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Near mass-shell double boxes

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Abstract: Two-loop multi-leg form factors in off-shell kinematics require knowledge of planar and nonplanar double box Feynman diagrams with massless internal propagators. These are complicated functions of Mandelstam variables and external particle virtualities. The latter serve as regulators of infrared divergences, thus making these observables finite in four space-time dimensions. In this paper, we use the method of canonical differential equations for the calculation of (non)planar double box integrals in the near mass-shell kinematical regime, i.e., where virtualities of external particles are much smaller than the Mandelstam variables involved. We deduce a basis of master integrals with uniform transcendental weight based on the analysis of leading singularities employing the Baikov representation as well as an array of complementary techniques. We dub the former asymptotically canonical since it is valid in the near mass-shell limit of interest. We iteratively solve resulting differential equations up to weight four in terms of multiple polylogarithms.

Keywords: Higher-Order Perturbative Calculations, Renormalization and Regularization, Scattering Amplitudes, Supersymmetric Gauge Theory

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Contents

1 Introduction

The infrared structure of off-shell observables in massless gauge theories attracted attention in the past couple of years. Within the context of the maximally supersymmetric Yang-Mills theory (aka $\mathcal{N} = 4$ sYM) this kinematical regime can be addressed in a fully gauge-invariant fashion by studying the theory on its Coulomb branch [1]. With a proper choice of vacuum expectation values for the model's scalar fields, one can mimic the off-shellness of the unbroken gauge symmetry phase with nonvanishing masses for external particles only, while keeping all states propagating in internal lines of Feynman graphs massless. This regime is of phenomenological interest in physical theories like QCD. As opposed to the fully massless case where infrared singularities arise as poles in the dimensional regularization parameter $\varepsilon = (4 - D)/2$, in the nearly mass-shell regime of virtual amplitudes, they are replaced by the logarithms of external states' virtualities. An orthodox universality of infrared physics would suggest that critical exponents in both cases will be given by the very same function of the Yang-Mills coupling constant. However, recently this was demonstrated to be far from the truth [2–5].

Four- [2] and five-leg [3] scattering amplitudes as well as two-particle form factors [4, 5] were the first few examples to exhibit a novel feature of the near mass-shell kinematics as opposed to the fully massless regime. While the infrared physics in the latter was known, since the inception of QCD [6], to be governed by the cusp anomalous dimension [7, 8] the former

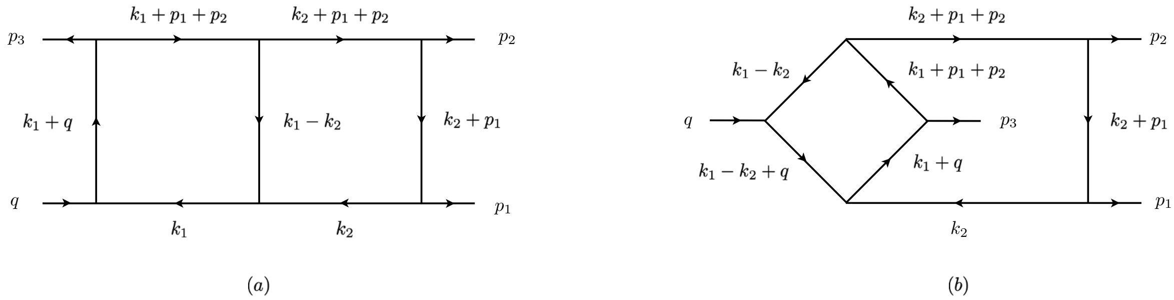

Figure 1. Planar and non-planar double box graphs in the left and right panels, respectively.

involved a different function of the coupling, the so-called octagon anomalous dimension [9–11]. To further elucidate its role, one needs to address more complicated observables containing more scales. They are of interest for several reasons. First, it is desirable to test the infrared factorization and off-shell universality in circumstances that involve multiple scales at the same time. Second, for near mass-shell scattering amplitudes with more than five legs and form factors with more than two, there is a residual finite contribution free from infrared logarithms but depending on Mandelstam-like variables. These are known as remainder functions. A natural question arises whether they are the same both in on- and off-shell regimes. Given that the critical exponents are different, one would expect them to differ as well. But one needs explicit verifications.

Remainder functions in the massless case of planar $\mathcal{N} = 4$ sYM are endowed with a stringy description [12, 13] in terms of an effective two-dimensional world-sheet [14, 15]. The string in question is the so-called GKP string [16] with its energy density determined by the cusp anomalous dimension. The string supports a set of elementary excitations of a T-dual theory, with their dispersion relations and scattering matrices known exactly in 't Hooft coupling constant [17]. One may wonder then, given the vacuum of off-shell observables is determined by the octagon anomalous dimension, whether the spectrum of excitations that live on it and their interactions remain the same as on the GKP background. This is a long-term goal. On the way toward it, one needs 'experimental' data from explicit field theoretical calculations to confirm or deny this expectation. The first step will be undertaken in this paper.

