by a factor of $\sqrt{2}$, and we have included a factor of $2c_\Gamma$ instead of $e^{\epsilon\gamma}$ due to a different normalization convention for the coupling expansion parameter (g^2 vs. Catani's $\alpha_s/(2\pi) = g^2/(8\pi^2)$).

For external gluons of positive helicity only, we can rewrite the predicted divergent part of the renormalized two-loop amplitude in our notation as

$$\mathcal{A}_n^{\text{2-loop, ren.}}(1^{a_1}, \dots, n^{a_n}) \Big|_{\text{pred. div.}} = g^2 \sum_{1 \leq i < j \leq n} \mathcal{A}_n^{(i,j)}(1, \dots, n), \quad (5.7)$$

where

$$\begin{aligned} \mathcal{A}_n^{(i,j)}(1, \dots, n) &= c_\Gamma (if^{a_i c b_i})(if^{a_j c b_j}) \left[\frac{1}{\epsilon^2} (-s_{ij})^{-\epsilon} + 2 \frac{b_0^{R_0}}{C_A} \frac{1}{\epsilon} \right] \\ &\quad \times \mathcal{A}_n^{\text{1-loop}}(1^{a_1}, \dots, i^{b_i}, \dots, j^{b_j}, \dots, n^{a_n}) \end{aligned} \quad (5.8)$$

acts on the colors of legs i and j . Specializing to four points, we only need to evaluate the case $(i, j) = (1, 2)$,

$$\begin{aligned}\mathcal{A}_4^{(1,2)}(1^{a_1}, 2^{a_2}, 3^{a_3}, 4^{a_4}) &= c_\Gamma(if^{a_1 cb_1})(if^{a_2 cb_2}) \left[\frac{1}{\epsilon^2}(-s)^{-\epsilon} + 2\frac{b_0^{R_0}}{C_A} \frac{1}{\epsilon} \right] \\ &\quad \times \mathcal{A}_4^{\text{1-loop}}(1^{b_1}, 2^{b_2}, 3^{a_3}, 4^{a_4}),\end{aligned}\quad (5.9)$$

as the other five cases are obtained by relabeling i and j .

It should be noted that there are two conventions for the placement of $(e^{-i\lambda_{ij}\pi}/s_{ij})^\epsilon$ in eq. (5.3). The other convention is to have it multiplying both powers of ϵ rather than just the ϵ^{-2} as in eq. (5.3). With our choice of the matter representation, the two choices are equivalent up to and including $\mathcal{O}(\epsilon^0)$, since the one-loop amplitude vanishes identically at ϵ^0 , i.e.

$$\left[\frac{1}{\epsilon^2}(-s_{ij})^{-\epsilon} + 2\frac{b_0}{C_A} \frac{1}{\epsilon} \right] \mathcal{A}_n^{\text{1-loop}} = \left[\frac{1}{\epsilon^2} + 2\frac{b_0}{C_A} \frac{1}{\epsilon} \right] (-s_{ij})^{-\epsilon} \mathcal{A}_n^{\text{1-loop}} + \mathcal{O}(\epsilon). \quad (5.10)$$

The one-loop amplitude with matter in the representation R_0 decomposes as

$$\begin{aligned}\mathcal{A}_4^{\text{1-loop}}(1, 2, 3, 4) &= g^4 \left[C_{G1234}^{\text{1-loop}} A_4^{[1]}(1, 2, 3, 4) + C_{G1243}^{\text{1-loop}} A_4^{[1]}(1, 2, 4, 3) + C_{G1423}^{\text{1-loop}} A_4^{[1]}(1, 4, 2, 3) \right. \\ &\quad \left. + C_{R1234}^{\text{1-loop}} A_4^{[1/2]}(1, 2, 3, 4) + C_{R1243}^{\text{1-loop}} A_4^{[1/2]}(1, 2, 4, 3) + C_{R1423}^{\text{1-loop}} A_4^{[1/2]}(1, 4, 2, 3) \right].\end{aligned}\quad (5.11)$$

Here, the $C_{X1234}^{\text{1-loop}}$ with $X \in \{G, R\}$ are given by ring graphs with the loop being in the representation X . They are depicted in the left-hand side of fig. 1 for $X = G$ and in fig. 3 for $X = R$.

The kinematic factors $A_4^{[j]}$ are the familiar one-loop color-ordered all-plus amplitudes for a particle of spin j propagating in the loop. However, unlike in eq. (3.9), here we will need the result to higher orders in ϵ :

$$A_4^{[1]}(1, 2, 3, 4) = -(D_s - 2)i\rho \mathcal{I}_4^{\text{1-loop}}[\lambda_\ell^4](s, t), \quad (5.12)$$

$$A_4^{[1/2]}(1, 2, 3, 4) = 2i\rho \mathcal{I}_4^{\text{1-loop}}[\lambda_\ell^4](s, t), \quad (5.13)$$

with

$$\mathcal{I}_4^{\text{1-loop}}[\lambda_\ell^4](s, t) = \int \frac{d^D \ell}{(2\pi)^D} \frac{\lambda_\ell^4}{\ell^2(\ell - k_1)^2(\ell - k_1 - k_2)^2(\ell + k_4)^2}, \quad (5.14)$$

and λ_ℓ represents the (-2ϵ) -dimensional components of the loop momentum ℓ . The box integral $\mathcal{I}_4^{\text{1-loop}}[\lambda_\ell^4]$ is finite as $\epsilon \rightarrow 0$ so that

$$A_4^{[1/2]}(1, 2, 3, 4) = -A_4^{[1]}(1, 2, 3, 4), \quad (5.15)$$

in this limit, or when $D_s = 4$. We will keep $A_4^{[1]}$ and $A_4^{[1/2]}$ distinct for now.

After inserting eq. (5.11) into eq. (5.9), the two structure constants from the operator $\mathbf{I}^{(1)}$ will be contracted with the different one-loop color coefficients, and these contractions give rise to two-loop color diagrams,

$$\begin{aligned}
(if^{b_1 a_1 c})(if^{c a_2 b_2}) C_{Gb_1 b_2 34}^{\text{1-loop}} &= C_{1234}^P, \\
(if^{b_1 a_1 c})(if^{c a_2 b_2}) C_{Gb_1 b_2 43}^{\text{1-loop}} &= C_{1243}^P, \\
(if^{b_1 a_1 c})(if^{c a_2 b_2}) C_{Gb_1 4 b_2 3}^{\text{1-loop}} &= C_{3412}^{NP}, \\
(if^{b_1 a_1 c})(if^{c a_2 b_2}) C_{Rb_1 b_2 34}^{\text{1-loop}} &= R_{1234}^{P_1}, \\
(if^{b_1 a_1 c})(if^{c a_2 b_2}) C_{Rb_1 b_2 43}^{\text{1-loop}} &= R_{1243}^{P_1}, \\
(if^{b_1 a_1 c})(if^{c a_2 b_2}) C_{Rb_1 4 b_2 3}^{\text{1-loop}} &= R_{3412}^{NP_3}.
\end{aligned} \tag{5.16}$$

These relations allow us to write $\mathcal{A}_4^{(1,2)}$ as

$$\begin{aligned}
\mathcal{A}_4^{(1,2)}(1, 2, 3, 4) &= -g^6 \left[\frac{1}{\epsilon^2} (-s)^{-\epsilon} + 2 \frac{b_0^{R_0}}{C_A} \frac{1}{\epsilon} \right] \\
&\times \left[C_{1234}^P A_4^{[1]}(1, 2, 3, 4) + C_{1243}^P A_4^{[1]}(1, 2, 4, 3) + C_{3412}^{NP} A_4^{[1]}(1, 3, 2, 4) \right. \\
&+ R_{1234}^{P_1} A_4^{[1/2]}(1, 2, 3, 4) + R_{1243}^{P_1} A_4^{[1/2]}(1, 2, 4, 3) + R_{3412}^{NP_3} A_4^{[1/2]}(1, 3, 2, 4) \left. \right].
\end{aligned} \tag{5.17}$$

Now we insert eq. (5.17) into eq. (5.7) and perform the sum over i and j by first adding the term with $(i, j) = (3, 4)$. We arrive at

$$\begin{aligned}
\mathcal{A}_n^{\text{2-loop, ren.}}(1, 2, 3, 4) \Big|_{\text{pred. div.}} &= -g^6 c_\Gamma \left[\frac{1}{\epsilon^2} (-s)^{-\epsilon} + 2 \frac{b_0^{R_0}}{C_A} \frac{1}{\epsilon} \right] \\
&\times \left[2C_{1234}^P A_4^{[1]}(1, 2, 3, 4) + 2C_{1243}^P A_4^{[1]}(1, 2, 4, 3) \right. \\
&+ (C_{3412}^{NP} + C_{1234}^{NP}) A_4^{[1]}(1, 3, 2, 4) \\
&+ 2R_{1234}^{P_1} A_4^{[1/2]}(1, 2, 3, 4) + 2R_{1243}^{P_1} A_4^{[1/2]}(1, 2, 4, 3) \\
&+ (R_{3412}^{NP_3} + R_{1234}^{NP_3}) A_4^{[1/2]}(1, 3, 2, 4) \left. \right] \\
&+ \mathcal{C}(234).
\end{aligned} \tag{5.18}$$

Let us compare the predicted two-loop divergences for matter in the representation R_0 eq. (5.18) to those appearing in the actual two-loop amplitude. There are two divergent integrals contributing to the this amplitude, namely $\mathcal{I}_4^P[\lambda_q^2 \lambda_{p+q}^2] = \mathcal{I}_4^P[\lambda_p^2 \lambda_{p+q}^2]$ and $\mathcal{I}_4^{NP}[\lambda_p^2 \lambda_q^2]$ [26]. The divergent parts of these integrals are proportional to the one-loop box integral,

$$\begin{aligned}
\mathcal{I}_4^P[\lambda_q^2 \lambda_{p+q}^2](s, t) \Big|_{\text{div.}} &= -ic_\Gamma \frac{1}{\epsilon^2} (-s)^{-1-\epsilon} \mathcal{I}_4^{\text{1-loop}}[\lambda_\ell^4](s, t), \\
\mathcal{I}_4^{NP}[\lambda_p^2 \lambda_q^2](s, t) \Big|_{\text{div.}} &= -ic_\Gamma \frac{1}{\epsilon^2} (-s)^{-1-\epsilon} \mathcal{I}_4^{\text{1-loop}}[\lambda_\ell^4](u, t),
\end{aligned} \tag{5.19}$$

as expected if eq. (5.18) is to be recovered. A heuristic reason for this factorization is given in ref. [26], but we briefly summarize it here. When loop momenta are simultaneously soft and collinear with two adjacent external legs, three consecutive propagators can go on shell. When they go on shell, the remaining propagators become exactly that of the finite box integral with external momenta k_1, k_2, k_3, k_4 in the planar case and k_1, k_4, k_2, k_3 in the nonplanar case. The (-2ϵ) -dimensional numerator in both cases becomes the numerator λ_ℓ^4 in eq. (5.14). The spacetime picture is then a small finite box times an enlarged divergent triangle.