In this work, we calculate Feynman integrals of double box families, see figure 1, relevant for the problem of three-leg form factors $\langle p_1, p_2, p_3 | \mathcal{O}(q) | 0 \rangle$ at two-loop perturbative order. As we advocated above, we are particularly interested in the kinematical situation where the off-shellness of external particles with momenta p_ℓ ($\ell = 1, 2, 3$) are equal and small compared to the virtuality q^2 associated with the operator $\mathcal{O}$, — the lowest super-component of the stress-tensor multiplet. To this end, we will rely on the method of differential equations [18, 19] in its modern-day incarnation that employs canonical bases [20]. To date, this is the most powerful and efficient technique to tackle multi-scale Feynman integrals. Recently, it was successfully applied to the planar double box integrals (left panel in figure 1) with three [22] and four [23] external squared momenta being off the light cone and all internal lines being massless. A basis of uniformly transcendental (UT) integrals was established and its symbol alphabet was analyzed. The latter was shown to be populated by letters expressed in terms of multiple square roots but no solution to the differential equations was offered. We will fill in this gap below for our kinematical situation and supplement it with an analysis of nonplanar graphs as well (right panel in figure 1) which are far more complex. We will demonstrate that the near mass-shell limit provides sufficient simplification of the structure of canonical differential equations to offer a solution in terms of multiple polylogarithms [24] with all square roots gone from their arguments.

Our subsequent presentation is organized as follows. In the next section, we set up the kinematics and classes of Feynman integrals to be studied both for planar and nonplanar families. Next, we move on to the construction of canonical bases. We will discuss the two cases in parallel providing necessary technical details as needed so that a curious reader could reproduce all results if desired. We start in section 3 by building an initial basis of master integrals (MIs) making use of the integration-by-parts (IBP) to deduce a primary basis. Then in section 4, we use leading singularities and a variety of other available techniques to cast them in the canonical form for the planar case. The nonplanar family is far more complex and while we manage to build a canonical basis for lower sectors, we encounter elliptic cases and thus turn to the asymptotic limit in question where these degenerate into poles. The asymptotically canonical basis for non-planar graphs is presented in section 5. We furnish solutions to the resulting differential equations and determine corresponding integration constants in section 6 making use of a variety of criteria that bypass the necessity for explicit evaluation of parametric integrals. In both situations, explicit results are given up to weight-four in terms of multiple polylogarithms and they are further recast in terms of classical Euler polylogarithms and an additional two-argument polylogarithm $\mathrm{Li}_{2,2}$ at weight-four. Finally, we conclude and outline directions for future developments. Mathematica notebooks files published as supplementary material provide the necessary details for the construction and solution of canonical differential equations for any (non-elliptic) family of Feynman graphs.

2 Setting up conventions

To begin with, let us establish our notations. The kinematics of interest correspond to the momentum flow from the operator source $\mathcal{O}(q)$ to off-shell external particles, obeying the conservation condition $q = p_1 + p_2 + p_3$. We introduce three Mandelstam variables according to

$$u \equiv -(p_1 + p_2)^2 , \qquad v \equiv -(p_2 + p_3)^2 , \qquad w \equiv -(p_3 + p_1)^2 , \tag{2.1}$$

which are related by the equation

$$u + v + w = -q^2 + 3\mu . \tag{2.2}$$

Nevertheless, throughout our subsequent analysis, we will treat u, v, and w as independent since this provides stringent checks on the correctness of our derivations. Above, we introduced equal Euclidean virtualities for all particle legs $p_\ell^2 \equiv -\mu$. Since the overall scale of a Feynman integral can be always unambiguously restored on dimensional grounds, we will set $q^2 = -1$ in what follows.

The families of graphs that take centre stage in this paper are shown in figure 1. Even though Feynman integrals contributing to physical observables are finite for nonvanishing off-shellness, nevertheless, we will work with a dimensionally regularized theory to be able to

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apply IBP reduction which requires a D-dimensional setup to render bases of sought-after MIs complete. We work in conventions of ref. [21]. The two-loop non- and planar integrals

$$G_{a_1 \dots a_9} = \mathrm{e}^{2\varepsilon\gamma_{\mathrm{E}}} \int \frac{d^D k_1}{i\pi^{D/2}} \frac{d^D k_2}{i\pi^{D/2}} \prod_{j=1}^{9} D_j^{-a_j} \tag{2.3}$$

are determined by a set of massless propagators $1/D_j$ (for $j = 2, \dots, 7$) and two irreducible scalar products $D_{8,9}$ defined according to the momentum flow exhibited in figure 1 as

$$\begin{aligned} &D_2 = -(k_1 + p_1 + p_2)^2 , && D_3 = -(k_1 + q)^2 , && D_4 = -(k_1 - k_2)^2 , && D_5 = -k_2^2 , \\ &D_6 = -(k_2 + p_1)^2 , && D_7 = -(k_2 + p_1 + p_2)^2 , && D_8 = -(k_1 + p_1)^2 , && D_9 = -(k_2 + q)^2 , \end{aligned} \tag{2.4}$$

with the remaining denominator

$$D_1 = -k_1^2 , \qquad \text{and} \qquad D_1 = -(k_1 - k_2 + q)^2 \tag{2.5}$$

corresponding to the planar and non-planar cases, respectively. All indices a_i are integers with $a_{8,9} \leq 0$. Let us turn to these two families one by one.

3 Primary basis of MIs and differential equations

Let us begin with the planar graph as a case study. Bases of integrals defining it were previously addressed in refs. [22, 23], however, we will use this more familiar family to set up our formalism so that we can be more concise in our following presentation of the non-planar graph, which is computationally more demanding but does not bring anything new to the table to a certain degree.

Preliminary counting of MIs can be done with a variety of available tools, say with `Mint` [25] or the modular component of `FIRE` [26], which was the go-to tool in our analysis. Constructing a list of integrals in the top, i.e., level-seven sector, obtained by inequivalent permutations of two indices equal to two $G_{221111100}$, we prepare start files and generate symmetry relations with `LiteRed` [27, 28]. A modular arithmetic IBP then yields an initial set of 74 MIs. We give preference to Laporta-reducible values of indices being equal to 2 since experience with canonical bases has taught us that these more likely than not be endowed with single leading singularities and thus serve as UT candidates. Next, we use `FindRules` command of `FIRE` to deduce 10 symmetry equations between MIs in our preferential basis, thus reducing their number to 64. However, this is not the end of the story. We can further determine 'hidden' relations as well. To accomplish this, we create lists of integrals sufficiently close to the preliminary set and containing these as a subset: it includes integrals with none, one, and two indices set to 2. Then an IBP reduction reveals additional two relations among them reducing their total number to 62. At this step, it is always advisable to verify that thus obtained basis does not yield the so-called 'bad' denominators according to the nomenclature of ref. [21]. In fact, we find none. But at level five, IBP yields quite lengthy denominator polynomials in the Mandelstam variables and the off-shellness and these can be traded however for significantly more compact ones. This provides us with a solid starting set of 62 preliminary MIs $\boldsymbol{I}$ for our subsequent analytical analysis which we will use from now on as the option `#masters` for IBP reduction with `FIRE`. These read

$$\begin{aligned}\boldsymbol{I}=\{&G_{001101000}, G_{001110000}, G_{010110000}, G_{100101000}, G_{001110100}, G_{001110200}, G_{001111000}, G_{001112000},\\
&G_{011011000}, G_{011101000}, G_{011102000}, G_{011110000}, G_{011120000}, G_{100101100}, G_{100101200}, G_{101010100},\\
&G_{101011000}, G_{101100100}, G_{101100200}, G_{101101000}, G_{101102000}, G_{110010100}, G_{110011000}, G_{110101000},\\
&G_{110102000}, G_{002111100}, G_{002211100}, G_{011011100}, G_{011101100}, G_{011110100}, G_{011111000}, G_{011112000},\\
&G_{011121000}, G_{011211000}, G_{012111000}, G_{012121000}, G_{012211000}, G_{202011100}, G_{101101100}, G_{101101200},\\
&G_{101102100}, G_{101201100}, G_{101201200}, G_{102102100}, G_{102201100}, G_{102110100}, G_{102211000}, G_{110011100},\\
&G_{110111000}, G_{111010100}, G_{111011000}, G_{111102000}, G_{111202000}, G_{011111100}, G_{101111100}, G_{111011100},\\
&G_{111101100}, G_{111111000}, G_{111111100}, G_{111111200}, G_{111211100}, G_{112111100}\}\,. \end{aligned} \tag{3.1}$$

All of the above steps are presented in sections 1 through 10 of the attached Mathematica notebook `A2Zdbox.nb` and the output is saved in the subdirectory `dbox`. An analysis identical to the one just discussed is performed then for the non-planar family to give us a set of 97 primary MIs $\boldsymbol{I}$

$$\begin{aligned}\boldsymbol{I}=\{&G_{001101000}, G_{001110000}, G_{010110000}, G_{101001000}, G_{110001000}, G_{001110100}, G_{001110200}, G_{001111000},\\
&G_{001112000}, G_{011010100}, G_{011011000}, G_{011101000}, G_{011102000}, G_{011110000}, G_{011120000}, G_{100110100},\\
&G_{101001100}, G_{101001200}, G_{101100100}, G_{101100200}, G_{101101000}, G_{101102000}, G_{110001100}, G_{110001200},\\
&G_{110101000}, G_{110102000}, G_{111001000}, G_{111002000}, G_{111100000}, G_{001111100}, G_{001111200}, G_{011011100},\\
&G_{011101100}, G_{011110100}, G_{011111000}, G_{011112000}, G_{011113000}, G_{011121000}, G_{011211000}, G_{012111000},\\
&G_{021111000}, G_{200211100}, G_{101101100}, G_{101101200}, G_{101101300}, G_{101102100}, G_{101201100}, G_{102101100},\\
&G_{201101100}, G_{101110100}, G_{101111000}, G_{110011100}, G_{110011200}, G_{110101100}, G_{110111000}, G_{110112000},\\
&G_{110113000}, G_{110121000}, G_{110211000}, G_{120111000}, G_{210111000}, G_{111001100}, G_{111001200}, G_{111001300},\\
&G_{111002100}, G_{112001100}, G_{121001100}, G_{211001100}, G_{111011000}, G_{111100100}, G_{111101000}, G_{111102000},\\
&G_{111103000}, G_{112101000}, G_{121101000}, G_{211101000}, G_{221101000}, G_{011111100}, G_{101111100}, G_{110111100},\\
&G_{111011100}, G_{111101100}, G_{111101200}, G_{111102100}, G_{111201100}, G_{112101100}, G_{121101100}, G_{111110100},\\
&G_{111111000}, G_{111112000}, G_{111121000}, G_{111211000}, G_{112111000}, G_{211111000}, G_{111111100}, G_{111111200},\\
&G_{111112100}\}\,. \end{aligned} \tag{3.2}$$

These are stored in the subdirectory `nbox`.