The divergences of the primitive amplitudes in terms of the one-loop amplitudes are given by

$$\begin{aligned} A_{G1234}^P \Big|_{\text{div.}} &= -2c_\Gamma \frac{1}{\epsilon^2} (-s)^{-\epsilon} A_4^{[1]}(1, 2, 3, 4), \\ A_{G1234}^{NP} \Big|_{\text{div.}} &= -c_\Gamma \frac{1}{\epsilon^2} (-s)^{-\epsilon} A_4^{[1]}(1, 3, 2, 4), \\ A_{F1234}^{P_1} \Big|_{\text{div.}} &= A_{F1234}^{P_2} \Big|_{\text{div.}} = -c_\Gamma \frac{1}{\epsilon^2} (-s)^{-\epsilon} A_4^{[1/2]}(1, 2, 3, 4), \\ A_{F1234}^{NP_3} \Big|_{\text{div.}} &= -c_\Gamma \frac{1}{\epsilon^2} (-s)^{-\epsilon} A_4^{[1/2]}(1, 3, 2, 4), \\ A_{F1234}^{D_i} \Big|_{\text{div.}} &= 0, \end{aligned} \quad (5.20)$$

where $D_i \in \{P_3, P_4, NP_1, NP_2\}$ for the last equality. Plugging these formulae into the sum of (4.12) and (4.4) yields

$$\begin{aligned} \mathcal{A}_4^{\text{2-loop}}(1, 2, 3, 4) \Big|_{\text{div.}} &= g^6 \left[C_{1234}^P A_{G1234}^P + C_{3421}^P A_{G3421}^P + C_{1234}^{NP} A_{G1234}^{NP} + C_{3421}^{NP} A_{G3421}^{NP} \right. \\ &\quad + R_{1234}^{P_1} A_{F1234}^{P_1} + R_{3421}^{P_1} A_{F3421}^{P_1} + R_{1234}^{P_2} A_{F1234}^{P_2} + R_{3421}^{P_2} A_{F3421}^{P_2} \\ &\quad \left. + R_{1234}^{NP_3} A_{F1234}^{NP_3} + R_{3421}^{NP_3} A_{F3421}^{NP_3} \right] \Big|_{\text{div.}} + \mathcal{C}(234) \\ &= -g^6 c_\Gamma \frac{1}{\epsilon^2} (-s)^{-\epsilon} \left[2C_{1234}^P A_4^{[1]}(1, 2, 3, 4) + 2C_{1243}^P A_4^{[1]}(1, 2, 4, 3) \right. \\ &\quad + (C_{3412}^{NP} + C_{1234}^{NP}) A_4^{[1]}(1, 3, 2, 4) \\ &\quad + 2R_{1234}^{P_1} A_4^{[1/2]}(1, 2, 3, 4) + 2R_{1243}^{P_1} A_4^{[1/2]}(1, 2, 4, 3) \\ &\quad \left. + (R_{3412}^{NP_3} + R_{1234}^{NP_3}) A_4^{[1/2]}(1, 3, 2, 4) \right] + \mathcal{C}(234), \end{aligned} \quad (5.21)$$

where we used the fact that $R_{1234}^{P_1} = R_{1234}^{P_2}$. This matches eq. (5.18) at the level of the $(-s)^{-\epsilon}/\epsilon^2$ term, i.e. except for the term proportional to $b_0^{R_0}$.

Now the expression (5.21) is for the unrenormalized two-loop amplitude, whereas the Catani formula (5.18) predicts the UV renormalized one. The renormalized amplitude $\mathcal{A}_4^{\text{2-loop, ren.}}$ is given by adding the $\overline{\text{MS}}$ counterterm

$$-4g^2 c_\Gamma b_0^{R_0} \frac{1}{\epsilon} \mathcal{A}_4^{\text{1-loop}}(1, 2, 3, 4). \quad (5.22)$$

No other terms are needed due to the vanishing of the all-plus helicity amplitude at tree level.

To arrive at the term proportional to $b_0^{R_0}$ in eq. (5.18), we use the color conservation identity

$$\sum_{i=1}^n \mathbf{T}_i = 0 \quad (5.23)$$

to write

$$nC_A |\mathcal{M}_n\rangle = \sum_{i=1}^n \mathbf{T}_i^2 |\mathcal{M}_n\rangle = -2 \sum_{1 \leq i < j \leq n} \mathbf{T}_i \cdot \mathbf{T}_j |\mathcal{M}_n\rangle. \quad (5.24)$$

This identity allows us to write the counterterm (5.22) in our notation as

$$\begin{aligned} -4g^2 c_\Gamma b_0^{R_0} \frac{1}{\epsilon} \mathcal{A}_4^{\text{1-loop}}(1, 2, 3, 4) &= -g^2 c_\Gamma \frac{b_0^{R_0}}{C_A \epsilon} (4C_A \mathcal{A}_4^{\text{1-loop}}(1, 2, 3, 4)) \\ &= -2g^2 c_\Gamma \frac{b_0^{R_0}}{C_A \epsilon} \sum_{1 \leq i < j \leq 4} (if^{b_i a_i c})(if^{c a_j b_j}) \\ &\quad \times \mathcal{A}_4^{\text{1-loop}}(1^{a_1}, \dots, i^{b_i}, \dots, j^{b_j}, \dots, 4^{a_4}). \end{aligned} \quad (5.25)$$

Now it matches precisely the $b_0^{R_0}$ -containing term of eq. (5.18), in the form of eqs. (5.7) and (5.8).

Thus, once the UV counterterm is included, we have exact agreement between the infrared divergences of the renormalized two-loop amplitude and the ones predicted by eq. (5.18). In other words, the non- $b_0^{R_0}$, $1/\epsilon^2$ term of eq. (5.18) precisely matches the divergences of the unrenormalized two-loop amplitude.

Next we evaluate eq. (5.18), but including also the $\mathcal{O}(\epsilon^0)$ terms. We subtract the result from the UV renormalized two-loop amplitude, in order to obtain the Catani finite remainder, $\mathcal{M}_4^{(2),\text{fin}}$. This result exactly yields the CCA bootstrap formula (1.3). In other words, eq. (1.3) gives the IR-subtracted two-loop amplitude. In the next section, we explore how to avoid an explicit IR divergence and subtraction.

6 Mass regularization

The requirement to subtract the IR divergences is unsatisfactory for the following reasons. Firstly, the CCA bootstrap requires no such subtraction; it is a completely finite procedure. Secondly, there is no dimensional regularization prescription for sdYM, since its definition requires the four-dimensional Levi-Civita tensor. In some sense, the IR subtraction remedies a problem that is introduced by our lack of understanding of how to regulate Feynman integrals in sdYM. We remedy this by regulating the internal propagators that give rise to IR divergences of the loop momenta with a particle mass. Then we can take $\epsilon \rightarrow 0$ without encountering any poles in ϵ .

There is a fundamental difference between mass regularization and dimensional regularization in when small terms can be neglected. In dimensional regularization, divergences are

powers of $1/\epsilon$, whose degree rises with the loop order. Therefore terms suppressed by powers of ϵ in lower-loop amplitudes generally have to be retained. On the other hand, when regulating with a particle mass m , divergences are logarithmic in m . Hence power-suppressed contributions can always be dropped, because any positive power of m vanishes much faster than (any power of) $\ln m$ increases, in the limit $m \rightarrow 0$.

Mass regularization has previously been used in planar $\mathcal{N} = 4$ supersymmetric YM [60–64]. Our method for assigning a mass to the propagators differs from these examples. Indeed, planar $\mathcal{N} = 4$ supersymmetric YM has dual conformal symmetry, which is closely related to these regularization schemes. It is not clear whether one can find a fully consistent massive regulator of nonplanar YM theory, given that the number of helicity states for massive vector bosons does not match the massless case. Hence, we do not claim that our method can consistently reproduce the correct IR divergences in the massless limit for more complicated amplitudes or integrals. We are merely regulating the few divergent integrals that appear in the all-plus four-point case.

In our scheme, a propagator is given a mass m when a limit of the loop momentum that puts it on shell also results in one or more of its neighboring propagators going on shell. The mass prevents the other propagators from diverging when the initial one does. For example, in the case of diagram (a) of fig. 6, when the loop momentum $p \rightarrow k_1$, all three of $(p - k_1)^2$, p^2 , and $(p - k_1 - k_2)^2$ approach zero. So the mass m is added to the first propagator $(p - k_1)^2 \mapsto (p - k_1)^2 - m^2$. Now, no two or more neighboring propagators can simultaneously diverge. We could have achieved the same result by adding a mass m to both the p^2 and $(p - k_1 - k_2)^2$ propagators; however, adding the mass to $(p - k_1)^2$ is the minimal solution and leads to very simple integrals.

It is unnecessary to add a mass to propagators containing loop momentum ℓ if the integral has a numerator factor of $(\lambda_\ell^2)^n$ for some positive integer n . This purely (-2ϵ) -component of ℓ vanishes when ℓ is purely four-dimensional, which in turn prevents the appearance of the soft or collinear IR singularity associated with the divergence of a propagator. This argument includes cases where ℓ is a sum (or difference) of loop momenta.

For the integrals appearing in eqs. (4.8) and (4.22) and depicted in fig. 6, only the following replacements are necessary:

$$\begin{aligned} \mathcal{I}_4^P[\lambda_p^2 \lambda_{p+q}^2] : & \quad (q - k_4)^2 \mapsto (q - k_4)^2 - m^2, \\ \mathcal{I}_4^P[\lambda_q^2 \lambda_{p+q}^2] : & \quad (p - k_1)^2 \mapsto (p - k_1)^2 - m^2, \\ \mathcal{I}_4^{NP}[\lambda_p^2 \lambda_{p+q}^2] : & \quad (q - k_2)^2 \mapsto (q - k_2)^2 - m^2, \\ \mathcal{I}_4^{NP}[\lambda_q^2 \lambda_{p+q}^2] : & \quad (p - k_1)^2 \mapsto (p - k_1)^2 - m^2, \\ \mathcal{I}_4^{NP}[\lambda_p^2 \lambda_q^2] : & \quad (p + q + k_3)^2 \mapsto (p + q + k_3)^2 - m^2. \end{aligned} \quad (6.1)$$

These new integrals can be evaluated directly using Feynman parameters, giving

$$\mathcal{I}_{4,m^2}^P[\lambda_p^2 \lambda_{p+q}^2] = \mathcal{I}_{4,m^2}^P[\lambda_q^2 \lambda_{p+q}^2] = \mathcal{I}_{4,m^2}^{NP}[\lambda_p^2 \lambda_q^2] = \frac{s^{-1}}{6(4\pi)^4} [\text{Li}_2(1 + s/m^2) - \zeta_2] + \mathcal{O}(\epsilon), \quad (6.2)$$

$$\mathcal{I}_{4,m^2}^{NP}[\lambda_p^2 \lambda_{p+q}^2] = \mathcal{I}_{4,m^2}^{NP}[\lambda_q^2 \lambda_{p+q}^2] = \mathcal{O}(\epsilon), \quad (6.3)$$

where $\zeta_2 = \zeta(2) = \text{Li}_2(1) = \pi^2/6$. The bow-tie integrals remain unchanged and are given in eq. (4.23). In the $m \rightarrow 0$ limit, eq. (6.2) has the asymptotic behavior

$$\frac{s^{-1}}{6(4\pi)^4} [\text{Li}_2(1 + s/m^2) - \zeta_2] \sim -\frac{s^{-1}}{6(4\pi)^4} \left[\frac{1}{2} \ln^2 \left(\frac{m^2}{-s} \right) + 2\zeta_2 \right] + \mathcal{O}(m^2). \quad (6.4)$$

The divergent log term agrees with the leading-order divergent term in the dimensionally-regulated integrals eqs. (D.1) and (D.4), i.e. the coefficient of the leading-order $1/\epsilon^2$ equals the coefficient of $\frac{1}{2} \ln^2(-m^2/s)$. Although it is necessary to take $m \rightarrow 0$ to make apparent the IR divergence, we will continue to work with the expression for generic m , eq. (6.2), as it will not affect our analysis below.

These mass-regulated integrals are much simpler than their purely dimensionally-regulated counterparts. We can understand these results heuristically by considering the IR divergences appearing in the original integrals.

First consider eq. (6.2). When $m = 0$, the divergent terms in ϵ are given by eq. (5.19), the massless triangle times the massless box. The mass-regulated planar integral in eq. (6.2) should factorize similarly when $m \rightarrow 0$. The mass-regulated triangle is

$$\mathcal{I}_{3,m^2}^{\text{1-loop}}[1](s) = \frac{i}{(4\pi)^2} s^{-1} [\text{Li}_2(1 + s/m^2) - \zeta_2] + \mathcal{O}(\epsilon), \quad (6.5)$$

and the box to zeroth order in ϵ is

$$\mathcal{I}_4^{\text{1-loop}}[\lambda_\ell^4] = -\frac{i}{(4\pi)^2} \frac{1}{6} + \mathcal{O}(\epsilon). \quad (6.6)$$

So, eq. (6.2) indeed agrees with the divergence statement when $m \rightarrow 0$. Surprisingly though, these mass-regulated two-loop integrals are *exactly* the product of the mass-regulated triangle and the massless box, even for generic mass m .

As a check on the results, consider the s -channel cut in four dimensions of $\mathcal{I}_{4,m^2}^P[\lambda_p^2 \lambda_{p+q}^2]$, where we cut the propagators neighboring the massive one, which corresponds to cutting the right box vertically in fig. 6(a). Indeed, the unitarity cuts can be performed in four dimensions since the mass-regulated double box is finite *a priori*. This produces a factor of the massless box within the phase-space integral, which is *constant* in four dimensions. So, the massless box can be factored out of the phase-space integral, and what remains within the integral is nothing more than the s -channel cut of the mass-regulated triangle. In other words,

$$\text{Disc}_{s>0} \mathcal{I}_{4,m^2}^P[\lambda_p^2 \lambda_{p+q}^2] = \mathcal{I}_4^{\text{1-loop}}[\lambda_p^4] \text{Disc}_{s>0} \mathcal{I}_{3,m^2}^{\text{1-loop}}[1]. \quad (6.7)$$

This is the only non-vanishing four-dimensional cut of the double-box, since all other cuts vanish due to the vanishing of the λ^2 numerator factors in four dimensions. The discontinuity of the mass-regulated triangle is easily computed from eq. (6.5) to be

$$\text{Disc}_{s>0} \mathcal{I}_{3,m^2}^{\text{1-loop}}[1] = \frac{i}{(4\pi)^2} 2\pi i \frac{\log(1 + s/m^2)}{s}. \quad (6.8)$$

Since $|\mathcal{I}_{3,m^2}^{\text{1-loop}}[1](s)| \rightarrow 0$ sufficiently fast as $|s| \rightarrow \infty$, we can use a dispersion relation to compute the triangle integral from its discontinuity along $s > 0$. In other words,

$$\mathcal{I}_{4,m^2}^P[\lambda_p^2 \lambda_{p+q}^2](s) = \frac{\mathcal{I}_4^{\text{1-loop}}[\lambda_p^4]}{2\pi i} \int_0^\infty dx \frac{\text{Disc}_{x \geq 0} \mathcal{I}_{3,m^2}^{\text{1-loop}}[1]}{x - s} = \mathcal{I}_4^{\text{1-loop}}[\lambda_p^4] \mathcal{I}_{3,m^2}^{\text{1-loop}}[1](s). \quad (6.9)$$

We can understand the vanishing of the integrals in eq. (6.3) by again understanding the IR divergences when $m = 0$. Consider the divergences of $\mathcal{I}_{4,m^2}^{NP}[\lambda_p^2 \lambda_{p+q}^2]$. The only propagators that are not suppressed by a (-2ϵ) -component of the loop momenta are q^2 and $(q - k_2)^2$. When the latter goes on shell, the former does as well. This gives a $\mathcal{O}(1/\epsilon)$ divergent term, since they are neighboring propagators, multiplied by a box with a doubled propagator, denoted by $\mathcal{I}_4^{\text{1-loop}}[\lambda^4/(p - k_1)^2]$, which is $\mathcal{O}(\epsilon)$ because it is related to an UV finite integral in six dimensions. The result is an integral that begins at $\mathcal{O}(\epsilon^0)$. Following our procedure for mass regularizing, the only propagator given a mass is $(q - k_2)^2$. This replaces the $\mathcal{O}(1/\epsilon)$ term by a $\mathcal{O}(\epsilon^0)$ one, but it is still multiplied by a box of $\mathcal{O}(\epsilon)$. Thus, the mass-regulated integral is $\mathcal{O}(\epsilon)$. Notice also that there is no four-dimensional unitarity cut of this integral, so its vanishing is consistent with the vanishing of its cuts.

Mass regularization of the integrals renders the primitive amplitudes (4.8) and (4.22) much simpler. Substituting eqs. (6.2) and (6.3) into eq. (4.22) yields

$$\begin{aligned} A_{F1234}^{P_1} &= \frac{\rho}{(4\pi)^4} \left\{ -\frac{1}{3} [\text{Li}_2(1 + s/m^2) - \zeta_2] + \frac{1}{9} \left(\frac{t}{s} - 4 \right) + 1 \right\} + \mathcal{O}(\epsilon), \\ A_{F1234}^{P_2} &= \frac{\rho}{(4\pi)^4} \left\{ -\frac{1}{3} [\text{Li}_2(1 + s/m^2) - \zeta_2] + \frac{1}{9} \left(\frac{t}{s} - 4 \right) + 1 \right\} + \mathcal{O}(\epsilon), \\ A_{F1234}^{P_3} &= -\frac{\rho}{(4\pi)^4} \frac{1}{2}, \\ A_{F1234}^{P_4} &= -\frac{\rho}{(4\pi)^4} \left\{ \frac{1}{9} \left(\frac{t}{s} - 4 \right) + \frac{1}{2} \right\}, \\ A_{F1234}^{NP_1} &= \mathcal{O}(\epsilon), \\ A_{F1234}^{NP_2} &= \mathcal{O}(\epsilon), \\ A_{F1234}^{NP_3} &= -\frac{\rho}{(4\pi)^4} \frac{1}{3} [\text{Li}_2(1 + s/m^2) - \zeta_2] + \mathcal{O}(\epsilon). \end{aligned} \quad (6.10)$$

The above primitive amplitudes are now a sum of rational terms and terms of uniform transcendental weight two, which contain the mass regulator m . In particular, $A_F^{NP_1}$ and $A_F^{NP_2}$ now vanish at $\mathcal{O}(\epsilon^0)$, and $A_F^{P_1} = A_F^{P_2}$ and $A_F^{NP_3}$ share the same transcendental terms. Inspection of eqs. (4.38) and (4.43) shows that no transcendental terms remain in $A_{4;1;1}$ and $A_{4;3;0}$ when eq. (6.10) is used,

$$A_{4;1;1}(1, 2, 3, 4) = \frac{12\rho}{(4\pi)^4} + \mathcal{O}(\epsilon), \quad (6.11)$$

and

$$A_{4;3;0}(1, 2, 3, 4) = \frac{24\rho}{(4\pi)^4} + \mathcal{O}(\epsilon), \quad (6.12)$$

and we now obtain complete agreement with eq. (1.3). Notice that this is true even without taking the limit $m \rightarrow 0$.