After these preparatory studies, we move on to the construction of the derivatives in the Mandelstam variables and the off-shellness by performing differentiations with `LiteRed`. The differential $d\boldsymbol{I} = du\,\partial_u \boldsymbol{I} + dv\,\partial_v \boldsymbol{I} + dw\,\partial_w \boldsymbol{I} + d\mu\,\partial_\mu \boldsymbol{I}$ then needs to be IBP-reduced back to the MIs $\boldsymbol{I}$ thus generating the sought-after differential equations

$$\partial_i \boldsymbol{I} = \boldsymbol{M}_i \cdot \boldsymbol{I}\,, \tag{3.3}$$

with $i = u, v, w, \mu$. While the analytic IBP reduction for the planar family takes a matter of hours on a typical machine, the non-planar case is far more computationally demanding. For instance, the reduction of level-seven integrals from the left-hand side of the differential

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equations (3.3) given in the accompanying file `intsde-nbox2.m` down to MIs #3 $G_{010110000}$ and #4 $G_{101001000}$ from `pr-nbox2.m` takes a staggering 7 and 10 days, respectively, on a typical compute node but with 700 GB of RAM. To cross-check that the resulting tables are indeed correct, we relied on modular arithmetic runs with `FIRE` with subsequent balanced rational reconstruction developed in ref. [29]. With an MPI parallelization of 1024 cores of ASU's `Sol` supercluster [30], the 7 → #3 IBP took 58 hours with `Flint` [31] and 46 hours with `Symbolica` [32] but indeed confirmed our earlier analytical findings. We provide a detailed account of the derivation in section 11 of the accompanying notebook `A2Zdbox.nb` for the planar graph. To ease navigation of the accompanying Mathematica notebooks, the reader is referred to appendix A for an itemized description of their contents.

4 Canonical basis

Now the main task at hand is to transform the basis of MIs $\boldsymbol{I} = \boldsymbol{T} \cdot \boldsymbol{J}$ such that the differential equations (3.3) admit their canonical form

$$\partial_i \boldsymbol{J} = \varepsilon \boldsymbol{A}_i \cdot \boldsymbol{J} \,, \qquad \varepsilon \boldsymbol{A}_i = \boldsymbol{T}^{-1} \cdot \boldsymbol{M} \cdot \boldsymbol{T} - \boldsymbol{T}^{-1} \cdot \partial_i \boldsymbol{T} \,, \tag{4.1}$$

with each element of the $\boldsymbol{A}$-matrices being Fuchsian, i.e., possessing simple poles only, and ε-independent [20]. To this end, we need to determine viable UT candidates from our primary list of MIs. Provided this procedure is successful, a differentiation of these pure UT integrals will reduce their transcendental weight by one and, thus, the right-hand side of (3.3) will have to be proportional to ε, which carries the transcendentality weight -1. To practically implement this strategy, we rely on the well-known conjecture that connects uniform weight integrals with the properties of their integrands, namely, that the singularities of an integrand are locally of logarithmic type [33, 34], see, e.g., [35] for a comprehensive review.

As the calculation of unitarity cuts is in general downright easier than a solution of integrals per se, the idea is to use the former for the identification of Feynman integrals that correspond to pure functions. To perform multidimensional unitarity cuts efficiently, one has to rely on an appropriate parametrization. Since Feynman integrals possess integrands which are rational functions of propagators and ISPs, it is only natural to choose these as integration parameters $z_i \equiv D_i$. To date, this is the most concise framework which is known as the Baikov representation [36, 37], see refs. [38, 39] for comprehensive reviews. This form of integrals trivializes the computation of unitarity cuts. The so-called leading singularities correspond to taking the maximal cut, i.e., successive residues in all $z_i = 0$, followed by residues in composite singularities emerging along the way from any Jacobian factors [40]. This completely localizes all integrations and provides a function of external kinematical variables, which once being divided out from the Feynman integral in question yields a pure UT candidate with constant leading singularity. Of course, for a given integral, there could be multiple ways to localize all integrations depending on the order of taking residues and this can yield different leading singularities. Only integrals with a single leading singularity can be autonomously recast as UT, while in cases where there is more that one, linear combinations of these have to be studied as well. It is important to realize that UT candidates found this way may not correspond to MIs of the traditional Laporta algorithm.

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This is the reason why we chose from the very beginning to favor MIs having indices equal to 2 in our IBP studies. Leading singularities analysis completely fixes the diagonal blocks of the $\boldsymbol{A}$-matrices, which do not mix MIs at different levels. Then we move on to study sub-maximal cuts to find corrections from lower-level subsectors.