7 Conclusions and outlook

In this paper, we used previously-derived results [26, 59] and color algebra to perform a check in dimensional regularization of the two-loop four-point all-plus result (1.3) from the CCA bootstrap. The primitive amplitudes of refs. [26, 59] begin at $\mathcal{O}(1/\epsilon^2)$ and contain transcendental functions. By placing the matter in the representation R_0 , we found that the color-ordered two-loop amplitudes in this theory contain both $1/\epsilon$ poles and transcendental terms. At first sight, this might seem to contradict eq. (1.3). However, Catani's universal factorization formula (5.1) exactly predicts these terms, and our computation agrees with (1.3) after we subtract the universal IR divergences.

The discrepancy arises due to the non-vanishing of the one-loop amplitude in this theory at $\mathcal{O}(\epsilon)$. We remedy this by mass-regulating the already dimensionally-regulated integrals comprising the primitive amplitudes (4.8) and (4.22). All appearances of the dimension regulator ϵ are replaced by expressions involving the mass regulator m , resulting in finite quantities when $m \neq 0$. The new mass-regulated amplitudes give exact agreement with eq. (2.4), even for generic mass m . Removing the dependence on ϵ is essential for comparing the YM and sdYM results. The self-dual equations explicitly depend on the Levi-Civita tensor, which does not have a sensible definition for non-integer dimensions. So, the CCA bootstrap must implicitly use a different IR regularization scheme that involves keeping all momenta in four dimensions. Mass regularization appears to be such a scheme, at least at four points, and a suitable mass regularization for higher-point all-plus amplitudes seems likely to lead to agreement with eq. (2.8) as well.

Despite the discrepancy between the sdYM form factor and the YM amplitude in dimensional regularization, we are confident in the validity of eq. (2.8) when using a suitable mass regulator. Taking all possible four-dimensional unitarity cuts of the two-loop all-plus sdYM form factor shows that it cannot have any branch cuts in the R_0 theory. Moreover, the vanishing of the one-loop form factor forces the two-loop one to behave like a tree-level form factor in collinear limits, suggesting that the two-loop one is finite. We believe that eq. (2.8) predicts the finite remainder of the YM amplitude in dimensional regularization. In particular, we predict that

$$\mathcal{A}_n^{\text{2-loop}} = \mathcal{A}_n^{\text{2-loop}}|_{\text{pred. div.}} + \mathcal{A}_{n,\text{sdYM}}^{\text{2-loop}}, \quad (7.1)$$

where $\mathcal{A}_n^{\text{2-loop}}|_{\text{pred. div.}}$ is the predicted IR divergence of Catani given by eqs. (5.7) and (5.8), including its $\mathcal{O}(\epsilon^0)$ parts, and $\mathcal{A}_{n,\text{sdYM}}^{\text{2-loop}}$ is the two-loop result computed from the CCA bootstrap given by eq. (2.8). Evaluating $\mathcal{A}_n^{\text{2-loop}}|_{\text{pred. div.}}$ to $\mathcal{O}(\epsilon^0)$ requires knowing the one-loop all-plus n -point amplitude to $\mathcal{O}(\epsilon^2)$. A closed-form formula is not known for this, but in principle it can be computed for each n by using a basis of scalar integrals. The complete basis

to all-orders in ϵ includes pentagons, boxes, bubbles and triangles [65–69], the coefficients of which can be computed using D -dimensional unitarity [70, 71].

The combination of the single-trace term computed in ref. [49] and the double-trace term that we have computed, eq. (2.8), is a complete two-loop n -point result for a non-supersymmetric gauge theory with matter. We have conjectured that the YM amplitude has the form given by (7.1) with dimensional regularization as the IR regulator. Mass regularization of the four-point integrals allows for complete agreement between the YM amplitudes and the sdYM form factor. We further conjecture that this scheme, and perhaps other IR regularization schemes which do not change the dimensions of spacetime, give complete agreement between the two approaches at higher points. In light of the simple behavior of the two-loop all-plus four-point amplitudes when dimensional regularization is combined with suitable mass regularization, it may be worth investigating similar mass regularization for other types of gauge theory amplitudes. Although the two-loop all-plus n -point amplitude was not computed in QCD, where the fermions are in the representation $N_F(F \oplus \bar{F})$, methods similar to the CCA bootstrap, perhaps when combined with other bootstrap methods, may lead to analytic progress in the computation of higher-order corrections in more realistic theories.

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A Colorful identities

In order to evaluate the color factors in terms of traces over the fundamental representation without any contracted indices, we make use of various $SU(N)$ identities. In this appendix, we let R be an arbitrary irreducible representation of $SU(N)$. The fundamental (defining) representation is denoted by F , and G denotes the adjoint representation.

In the main text, we normalize the generators such that the Dynkin index of the fundamental representation T_F is unity, i.e.

$$\text{tr}(t^a t^b) = \delta^{ab} \quad \Longleftrightarrow \quad T_F = 1. \quad (\text{A.1})$$

Furthermore, we define the the $SU(N)$ structure constants f^{abc} to be real and normalized such that

$$i f^{abc} = \text{tr}([t^a, t^b] t^c). \quad (\text{A.2})$$

We will make use of color diagrams to describe one- and two-loop color factors. The rules for evaluating color diagrams are

$$\begin{aligned}
& b \swarrow \swarrow \curvearrowleft c = if^{abc} \\
& a \curvearrowleft a = \delta^{ab} \\
& j \xleftarrow[R]{\curvearrowleft} i = (t_R^a)^i_j \\
& a \curvearrowleft a
\end{aligned} \tag{A.3}$$

$$i \xrightarrow[R]{\curvearrowright} j = (\delta_R)^i_j$$

where t_R^a is an $SU(N)$ generator in a representation R . If the “ R ” is omitted, then it is implied that the generators are in the fundamental/anti-fundamental representation. The graphical depiction of the antisymmetric tensor product of the fundamental $\wedge^2 F$ is given in fig. 4.

In this appendix, we will keep the Dynkin index of the fundamental representation T_F arbitrary. It is set to 1 outside this appendix.

Recall that the quadratic Casimir in R is defined by

$$t_R^a t_R^a = C_R \cdot \text{id}_R. \tag{A.4}$$

Two other contractions of generators that appear in the computations are

$$t_R^c t_R^a t_R^c = \left(C_R - \frac{C_G}{2} \right) t_R^a, \tag{A.5}$$

$$t_R^c t_R^a t_R^b t_R^c = (C_R - C_G) t_R^a t_R^b + (if^{adc})(if^{ceb}) t_R^d t_R^e. \tag{A.6}$$

The $SU(N)$ Fierz identity,

$$(t^a)_j^i (t^a)_l^k = T_F \delta_l^i \delta_j^k - \frac{T_F}{N} \delta_j^i \delta_l^k, \tag{A.7}$$

when in the presence of other matrices and inside traces is given by

$$\text{tr}(X t^a Y t^a Z) = T_F \text{tr}(Y) \text{tr}(XZ) - \frac{T_F}{N} \text{tr}(XYZ), \tag{A.8}$$

$$\text{tr}(W t^a X) \text{tr}(Y t^a Z) = T_F \text{tr}(ZYXW) - \frac{T_F}{N} \text{tr}(WX) \text{tr}(YZ), \tag{A.9}$$

$$\text{tr}(W t^a X) Y t^a Z = T_F Y X W Z - \frac{T_F}{N} \text{tr}(WX) Y Z. \tag{A.10}$$

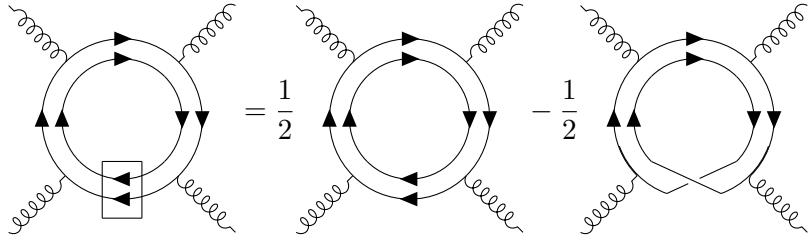


Figure 9: Color diagram for the trace over the representation $\wedge^2 F$ in terms of traces over the fundamental F .

The trace over the exterior square of the fundamental $\wedge^2 F$ has a realization as traces over F . Letting $P : F \otimes F \rightarrow F \otimes F$ be the permutation operator, the exterior square is the image of the projector $\frac{1}{2}(1 - P)$. Thus, the trace over $\wedge^2 F$ is given by

$$\text{tr}_{\wedge^2 F}(t^{a_1} \cdots t^{a_n}) = \text{tr}_{F \otimes F}(t^{a_1} \cdots t^{a_n} \frac{1}{2}(1 - P)). \quad (\text{A.11})$$

The generators of $F \otimes F$ are related to the generators of F by

$$t_{F \otimes F}^a = t^a \otimes 1 + 1 \otimes t^a, \quad (\text{A.12})$$

which implies that there are 2^n contributions to the trace over n generators $t_{F \otimes F}^{a_i}$, according to the choice of first or second term in eq. (A.12). In other words,

$$\text{tr}_{F \otimes F}(t^{a_1} \cdots t^{a_n}) = \sum_{I \subset (1, \dots, n)} \text{tr}(t_I) \text{tr}(t_{I^c}), \quad (\text{A.13})$$

where t_I denotes the product $t^{a_{i_1}} \cdots t^{a_{i_m}}$ for $I = (i_1, \dots, i_m)$ with the ordering inherited from the ordered list $(1, \dots, n)$, and I^c is the complement of I , again with the inherited ordering. Similarly,

$$\text{tr}_{F \otimes F}(t^{a_1} \cdots t^{a_n} P) = \sum_{I \subset (1, \dots, n)} \text{tr}(t_I t_{I^c}), \quad (\text{A.14})$$

so that

$$\text{tr}_{\wedge^2 F}(t^{a_1} \cdots t^{a_n}) = \frac{1}{2} \sum_{I \subset (1, \dots, n)} [\text{tr}(t_I) \text{tr}(t_{I^c}) - \text{tr}(t_I t_{I^c})]. \quad (\text{A.15})$$

Note that

$$t_\emptyset = \mathbf{1}, \quad (\text{A.16})$$

with this notation, so

$$\text{tr}(t_\emptyset) = \text{tr}(\mathbf{1}) = N. \quad (\text{A.17})$$

The associated color diagram for the trace over $\wedge^2 F$ is shown in fig. 9. It uses the diagrammatic rules for antisymmetrizing two lines shown in fig. 4.

The Dynkin index of $\wedge^2 F$ is read off from

$$\mathrm{tr}_{\wedge^2 F}(t^a t^b) = \frac{1}{2} [2N \mathrm{tr}(t^a t^b) - 4 \mathrm{tr}(t^a t^b)] = T_F(N-2) \delta^{ab}, \quad (\mathrm{A}.18)$$

i.e.

$$T_{\wedge^2 F} = T_F(N-2). \quad (\mathrm{A}.19)$$

The quadratic Casimir is then

$$C_{\wedge^2 F} = \frac{T_{\wedge^2 F} \dim G}{\dim \wedge^2 F} = 2T_F(N-1-2N^{-1}). \quad (\mathrm{A}.20)$$

B Computation of the double-trace kinematic terms in eq. (2.8)

The color factors computed in ref. [49] leave out the double-trace terms. Here, we recompute these color factors while keeping track of the double-trace structure. Afterwards, we use the CCA bootstrap to prove eq. (2.9). In order to do this, we first introduce some notation from ref. [49].

The momenta for massless states satisfy

$$p_{\alpha\dot{\alpha}} = \lambda_\alpha \tilde{\lambda}_{\dot{\alpha}}, \quad (\mathrm{B}.1)$$

where $\lambda, \tilde{\lambda}$ are two-component Weyl spinors. We can scale $\lambda, \tilde{\lambda}$ while keeping the momentum p fixed such that

$$\lambda = (1, z). \quad (\mathrm{B}.2)$$

The parameter z is then the coordinate on the \mathbb{CP}^1 where the chiral algebra lives. A massless state of energy ω is described by a function of z and $\tilde{\lambda}$. For a set of n outgoing momenta $\{p_i\}$, the familiar spinor brackets are defined by

$$\langle ij \rangle = 2\pi i(z_i - z_j), \quad (\mathrm{B}.3)$$

$$[ij] = -\epsilon_{\dot{\alpha}\dot{\beta}} \tilde{\lambda}_i^{\dot{\alpha}} \tilde{\lambda}_j^{\dot{\beta}}. \quad (\mathrm{B}.4)$$

Positive- and negative-helicity states of a gauge theory are denoted by

$$J^a[\omega \tilde{\lambda}](z) \text{ and } \tilde{J}^a[\omega \tilde{\lambda}](z), \quad (\mathrm{B}.5)$$

respectively, where a is the color index. The states can be expanded in a series in ω as

$$\begin{aligned} J^a[\omega \tilde{\lambda}](z) &= \sum_k \omega^k J^a[k](z), \\ \tilde{J}^a[\omega \tilde{\lambda}](z) &= \sum_k \omega^k \tilde{J}^a[k](z), \end{aligned} \quad (\mathrm{B}.6)$$

where $J^a[k]$, $\tilde{J}^a[k]$ are homogeneous polynomials of order k in $\tilde{\lambda}$. These quantities are expanded further as

$$\begin{aligned} J^a[k](z) &= \sum_{r+s=k} \frac{1}{r!s!} (\tilde{\lambda}_1)^r (\tilde{\lambda}_2)^s J^a[r,s](z), \\ \tilde{J}^a[k](z) &= \sum_{r+s=k} \frac{1}{r!s!} (\tilde{\lambda}_1)^r (\tilde{\lambda}_2)^s \tilde{J}^a[r,s](z). \end{aligned} \quad (\text{B.7})$$

The states $J^a[r,s]$, $\tilde{J}^a[r,s]$ generate the (extended) chiral algebra for pure sdYM living on the z -plane. These states should be thought of as soft modes, since they result from an expansion in ω .

The OPEs in the chiral algebra correspond to collinear limits of states in sdYM. At tree-level, the OPEs are

$$J^a[\tilde{\lambda}_i](z_i) J^b[\tilde{\lambda}_j](z_j) \sim i f^{abc} \frac{1}{\langle ij \rangle} J^c[\tilde{\lambda}_i + \tilde{\lambda}_j](z_i), \quad (\text{B.8})$$

$$J^a[\tilde{\lambda}_i](z_i) \tilde{J}^b[\tilde{\lambda}_j](z_j) \sim i f^{abc} \frac{1}{\langle ij \rangle} \tilde{J}^c[\tilde{\lambda}_i + \tilde{\lambda}_j](z_i). \quad (\text{B.9})$$

We have redefined the normalization of the $\tilde{\lambda}$ in order to remove the appearance of the energy ω . Notice that the structure constants used here differ from that of ref. [49] by a factor of i . The higher loop-order OPEs (including those with matter) are found in ref. [49], but they are not necessary for our purposes here.

As mentioned in the main body of the paper, correlation functions of the chiral algebra in a given conformal block are form factors of sdYM with an operator insertion \mathcal{O} at a point in spacetime corresponding to the conformal block. We denote these correlators as

$$\langle \mathcal{O} | J[\tilde{\lambda}_1](z_1) \cdots \tilde{J}[\tilde{\lambda}_k](z_k) \cdots \rangle. \quad (\text{B.10})$$

Expanding the external states as a sum of soft modes, we are left with computing correlators of the form

$$\langle \mathcal{O} | J[k_1](z_1) \cdots \tilde{J}[k_2](z_k) \cdots \rangle. \quad (\text{B.11})$$

Since correlators on twistor space must not scale with dilations of \mathbb{R}^4 , the scaling dimensions of the external states must sum to minus the scaling dimension of the operator. Positive-helicity states $J[k]$ contribute dimension $-k$, while negative-helicity states $\tilde{J}[k]$ contribute $-k-2$.

The OPEs constrain the poles of the correlators. In order to compute the two-loop amplitude eq. (2.8), only knowledge of tree-level and one-loop OPEs are needed. In particular, poles that involve $J[0]$ and $J[1]$ insertions are dictated by tree-level and one-loop OPEs, respectively.

The chiral algebra also places constraints on terms which are regular in a given limit. The algebra can be derived directly via Koszul duality [48]. This involves coupling $J[k]$ and $\tilde{J}[k]$ to the gauge field and the auxiliary field of sdYM on twistor space, which requires $J[k]$

to have a zero of order $2 - k$ at $z = \infty$ and $\tilde{J}[k]$ to have a pole of order $2 + k$ at $z = \infty$ in order for the coupling to be well-defined.

Form factors of sdYM with the operator $\mathcal{O} = \frac{1}{2}\text{tr}(B \wedge B)$ inserted at the origin give YM amplitudes when the sum of the gluon momenta vanishes. However, at two loops, the operator is chosen to be

$$\frac{1}{2}\text{tr}(B \wedge B) + \hbar^2 C \text{tr}(F \wedge F), \quad (\text{B.12})$$

where C is some constant. The $\text{tr}(F \wedge F)$ term is added as a two-loop counterterm, with \hbar^2 to remind us that the term is added at two loops. This term is added in order to remove an all-plus-helicity two-loop two-point correlator that can only be determined up to an overall constant C ; this addition also forces the two-loop three-point correlators to vanish. The operator $\text{tr}(F \wedge F)$ is a total derivative, which means that form factors with this operator vanish when we impose that the momenta of the gluons add up to zero, which we do when we pass to a scattering amplitude. So in practice we can neglect the second term in eq. (B.12).

Since \mathcal{O} has dimension four, and $J[1]$ dimension -1 , we consider the scale-invariant four-point correlator

$$\langle \mathcal{O} | J^{a_1}[1](z_1) J^{a_2}[1](z_2) J^{a_3}[1](z_3) J^{a_4}[1](z_4) \rangle, \quad (\text{B.13})$$

where \mathcal{O} means eq. (B.12) from now on. Eq. (B.13) is determined by one-loop OPEs between any two $J[1]$'s; hence we get a two-loop result. It evaluates to (see ref. [49] for how this is computed)

$$\begin{aligned} & \langle \mathcal{O} | J^{a_1}[1](z_1) J^{a_2}[1](z_2) J^{a_3}[1](z_3) J^{a_4}[1](z_4) \rangle \\ &= \frac{i}{(4\pi)^4} \frac{[12][34]}{\langle 12 \rangle \langle 34 \rangle} \frac{R^{a_1 a_2 a_3 a_4}}{4} \\ & \quad - \frac{2i}{(4\pi)^4} \frac{[12][34]}{\langle 12 \rangle \langle 34 \rangle} \frac{\langle 13 \rangle \langle 24 \rangle + \langle 14 \rangle \langle 23 \rangle}{\langle 12 \rangle \langle 34 \rangle} (\text{tr}(1234) + \text{tr}(1432) - \text{tr}(1243) - \text{tr}(1342)) \\ & \quad + (1324) + (1423), \end{aligned} \quad (\text{B.14})$$

where the last line adds two more permutations, and the color factor $R^{a_1 a_2 a_3 a_4}$ is given by

$$\begin{aligned} R^{a_1 a_2 a_3 a_4} &= 4 \left(t_G^{(a_1} t_G^{a_2)} \right)_{b_1 b_2} \left(t_G^{(a_3} t_G^{a_4)} \right)_{b_3 b_4} \left(-2\text{tr}((b_1 b_2)(b_3 b_4)) + \text{tr}(b_1 b_3 b_2 b_4) + \text{tr}(b_1 b_4 b_2 b_3) \right) \\ & \quad + 4 \left(t_G^{(a_1} t_G^{a_2)} \right)_{b_1 b_2} \text{tr}_{R_0}((a_3 a_4)(b_1 b_2)) + 4 \left(t_G^{(a_3} t_G^{a_4)} \right)_{b_1 b_2} \text{tr}_{R_0}((a_1 a_2)(b_1 b_2)) \\ & \quad - 4\text{tr}_{R_0}(c(a_1 a_2)c(a_3 a_4)). \end{aligned} \quad (\text{B.15})$$

The parentheses around color indices means to symmetrize on said indices. Recall that t_G^a are the generators of $SU(N)$ in the adjoint representation defined by

$$(t_G^a)_{bc} = -i f^{abc}. \quad (\text{B.16})$$

Writing eq. (B.15) as traces over the fundamental without contracted indices requires the use of the identities in Appendix A. Doing so results in

$$\begin{aligned} R^{a_1 a_2 a_3 a_4} = & (24N - 16 - 32N^{-1}) (\text{tr}(1234) + \text{tr}(1243) + \text{tr}(1342) + \text{tr}(1432)) \\ & - (16 + 32N^{-1}) (\text{tr}(1324) + \text{tr}(1423)) \\ & + (32 + 32N^{-1}) (\text{tr}(12)\text{tr}(34) + \text{tr}(13)\text{tr}(24) + \text{tr}(14)\text{tr}(23)). \end{aligned} \quad (\text{B.17})$$

With this formula, eq. (B.14) can now be expressed as a sum over permutations of different trace structures, resulting in eqs. (2.4)–(2.6).