In our analysis, we relied on the Mathematica implementation of the Baikov parametrization via `Baikov.m` package developed in ref. [41]. We provide thorough details of it use in section 12 of the accompanying `Mathematica` notebook `A2Zdbox.nb` for a subsector of the planar double box integral as described in appendix A.1. This is followed by an iterative construction of the canonical basis of MIs starting from the lowest sector and going up. The essence of the method consists of finding leading singularities of primary MIs and factoring them out (sometimes in linear combinations) to construct potential candidates of UT MIs. These are then used for IBP reductions to verify whether they are indeed UT. Since a more general case was already studied in the literature [23], we provide only sporadic details for the latter in sections 13–14 of the same supplementary material file with final results for the canonical basis and all $\boldsymbol{A}$-matrices given in `dboxCan62.m` and `AuPC.m`, `AvPC.m`, `AwPC.m`, `AmPC.m`, respectively.

5 Asymptotically canonical basis

The Baikov representation analysis akin to the one used above immediately convinces us that the non-planar graph (right panel in figure 1) possesses elliptic sectors [42], see ref. [43] for a thorough review, implying that some leading singularities reside on elliptic curves [44, 45] rather being merely algebraic. However, they smoothly degenerate into the latter as we send the off-shellness μ down to zero since the ends of branch cuts collide and reduce to poles. Since at the end of the day, all we are after is the asymptotic behavior of our MIs as $\mu \to 0$ up to terms that vanish in μ, we can implement this limit on differential equations for the primary set of 97 MIs and then construct what we call as the *asymptotically* canonical basis. The latter solves the singular limit of the off-shellness equation but treats all variables exactly. This will become transparent from the discussion that follows.

Thus, we change the strategy for basis construction in the non-planar case. Namely, we tend to assume generic values for all variables (u, v, w as well as μ) as long as we encounter only algebraic leading singularities and swiftly pass to the asymptotic consideration when it is no longer the case. The Baikov representation is again used for this purpose. In elliptic sectors uncovered via this procedure, we do not attempt the construction of UT elements. Instead, we go back to their differential equations and expand/solve them to the leading order in the off-shellness μ. In particular, this occurs in the two level-six sectors $G_{111101100}$ and $G_{111111000}$, and the top level-seven sector $G_{111111100}$. For these, we require the following properties to be fulfilled by the differential equations: (i) the off-shellness matrix $\boldsymbol{M}_\mu$ can be cast in the form

$$\boldsymbol{M}_\mu \to \boldsymbol{A}_\mu = \frac{\varepsilon}{\mu}\boldsymbol{A}^0_\mu + O(\mu^0)\,, \tag{5.1}$$

with $\boldsymbol{A}^0_\mu$ being a matrix of rational numbers, i.e., its elements are strictly independent of u, v, and w; (ii) $\boldsymbol{M}_i$ matrices for the Mandelstam variables $i = (u, v, w)$ have well-defined finite limit as $\mu \to 0$ and do not possess elements with square roots; (iii) last but not least, resulting differential equations in u, v, and w are canonical or can be made canonical with an appropriate similarity transformation.

As usual, we focus on diagonal blocks first but use now the leading order form of the elements of the matrices $\boldsymbol{M}_i$ (with $i = u, v, w, \mu$) as μ goes to zero for a proper choice of asymptotically canonical elements. It is easier to demonstrate it with an example of the $G_{111101100}$ sector. The primary set of MIs defining this sector is

$$\{G_{111101100}\,,\ G_{111101200}\,,\ G_{111102100}\,,\ G_{111201100}\,, G_{112101100}\,,\ G_{121101100}\}\,. \tag{5.2}$$

To start with we utilize the form of $\boldsymbol{M}_\mu = \boldsymbol{M}_\mu^0/\mu + O(\mu)$, with $\boldsymbol{M}_\mu^0$ being a function of u, v, w and ε, to conclude that if we are to multiply the elements 2,3,5,6 with μ, after a similarity transformation the off-shellness matrix will take the required form (5.1). We know a priori, however, that the ε-dependence of this seed basis will have to be adjusted later since, as rule of thumb, one associates ε^4 with MIs without any twos and ε^{2-n} for MIs with n twos in the first 7 positions. For now, it will do the job, however. Next, we change the basis by multiplying each element in it with an unknown function of the Mandelstam variables

$$G \to f(u, v, w)G\,. \tag{5.3}$$

Enforcing the ε-form on the resulting differential equations for this new basis, we solve the arising differential equations on the functions $f(u, v, w)$ and get, after a gentle mixture of elements with each other and re-arrangement,

$$\begin{aligned}\{&\mu v(u+v+w)^2/(u+v)G_{111101200},\ \mu v[wG_{111102100} + (u+v+w)G_{111101200}],\\ &\mu v[uG_{112101100} + (u+v+w)G_{121101100}],\ \mu v(u+v+w)^2/(v+w)G_{121101100},\\ &f_5 G_{111101100},\ f_6 G_{111201100}\}\,.\end{aligned} \tag{5.4}$$

The last two elements of this naive basis contain square roots of Mandelstam variables in functions $f_{5,6}$. This is hardly a surprise since we completely ignored up to now the correct ε-dependence of the basis elements which resulted in erroneous differential equations for $f_{5,6}$. If we do it in a proper manner, we observe a violation of the canonical form of the differential equations in u, v, and w. Details on this calculation can be found in section 1 of the accompanying Mathematica notebook `AsyClevel6.nb`.