We now prove the formula (2.9) for the n -point double-trace term by induction. Eq. (2.9) clearly reproduces the $n = 4$ case. For the $n > 4$ case, the correlator giving rise to $A_{n;c}^{\text{2-loop}}(i_1, i_2, i_3, i_4)$ is

$$\langle \mathcal{O} | \cdots J^{a_1}[1](z_{i_1}) \cdots J^{a_2}[1](z_{i_2}) \cdots J^{a_3}[1](z_{i_3}) \cdots J^{a_4}[1](z_{i_4}) \cdots \rangle, \quad (\text{B.18})$$

where ellipses indicate $J[0]$ insertions. Assume the n -th insertion is a $J[0]$. Viewing eq. (B.18) as a function of z_n , the poles with respect to z_n are dictated by the OPEs of $J^{a_n}[0](z_n)$ with the other insertions. The OPEs are

$$J^{a_m}[0](z_m) J^{a_n}[0](z_n) \sim i f^{a_m a_n b} \frac{1}{\langle m n \rangle} J^b[0](z_m), \quad (\text{B.19})$$

$$J^{a_m}[1](z_m) J^{a_n}[0](z_n) \sim i f^{a_m a_n b} \frac{1}{\langle m n \rangle} J^b[1](z_m). \quad (\text{B.20})$$

The OPEs dictate that the residues at the simple poles $\langle m n \rangle$ will be $(n-1)$ -point correlators.

The double-trace structures in eq. (B.18) for $(n-1)$ points with the ordering $1, 2, \dots, n-1$ are

$$\sum_{c=3}^{n-2} A_{n-1;c}^{\text{2-loop}}(i_1, i_2, i_3, i_4) \text{tr}(1 \cdots c-1) \text{tr}(c \cdots n-1). \quad (\text{B.21})$$

Since we are only concerned with the ordering $1, 2, \dots, n$ in the trace structures for n points, to determine the dependence on z_n we only need to consider two OPEs, where the point z_n is near z_c and where it is near z_{n-1} , for a given $c \in \{3, \dots, n-2\}$. Then the double-trace structure of eq. (B.18) at a given c has the form

$$\begin{aligned} & i f^{a_{n-1} a_n b} \frac{1}{\langle n-1, n \rangle} A_{n-1;c}^{\text{2-loop}}(i_1, i_2, i_3, i_4) \text{tr}(1 \cdots c-1) \text{tr}(c \cdots (n-2)b) \\ & + i f^{a_n a_c b} \frac{1}{\langle n c \rangle} A_{n-1;c}^{\text{2-loop}}(i_1, i_2, i_3, i_4) \text{tr}(1 \cdots c-1) \text{tr}(b(c+1) \cdots n-1) \\ & = A_{n-1;c}^{\text{2-loop}}(i_1, i_2, i_3, i_4) \left(\frac{1}{\langle n-1, n \rangle} + \frac{1}{\langle n c \rangle} \right) \text{tr}(1 \cdots c-1) \text{tr}(c \cdots n) \\ & = A_{n-1;c}^{\text{2-loop}}(i_1, i_2, i_3, i_4) \frac{\langle n-1, c \rangle}{\langle n-1, n \rangle \langle n c \rangle} \text{tr}(1 \cdots c-1) \text{tr}(c \cdots n) \\ & = A_{n;c}^{\text{2-loop}}(i_1, i_2, i_3, i_4) \text{tr}(1 \cdots c-1) \text{tr}(c \cdots n). \end{aligned} \quad (\text{B.22})$$

In the first equality, we performed the contractions between the structure constants and the generators within the traces and kept only the double-trace terms with the ordering $1, 2, \dots, n$. In the second equality, we used the definition of the angle spinor brackets in terms of the z_i variables, eq. (B.3). The last equality follows by induction from the definition (2.9).

Summing over c then yields

$$\begin{aligned} & \sum_{c=3}^{n-2} A_{n;c}^{\text{2-loop}}(i_1, i_2, i_3, i_4) \text{tr}(1 \cdots c-1) \text{tr}(c \cdots n) \\ &= \sum_{c=3}^{n-1} A_{n;c}^{\text{2-loop}}(i_1, i_2, i_3, i_4) \text{tr}(1 \cdots c-1) \text{tr}(c \cdots n), \end{aligned} \quad (\text{B.23})$$

where we added $0 = A_{n;n-1}^{\text{2-loop}}(i_1, i_2, i_3, i_4)$ in the second line, which agrees with eq. (2.9), since the condition $c = n-1 \leq i_3 < i_4 \leq n$ is incompatible with $i_4 < n$, which holds because a $J[0]$ is inserted at the n -th position.

In the above, we ignored the terms regular in $\langle n-1, n \rangle$ and $\langle nc \rangle$; however, these terms are null since they would not allow $J^{a_n}[0](z_n)$ to have a second-order zero at $z_n = \infty$. Eq. (B.23) shows that the dependence on z_n is compatible inductively with eq. (2.9).

Next we consider the dependence on z_m , when there is a $J[0]$ inserted into eq. (B.18) at z_m for $m < n$. The computation goes very similarly for the three cases: $1 \leq m < i_1$, $i_1 < m < i_2$, and $i_3 < m < i_4$. The vanishing conditions for eq. (2.9) mean that the $J^{a_m}[0]$ contributes to only one of the two traces in the double-trace structure when only considering the ordering $1, 2, \dots, n$. The case $i_2 < m < i_3$ differs slightly. Taking $m = i_2 + 1$, the OPEs involving $J^{a_{i_2+1}}[0](z_{i_2+1})$ dictate that there are simple poles at $z_{i_2+1} = z_j$ for $j \in \{1, \dots, n\} \setminus \{i_2 + 1\}$, and their residues are $(n-1)$ -point correlators with $J^{a_{i_2+1}}[0](z_{i_2+1})$ removed.

The double-trace structure in the ordering $1, 2, \dots, n$ of the $(n-1)$ -point correlator with this operator removed is

$$\sum_{j=3}^{n-2} A_{n;c_j}^{\text{2-loop}}(i_1, i_2, i_3, i_4) \text{tr}(c_1 \cdots c_{j-1}) \text{tr}(c_j \cdots c_{n-1}), \quad (\text{B.24})$$

where c_j is the j -th element of the ordered list $(1, \dots, i_2, i_2 + 2, \dots, n)$. We can ignore terms with $j < i_2 + 1$, since $A_{n-1;c_j}^{\text{2-loop}}(i_1, i_2, i_3, i_4)$ vanishes with this condition. For $j > i_2 + 1$, the insertion $J^{a_{i_2+1}}[0](z_{i_2+1})$ only contributes to the right trace in the double-trace structure. So the computation is very similar to the z_n case described above.

For $j = i_2 + 1$, $J^{a_{i_2+1}}[0](z_{i_2+1})$ must contribute to both traces in the double-trace structure, since the generator $t^{a_{i_2+1}}$ can be inserted in either of the traces in

$$\text{tr}(1 \cdots i_2) \text{tr}(i_2 + 2 \cdots n) \quad (\text{B.25})$$

while preserving the ordering $1, \dots, n$. Correspondingly, there are four poles instead of two,

at $z_{i_2+1} \in \{z_1, z_{i_2}, z_{i_2+2}, z_n\}$, with residues dictated by the OPEs:

$$\begin{aligned}
& if^{a_{i_2}a_{i_2+1}b} \frac{1}{\langle i_2, i_2+1 \rangle} A_{n-1; c_{i_2+1}}^{\text{2-loop}}(i_1, i_2, i_3, i_4) \text{tr}(1 \cdots (i_2-1)b) \text{tr}(i_2+2 \cdots n) \\
& + if^{a_{i_2+1}a_1b} \frac{1}{\langle i_2+1, 1 \rangle} A_{n-1; c_{i_2+1}}^{\text{2-loop}}(i_1, i_2, i_3, i_4) \text{tr}(b2 \cdots i_2) \text{tr}(i_2+2 \cdots n) \\
& + if^{a_{i_2+1}a_{i_2+2}b} \frac{1}{\langle i_2+1, i_2+2 \rangle} A_{n-1; c_{i_2+1}}^{\text{2-loop}}(i_1, i_2, i_3, i_4) \text{tr}(1 \cdots i_2) \text{tr}(b(i_2+3) \cdots n) \\
& + if^{a_n a_{i_2+1}b} \frac{1}{\langle n, i_2+1 \rangle} A_{n-1; c_{i_2+1}}^{\text{2-loop}}(i_1, i_2, i_3, i_4) \text{tr}(1 \cdots i_2) \text{tr}(i_2+2 \cdots (n-1)b) \\
& = A_{n-1; c_{i_2+1}}^{\text{2-loop}}(i_1, i_2, i_3, i_4) \frac{\langle i_2 1 \rangle}{\langle i_2, i_2+1 \rangle \langle i_2+1, 1 \rangle} \text{tr}(1 \cdots i_2+1) \text{tr}(i_2+2 \cdots n) \\
& + A_{n-1; c_{i_2+1}}^{\text{2-loop}}(i_1, i_2, i_3, i_4) \frac{\langle n, i_2+2 \rangle}{\langle i_2+1, i_2+2 \rangle \langle n, i_2+1 \rangle} \text{tr}(1 \cdots i_2) \text{tr}(i_2+1 \cdots n) \\
& = A_{n; i_2+2}^{\text{2-loop}}(i_1, i_2, i_3, i_4) \text{tr}(1 \cdots i_2+1) \text{tr}(i_2+2 \cdots n) \\
& + A_{n; i_2+1}^{\text{2-loop}}(i_1, i_2, i_3, i_4) \text{tr}(1 \cdots i_2) \text{tr}(i_2+1 \cdots n).
\end{aligned} \tag{B.26}$$

The first equality follows from taking only the double-traces with the ordering $1, \dots, n$ after removing the index contraction. The second equality follows from the definition (2.9). This exhausts all cases, and the result follows by induction.

C Proof of eq. (3.14)

In this section, we prove that the single-trace color-ordered one-loop subamplitude when matter lives in the representation (1.1) is given by eq. (3.14), which we repeat here for convenience:

$$-8A_n^{[1]}(1, \dots, n) + \sum_{k=1}^n \sum_{\sigma \in \alpha_k \sqcup \beta_k} A_n^{[1]}(1, \sigma), \tag{C.1}$$

where $\alpha_k = (2, \dots, k)$ and $\beta_k = (k+1, \dots, n)$. The first term immediately follows from the eight copies of the fundamental representation for the fermions, together with the sign flip associated with the SWI (3.10). The second term must then come from the single copy of the antisymmetric tensor representation, in particular from the exchange graph shown in figure 9. (The gluon loop only generates double traces, and single traces with a factor of N which cancel against non-exchange contributions from $\wedge^2 F$.) Figure 10 provides an example, for $n=6$, of how a particular shuffle of α_4 and β_4 , i.e. an element of $\alpha_k \sqcup \beta_k$ for $k=4$, can contribute to the trace ordering $\text{tr}(1 \cdots n)$.

We now provide a rigorous argument for the validity of eq. (3.14). That is, we will show that the contributing color-orderings for the exchange terms are in bijection with the shuffles $\alpha_k \sqcup \beta_k$ for some k . Recall that the single-trace terms of the one-loop amplitude with matter

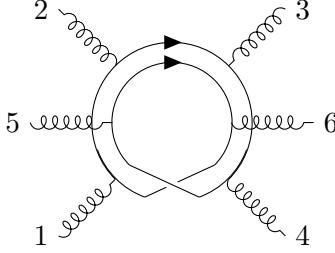


Figure 10: An example for $n = 6$ which illustrates how the color-ordered sub-amplitude $A_6^{[1]}(1, 5, 2, 3, 6, 4)$ can contribute to the color factor $\text{tr}(123456)$ via the exchange term P . The ordering $(1, 5, 2, 3, 6, 4)$ corresponds to a shuffle of $\alpha_4 = (2, 3, 4)$ and $\beta_4 = (5, 6)$.

in the representation (1.1) is given by

$$\begin{aligned} \sum_{\sigma \in S_n / \mathbb{Z}_n} \left[-8 \text{tr}(\sigma_1 \cdots \sigma_n) A_n^{[1]}(\sigma_1, \dots, \sigma_n) \right. \\ \left. + \frac{1}{2} \sum_{I \subset (1, \dots, n)} \text{tr}(\sigma(I \cdot I^c)) A_n^{[1]}(\sigma_1, \dots, \sigma_n) \right]. \end{aligned} \quad (\text{C.2})$$

The sum is over the group $S_n / \mathbb{Z}_n \cong S_{n-1}$, allowing us to choose an element from $1, \dots, n$ which can be fixed by all $\sigma \in S_{n-1}$. We choose 1 to be this fixed element. After summing over S_{n-1} and collecting on the traces, the color-ordered term multiplying $\text{tr}(1 \cdots n)$ is generically

$$-8A_n^{[1]}(1, \dots, n) + \frac{1}{2} \sum_{\sigma \in S} A_n^{[1]}(1, \sigma), \quad (\text{C.3})$$

where $S \subset S_{n-1}$ is

$$S = \{\sigma \in S_{n-1} \mid \sigma(I \cdot I^c) \in [(1, \dots, n)] \text{ for some } I \subset (1, \dots, n)\}, \quad (\text{C.4})$$

where $[(1, \dots, n)]$ is an equivalence class containing all cycles of $(1, \dots, n)$. Here S is written as a set, but we are counting multiplicities, meaning that σ is included in the sum the same number of times there is an instance of a sublist $I \subset (1, \dots, n)$ with $\sigma(I \cdot I^c) \in [(1, \dots, n)]$.

The set S can be written as a disjoint union over subsets \hat{S}_k which require the sublist I to be of size k , allowing for the sum over S to be written as a sum over k ,

$$\frac{1}{2} \sum_{\sigma \in S} A_n^{[1]}(1, \sigma) = \frac{1}{2} \sum_{k=0}^n \sum_{\sigma \in \hat{S}_k} A_n^{[1]}(1, \sigma), \quad (\text{C.5})$$

where the collection of permutations \hat{S}_k is

$$\hat{S}_k = \{\sigma \in S_{n-1} \mid \sigma(I \cdot I^c) \in [(1, \dots, n)] \text{ for some } I \subset (1, \dots, n) \text{ with } |I| = k\}. \quad (\text{C.6})$$

Notice that if $\sigma \in \hat{S}_k$ then $\sigma \in \hat{S}_{n-k}$, which follows from the fact that if $\sigma(I \cdot I^c) \in [(1, \dots, n)]$ then $\sigma(I^c \cdot I) \in [(1, \dots, n)]$, since $I^c \cdot I$ is related to $I \cdot I^c$ by a cyclic transformation. We can use this pairing between I and I^c to require that $1 \in I \subset (1, \dots, n)$. This restriction removes the overall factor of $1/2$ and the sum becomes

$$\frac{1}{2} \sum_{k=0}^n \sum_{\sigma \in \hat{S}_k \subset S_{n-1}} A_n^{[1]}(1, \sigma) = \sum_{k=1}^n \sum_{\sigma \in \tilde{S}_k} A_n^{[1]}(1, \sigma), \quad (\text{C.7})$$

where the new subset \tilde{S}_k is

$$\tilde{S}_k = \{\sigma \in S_{n-1} \mid \sigma(I \cdot I^c) \in [(1, \dots, n)] \text{ for some } I \subset (1, \dots, n) \text{ with } |I| = k \text{ and } 1 \in I\} \quad (\text{C.8})$$

for all $1 \leq k \leq n$.

We will show that $\tilde{S}_k = \alpha_k \sqcup \beta_k$, which will complete the proof of eq. (3.14). As a reminder, $\alpha_k = (2, \dots, k)$ and $\beta_k = (k+1, \dots, n)$. Consider an element $\tau \in \alpha_k \sqcup \beta_k$, and set $J = (1, \tau^{-1}(\alpha_k))$. The permutation τ is generically of the form

$$\tau = (\beta_{I_1}, 2, \beta_{I_2}, 3, \dots, \beta_{I_{k-1}}, k, \beta_{I_k}), \quad (\text{C.9})$$

where β_{I_j} represents some sublist of β_k such that $\beta_{I_1} \cdot \beta_{I_2} \cdots \beta_{I_k} = \beta_k$. Since $\tau \in S_{n-1}$, we can identify τ with $(1, \tau) \in S_n$. So the j -th element of τ is in the $(j+1)$ -th position in $(1, \tau)$. Letting j_i be the position of i in τ for $2 \leq i \leq n$, we then have that

$$J = (1, j_2 + 1, j_3 + 1, \dots, j_k + 1). \quad (\text{C.10})$$

Also, $j_i < j_l$ for $i < l$, since $(\alpha_k)_i = i+1 < l+1 = (\alpha_k)_l$ and the shuffle product preserves the ordering of α_k . This means that J is ordered with respect to $(1, \dots, n)$. It follows that the complement of J^c is

$$J^c = (j_{k+1} + 1, \dots, j_n + 1) = \tau^{-1}(\beta_k). \quad (\text{C.11})$$

Thus,

$$\tau(J \cdot J^c) = (1, \alpha_k, \beta_k) = (1, 2, \dots, n), \quad (\text{C.12})$$

which implies that $\tau \in \tilde{S}_k$, i.e. $\alpha_k \sqcup \beta_k \subseteq \tilde{S}_k$.

The shuffle product $\alpha_k \sqcup \beta_k$ has size

$$|\alpha_k \sqcup \beta_k| = \binom{|\alpha_k| + |\beta_k|}{|\alpha_k|} = \binom{n-1}{k-1}. \quad (\text{C.13})$$

The size of \tilde{S}_k is at most the number of size- k sublists of $(1, \dots, n)$ containing 1, i.e.

$$|\tilde{S}_k| \leq \binom{n-1}{k-1}. \quad (\text{C.14})$$

It cannot be larger, because $\sigma \in \tilde{S}_k$ if and only if there exists $I \subset (1, \dots, n)$ containing 1 such that $\sigma(I \cdot I^c) \in [(1, \dots, n)]$. Since $\sigma \in S_{n-1}$ has 1 as a fixed point, it must be that $\sigma(I \cdot I^c) = (1, \dots, n)$. By uniqueness, this means there is only one such σ for a given I . So the size of \tilde{S}_k is bounded by eq. (C.14). Given that $\alpha_k \sqcup \beta_k \subseteq \tilde{S}_k$, and eq. (C.13), the bound must be saturated, and then $\tilde{S}_k = \alpha_k \sqcup \beta_k$ follows. This proves the equality.