The above finding instructs us to look further for a better choice of elements 5 and 6 of this sector. The method of trial and error is quite tedious and exhausting, so we turn to the massless non-planar double box for inspiration. In the strict limit $\mu \to 0$, the first four elements if (5.4) vanish and one is left with just two elements. The massless non-planar box analysis demonstrates that indeed it possesses two level-six sectors with one of them containing two primary elements $G_{111101100}$ and $G_{111101200}$. Construction of the canonical basis in this sector is performed in section 2 of the notebook `AsyClevel6.nb` and offers two options for UT elements, namely,

$$\{v(u+v+w)G_{111101100}\,,\ (v+w)G_{1111011-10}\}\,, \tag{5.5}$$

or

$$\{v(u+v+w)G_{111101100}\,,\ (u+v)G_{11110110-1}\}\,. \tag{5.6}$$

We then build upon (5.5) to lift the analysis to the off-shell case in the asymptotic limit and construct the final form of the diagonal block of this sector in section 3 of `AsyClevel6.nb` such that the last two elements in eq. (5.4) are replaced with

$$\begin{aligned}(1+4\varepsilon)\varepsilon v(u+v+w)G_{111101100}\\ +\varepsilon\mu v(u+v+w)/(u+v)[wG_{111102100}-(u+v+w)G_{111101200}]\\ +\varepsilon\mu v(u+v+w)/(v+w)[uG_{112101100}-(u+v+w)G_{121101100}]\end{aligned} \tag{5.7}$$

and

$$\begin{aligned}&(1+4\varepsilon)\varepsilon(v+w)G_{1111011-10}\\ &+\frac{1}{4}\varepsilon\mu v/(v+w)[u(2u+5v+5w)G_{112101100}-(u+v+w)(2u+v+w)G_{121101100}]\,,\end{aligned} \tag{5.8}$$

respectively, and we simultaneously restored a proper relative ε-normalization of these elements. All other sectors can be analyzed in the same fashion.

Though all diagonal sectors were brought by us to the ε-form, not all elements of the $\boldsymbol{A}$-matrices are Fuchsian. Moreover, the off-diagonal blocks are not even close to the required ε-form. However, their transformation to the canonical form is now purely algorithmic. The Fuchsian form is easily obtained by making use of the code `Canonica.m` [46–48]. The latter cannot handle, however, the transformation of all off-diagonal elements in the differential equations to the ε-form using Lee's trick [49]. The latter is implemented in a powerful package `Libra.m` [50], which calls for an external `Fermat` [51] computer algebra system, though it works just as fine[1] even with built-in Mathematica commands. This systematic procedure is demonstrated step-by-step in the supplementary material notebook file `AsyCnbox.nb` proving the output in the file `nboxAsyCan97.m` in the `Canonica` format. This culminates our quest to reach the asymptotically canonical basis in the non-planar case.

6 Integration and determination of integration constants

To summarize, in the previous section we determined the asymptotically canonical form of the differential equation with the one in the off-shellness μ being

$$\partial_\mu \boldsymbol{J} = \frac{\varepsilon}{\mu}\boldsymbol{A}^0_\mu \boldsymbol{J}\,, \tag{6.1}$$

up to terms vanishing as $\mu \to 0$, with $\boldsymbol{A}^0_\mu$ being a purely numerical matrix. Solving this leading order equation is simple and it provides a transformation

$$\boldsymbol{J}(u,v,w,\mu) = \mu^{\varepsilon \boldsymbol{A}^0_\mu}\cdot \boldsymbol{J}_0(u,v,w)\,, \tag{6.2}$$

to the μ-independent basis $\boldsymbol{J}_0$ via a matrix exponent whose entries are expressed as linear combinations of $\mu^{-n\varepsilon}$-terms accompanied by rational number coefficients. The basis $\boldsymbol{J}_0$ solves in turn the asymptotically canonical equations

$$\partial_i \boldsymbol{J}_0 = \varepsilon \boldsymbol{A}^0_i \boldsymbol{J}_0 \qquad \text{with} \qquad i=(u,v,w)\,, \tag{6.3}$$

[1]Though ten times slower.

where the elements of $\boldsymbol{A}_i^0 = \boldsymbol{A}_i|_{\mu=0}$ are expressed in terms of rational functions of the Mandelstam invariants u, v and w only.

The main advantage of the canonical form of differential equations (6.3) is that their solution can be written in terms of a path-ordered exponential and explicitly calculated via Chen's iterative integrals theory [52],

$$\boldsymbol{J}_0 = P_\gamma \exp\left(\varepsilon \int_\gamma \boldsymbol{A}^0\right) \boldsymbol{J}_{00} \,, \tag{6.4}$$

where $\boldsymbol{A}^0 = du\boldsymbol{A}_u^0 + dv\boldsymbol{A}_v^0 + dw\boldsymbol{A}_w^0$ and $\boldsymbol{J}_{00}$ is a vector of integration constants. At each order in the ε-expansion it receives an independent set of unknowns

$$\boldsymbol{J}_{00} = \sum_{p\geq 0} \varepsilon^p \boldsymbol{c}^{(p)} \,. \tag{6.5}$$

The solution (6.4) is independent of the choice of the path γ since the integrability of the differential equations is a zero-curvature condition, $\mathrm{d}\boldsymbol{A}^0 - \varepsilon \boldsymbol{A}^0 \wedge \boldsymbol{A}^0 = 0$. In our analysis, we chose a piece-wise path

$$\gamma = [0, u] \cup [0, v] \cup [0, w] \,. \tag{6.6}$$

In more practical terms, we take the first equation with $i = u$ in (6.3) and solve it with respect to u. Then we turn to the v-variable. To eliminate the u-dependence from the differential equation, we form a difference between the right-hand side of (6.3) for $i = v$ and the derivative in v of the solution found in the previous step. We then find its primitive in v. Finally, we repeat the procedure for w. This procedure is cast in a Mathematica module `Integrator` in the attached notebook `AsySolCnbox.nb`. The result is then given in terms of multiple polylogarithms (MPLs) [24]. The latter are defined recursively via an integral iteration, e.g.,

$$G(a_0, \boldsymbol{a}; u) = \int_{[0,u]} du' \frac{G(\boldsymbol{a}; u')}{u' - a_0} \,.$$

However, in order to have a better handle on the analytical structure of our results, we recast them in terms of classical Euler polylogarithms[2] whenever possible. It is well known that for the weight up to three, all MPLs can be traded to Li_n's, see, e.g., [53–55] (Chapter 2 on MPLs of the latter reference is available at [56]). At weight four, one needs to include an additional two variable MPL $\mathrm{Li}_{2,2}$ to the minimal basis of classical polylogarithms as was observed in ref. [57]. This basis transformation was worked out and is conveniently implemented into the routine `gtolrules.m` devised in ref. [58]. We need to make sure that a proper 'branch' of MPLs is taken into account at a given point in the (u, v, w)-space since a single expression in terms of Li_n's and $\mathrm{Li}_{2,2}$ is not sufficient to cover the entire space of (complexified) Mandelstam variables.

At each p-order of the ε-expansion, arrays of integration constants $\boldsymbol{c}^{(p)}$ have to be determined from a set of boundary conditions. However, we would like to avoid an explicit calculation of any Feynman integrals since, even in some corners of the phase space, they are very complex and, which is worse, quite numerous. Instead, we relied on several criteria to fix them such as (i) numerology, (ii) cancellation of unphysical poles, (iii) absence of imaginary parts, and (iv) finite integrals.

[2]These are readily encoded in Mathematica.

(i) The first condition is self-explanatory. Using the fact that our asymptotically canonical MIs obey the property of being UT, we cast the integration constants into a product of rational numbers times values of the Riemann zeta function $\zeta_p = \zeta(p)$ of the same transcendental weight,

$$\boldsymbol{c}^{(p)} = \boldsymbol{r}^{(p)} \zeta_p \,, \tag{6.7}$$

with the employed convention $\zeta_0 = 1$ and $\zeta_1 = 0$ for the first two values of p. Then, computing the MIs at a random point for the Mandelstam variables with FIESTA [59], we confronted its results against the numerical evaluation of our solutions. In this manner, we managed to confidently determine 84 $r_j^{(p)}$ for $p = 0, 2$, 81 $r_j^{(3)}$'s and 79 $r_j^{(4)}$'s. The monotonically decreasing number of rationally reconstructed constants with increasing p is related to the loss of FIESTA's numerical precision and emergence of large rationals at higher orders in ε.

(ii) To alleviate the aforementioned problem and cross check correctness of previous numerological findings, we employed conditions for unphysical pole cancellation in the right-hand side of the canonical differential equations, namely, at $u + v = 0$, $v + w = 0$ and $w + u = 0$. Then, decomposing the A-matrices in explicitly Fuchsian form

$$\boldsymbol{A}_i^0 = \frac{\boldsymbol{a}_{i,u+v}}{u+v} + \frac{\boldsymbol{a}_{i,v+w}}{v+w} + \frac{\boldsymbol{a}_{i,w+u}}{w+u} + \dots \,, \tag{6.8}$$

we imposed the following equations on our basis

$$\boldsymbol{a}_{i,\alpha} \boldsymbol{J}_0 |_{\alpha=0} = 0 \,. \tag{6.9}$$

These provided a further set of 10,7,9 and 10 identifications/relations between integration constants at levels $p = 0, 2, 3$ and 4, respectively.

(iii) To further constrain the integration constants at order p, we used solutions at order $p+1$ and required the vanishing of imaginary parts as one approaches unphysical poles in eqs. (6.9). This provided the value on the last $r_{90}^{(3)}$ element from the solution at order ε^4. The solution at fifth order in ε was used in conjunction with high-precision numerical computations of MPLs with the C++ package `GiNaC` [60] making use of a Mathematica interface from ref. [61] and subsequent reconstruction of analytical expressions with the PSLQ algorithm [62]. This allowed us to deduce 3 equations for $r_j^{(4)}$ ($j = 86, 92, 97$).