D Integrals

In this section, we reproduce the evaluated integrals from ref. [26] that enter the two-loop primitive amplitudes in eqs. (4.8) and (4.22). The results for the two-loop integrals are given in the Euclidean region $s, t < 0$ and $u > 0$, for which $\chi = t/s > 0$. They can be analytically continued to other regions by substituting $(-s)^{-\epsilon} \mapsto s^{-\epsilon} e^{\epsilon i\pi}$ and $\ln \chi \mapsto \ln |\chi| + i\pi$. The planar double-box integral, expressed in terms of the one-loop box integral, is

$$\begin{aligned} \mathcal{I}_4^P[\lambda_p^2 \lambda_{p+q}^2](s, t) &= \mathcal{I}_4^P[\lambda_q^2 \lambda_{p+q}^2](s, t) \\ &= -ic\Gamma \frac{1}{\epsilon^2} (-s)^{-1-\epsilon} \mathcal{I}_4^{\text{1-loop}}[\lambda_p^4](s, t) + \frac{FR_{p+q,q}^P}{(4\pi)^4(-s)} + \mathcal{O}(\epsilon). \end{aligned} \quad (\text{D.1})$$

The one-loop box integral to $\mathcal{O}(\epsilon^2)$ is

$$\begin{aligned} \mathcal{I}_4^{\text{1-loop}}[\lambda_p^4](s, t) &= ic\Gamma(-s)^{-\epsilon}(-\epsilon)(1-\epsilon) \frac{1}{6} \left\{ \frac{1}{\epsilon} - \frac{1}{2} \frac{\chi(\ln^2 \chi + \pi^2)}{(1+\chi)^2} - \frac{\chi \ln \chi}{1+\chi} + \frac{11}{3} \right. \\ &\quad + \epsilon \left[\frac{\chi}{(1+\chi)^2} \left[\text{Li}_3(-\chi) - \zeta_3 - \ln \chi \text{Li}_2(-\chi) + \frac{1}{3} \ln^3 \chi - \frac{1}{2} \ln^2 \chi \ln(1+\chi) \right. \right. \\ &\quad \left. \left. + \frac{\pi^2}{2} \ln \left(\frac{\chi}{1+\chi} \right) + \frac{1}{2} \left((2+\chi) \ln^2 \chi + \pi^2 \right) \right] \right. \\ &\quad \left. \left. + \frac{11}{3} \left(-\frac{1}{2} \frac{\chi(\ln^2 \chi + \pi^2)}{(1+\chi)^2} - \frac{\chi \ln \chi}{1+\chi} + \frac{11}{3} \right) - 4 \right] \right\} + \mathcal{O}(\epsilon^3). \end{aligned} \quad (\text{D.2})$$

The planar finite remainder $FR_{p+q,q}^P$ is

$$FR_{p+q,q}^P = \frac{1}{18} \frac{\chi}{(1+\chi)^2} \left[-\ln \chi (\ln^2 \chi + \pi^2) + \left(\chi - \frac{1}{\chi} \right) \pi^2 \right]. \quad (\text{D.3})$$

The divergent non-planar integral in terms of the one-loop box integral is

$$\mathcal{I}_4^{NP}[\lambda_p^2 \lambda_q^2](s, t) = -ic\Gamma \frac{1}{\epsilon^2} (-s)^{-1-\epsilon} \mathcal{I}_4^{\text{1-loop}}[\lambda_p^4](u, t) + \frac{FR_{p,q}^{NP}}{(4\pi)^4(-s)}, \quad (\text{D.4})$$

where the finite remainder is

$$\begin{aligned} FR_{p,q}^{NP} &= \frac{1}{6} \left\{ -2\chi(1+\chi) \left[\text{Li}_3 \left(\frac{\chi}{1+\chi} \right) - \zeta_3 - \ln \left(\frac{\chi}{1+\chi} \right) \left(\text{Li}_2 \left(\frac{\chi}{1+\chi} \right) + \frac{\pi^2}{2} \right) - \frac{1}{6} \ln^3 \left(\frac{\chi}{1+\chi} \right) \right] \right. \\ &\quad + 3\chi(1+\chi) \ln(1+\chi) \ln \chi - \frac{1}{2}(1+\chi)^2 \left(-\frac{1}{\chi} + 3 \right) \ln^2(1+\chi) - \frac{1}{2}\chi^2 \left(\frac{1}{1+\chi} + 3 \right) \ln^2 \chi \\ &\quad \left. + \pi^2 \left(\chi - \frac{1}{2} \frac{1}{1+\chi} + \frac{5}{6} \right) + (1+\chi) \ln(1+\chi) - \chi \ln \chi \right. \\ &\quad \left. + i\pi \left(2\chi(1+\chi) \left[\text{Li}_2 \left(\frac{\chi}{1+\chi} \right) - \frac{\pi^2}{6} - \frac{3}{2} \ln \chi \right] + (1+\chi) \left[(1+\chi) \left(-\frac{1}{\chi} + 3 \right) \ln(1+\chi) - 1 \right] \right) \right\}. \end{aligned} \quad (\text{D.5})$$

The finite non-planar integral $\mathcal{I}_4^{NP}[\lambda_q^2 \lambda_{p+q}^2] = \mathcal{I}_4^{NP}[\lambda_p^2 \lambda_{p+q}^2]$ is

$$\begin{aligned}
\mathcal{I}_4^{NP}[\lambda_q^2 \lambda_{p+q}^2](s, t) = & \frac{1}{(4\pi)^4(-s)} \frac{1}{6} \left\{ \frac{\chi}{(1+\chi)^2} \left[\text{Li}_3(-\chi) - \zeta_3 - \ln \chi \left(\text{Li}_2(-\chi) - \frac{\pi^2}{6} \right) - \frac{3}{4} \chi (\ln^2 \chi - \pi^2) \right] \right. \\
& - \frac{1+\chi}{\chi^2} \left[\text{Li}_3\left(\frac{1}{1+\chi}\right) - \zeta_3 + \ln(1+\chi) \left(\text{Li}_2\left(\frac{1}{1+\chi}\right) + \frac{\pi^2}{6} \right) \right. \\
& + \frac{3}{4} (1+\chi) \ln^2(1+\chi) + \frac{1}{3} \ln^3(1+\chi) \left. \right] + \left(\frac{1}{\chi(1+\chi)} + \frac{3}{2} \right) \ln(1+\chi) \ln \chi \\
& + \pi^2 \left(\frac{1}{6\chi} + \frac{4}{3(1+\chi)} + \frac{3}{2} \frac{\chi}{(1+\chi)^2} - \frac{3}{4} \right) + \frac{\ln(1+\chi)}{2\chi} - \frac{\ln \chi}{2(1+\chi)} \\
& + i\pi \left(-\frac{1+\chi}{\chi^2} \left[\text{Li}_2\left(\frac{\chi}{1+\chi}\right) - \ln(1+\chi) \ln \chi + \frac{1}{2} \ln^2(1+\chi) - \frac{3}{2} (1+\chi) \ln(1+\chi) \right] \right. \\
& \left. \left. - \frac{1}{2} \frac{\chi}{(1+\chi)^2} (\ln^2 \chi + \pi^2) - \left(\frac{1}{\chi(1+\chi)} + \frac{3}{2} \right) \ln \chi - \frac{1}{2\chi} \right) \right\}. \quad (\text{D.6})
\end{aligned}$$

Finally, we provide parts of the explicit expressions for eqs. (4.48) and (4.49). They are

$$\begin{aligned}
A_{4;1;1}(1, 2, 3, 4) = & \frac{4}{3} \rho c_\Gamma^2 \frac{(-s)^{-2\epsilon}}{\chi^2(1+\chi)^2} \frac{1}{\epsilon} \\
& \times \left[\chi^3 (3 + 3\chi + 3\chi^2 + \chi^3) \ln^2 \left(\frac{\chi}{1+\chi} \right) + 4\chi^3 \ln(1+\chi) \ln \left(\frac{\chi}{1+\chi} \right) \right. \\
& + (1 + 3\chi + 3\chi^2 + 3\chi^3) \ln^2(1+\chi) + 2\pi^2 \chi^3 \\
& + 2\chi^3 (1+\chi) (3+\chi) \ln \left(\frac{\chi}{1+\chi} \right) - 2\chi (1+\chi) (1+3\chi) \ln(1+\chi) \\
& \left. + 2i\pi (1+\chi)^3 \left\{ \chi^3 \ln \left(\frac{\chi}{1+\chi} \right) - \ln(1+\chi) + \chi (1+\chi) \right\} \right] + \mathcal{O}(\epsilon^0) \quad (\text{D.7})
\end{aligned}$$

and

$$\begin{aligned}
A_{4;3;0}(1, 2, 3, 4) = & \frac{4}{3} \frac{\rho}{(4\pi)^4} \frac{1}{\chi^2(1+\chi)^2} \\
& \times \left\{ \chi^4(3+3\chi+\chi^2) \ln^3\left(\frac{\chi}{1+\chi}\right) - (1+3\chi+3\chi^2) \ln^3(1+\chi) \right. \\
& + \chi^3(1+6\chi+6\chi^2+2\chi^3) \left(\ln(1+\chi) \ln\left(\frac{\chi}{1+\chi}\right) + \pi^2 \right) \ln\left(\frac{\chi}{1+\chi}\right) \\
& - (2+6\chi+6\chi^2+\chi^3) \left(\ln(1+\chi) \ln\left(\frac{\chi}{1+\chi}\right) + \pi^2 \right) \ln(1+\chi) \\
& + 2\chi^4(1+\chi) \ln^2\left(\frac{\chi}{1+\chi}\right) + 2\chi(1+\chi) \ln^2(1+\chi) \\
& + 2\chi(2+\chi+2\chi^2)(1+\chi)^2 \ln(1+\chi) \ln\left(\frac{\chi}{1+\chi}\right) \\
& + 2\pi^2\chi(1+\chi)^4 + 18\chi^2(1+\chi)^2 \\
& + i\pi \left[4(1+3\chi+3\chi^2+\chi^3+3\chi^4+3\chi^5+\chi^6) \ln(1+\chi) \ln\left(\frac{\chi}{1+\chi}\right) \right. \\
& + \chi^3(-1+3\chi+3\chi^2+\chi^3) \ln^2\left(\frac{\chi}{1+\chi}\right) + (1+3\chi+3\chi^2-\chi^3) \ln^2(1+\chi) \\
& \left. - 2\chi(1+\chi)(2+3\chi+3\chi^2) \ln\left(\frac{\chi}{1+\chi}\right) + 2\chi^2(1+\chi)(3+3\chi+2\chi^2) \ln(1+\chi) - 2\pi^2\chi^3 \right] \left. \right\} + \mathcal{O}(\epsilon).
\end{aligned} \tag{D.8}$$

We only give the lowest order in ϵ term for $A_{4;1;1}$ due to the complexity of the $\mathcal{O}(\epsilon^0)$ term. It is already evident at this order that the dimensionally-regulated YM amplitude does not agree with eq. (2.4), the sdYM form-factor result. The predicted answer from the CCA bootstrap for $A_{4;3;0}$ is merely the $18\chi^2(1+\chi^2)$ term in eq. (D.8).

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