(iv) The implementation of the above three conditions fixed all but 3,6,7 and 8 integration constants for $p = 0, 2, 3$ and 4, correspondingly. Then, by a judicious choice, we found a set of 26 finite (in ε) integrals

$$\begin{array}{lllll}
G_{011111100}\,, & G_{101111100}\,, & G_{110111100}\,, & G_{111011100}\,, & G_{111110100}\,, \\
G_{111111000}\,, & G_{1111111-10}\,, & G_{11111110-1}\,, & G_{111111100}\,, & G_{1111111-1-1}\,, \\
G_{011101100}\,, & G_{011110100}\,, & G_{011111000}\,, & G_{101101100}\,, & G_{101110100}\,, \\
G_{101111000}\,, & G_{110101100}\,, & G_{110111000}\,, & G_{111001100}\,, & G_{111011000}\,, \\
G_{111100100}\,, & G_{111101000}\,, & G_{1111011-10}\,, & G_{111101100}\,, & G_{1111110-10}\,, \\
G_{11111100-1}\,, & & & &
\end{array} \tag{6.10}$$

which were reduced with IBP identities to our set of 97 MIs. The resulting relations are divergent and pole cancellation in the Laurent ε-expansion provided an ultimate set of equations to completely fix the solutions at orders one through three. In fourth order, we obtained the last five integration constants whose numerical value to $O(10^{-3})$ were determined to be

$$r_{83}^{(4)} = 1515.669\,, \; r_{84}^{(4)} = 26.958\,, \; r_{90}^{(4)} = -50645.784\,, \; r_{91}^{(4)} = 6.659\,, \; r_{95}^{(4)} = -576.338\,. \tag{6.11}$$

To rationalize these, one has to either perform an analytic calculation of a very large set of Feynman integrals or increase the accuracy of their numerical evaluation to twelve decimal places with FIESTA or any other program. Currently, alas, this is beyond our reach. However, a particular combination of these constants shows up in the three-leg form factor [63], which allows us to eliminate one of them from the above list. It reads

$$\frac{r_{83}^{(4)}}{42} - r_{84}^{(4)} + \frac{r_{90}^{(4)}}{252} - \frac{r_{91}^{(4)}}{6} + \frac{r_{95}^{(4)}}{8} = -\frac{62683849}{236544}\,. \tag{6.12}$$

All steps of the above analysis for the non-planar family are thoroughly presented in the accompanying Mathematica notebook `AsySolCnbox.nb`. For the planar graph, it suffices to use just the first two conditions (i) and (ii). All solutions up to the same order in ε are quoted in the supplementary material file `AsySolCdbox.nb`.

7 Conclusions

With this paper, we initiate a series of studies of multi-scale two-loop observables in $\mathcal{N}=4$ sYM. Currently, we constructed bases of UT MIs for double box planar and non-planar graphs in the kinematical limit of small virtualities of three external particles and an arbitrary invariant mass for the last leg. This is a preparatory study for a full-fledged analysis of the three-leg form factor of the stress tensor multiplet to be published separately [63]. The bases in question were used to determine the canonical form of differential equations in the Mandelstam variables u, v, w as well as the off-shellness μ. Solutions to these equations were constructed up to terms vanishing as $\mu \to 0$. The results for all master integrals were obtained as a double Laurent/Taylor expansion in $\varepsilon/\log\mu$ up to (and including) weight four contributions. All integration constants were successfully fixed analytically with the exception of 5 coefficients at level four where they were found numerically with the accuracy 10^{-3}. Future more precise numerical studies with FIESTA could potentially fix them unambiguously as rational coefficients accompanying the value of ζ_4.

Consideration performed in this work will be generalized in several avenues. From the point of view of identifying two-dimensional integrable physics of the octagon flux-tube, form factors of super-descendants of the stress-tensor multiplet could provide simpler circumstances for its elucidation since they are sensitive to contribution from single charged flux-tube excitations [64] as opposed to singlet pairs determining the lowest half-BPS operator [15]. So far the limitation to form factor observables was solely driven by a lower multiplicity requirement on the number of external legs in a graph to attain a non-trivial remainder

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function. It is well-known that in the case of scattering amplitudes, nontrivial remainder functions emerge starting from six legs. Thus, it is important to analyze these in the near mass-shell kinematics introduced in this paper and compare them both functionally as well as from the microscopic stringy point of view.

Regarding the development of computational techniques of multi-loop Feynman integrals per se, we are currently capable of breaking free from the simplifying assumption of the near mass-shell limit and uplifting our asymptotically canonical basis for the non-planar graph to the situation of arbitrary virtualities. The solution to the resulting equations is a very different issue though.

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A Summary of `Mathematica` notebooks

To make our presentation self-contained, the Arxiv submission of this paper is accompanied by several notebooks. The latter contains all mathematical derivations and results. Let us briefly summarize their contents.

A.1 `A2Zdbox.nb`

This notebook describes the derivation of the canonical basis of MIs for the planar graph in figure 1 (a). In particular,

- 'How many MIs to expect from `Mint`?' uses the software from ref. [25] to get an estimate on the expected number of primary MIs.
- 'Initial list of integrals for IBP' creates an initial set of integrals with two indices set to 2 for an initial IBP reduction.
- 'Preparation of the start file' as a necessary input for `FIRE` [26] and saving resulting files in the `dbox` directory.
- 'Generation of LiteRed rules' uses the code from ref. [27, 28] to automatically find symmetries among primary MIs.
- ' IBP reduction for a family of test integrals and search for (74) MIs' uses the modular component of `FIRE` for fast detection of primary MIs.

- ‘Initial (74) MIs and equivalence rules to reduce them to 64 MIs’ describes how to use the command `FindRules` to detect equivalences among some of the integrals and reduce the number of elements in the initial basis.
- ‘A list of sample integrals [close to 74 MIs found before]’ generates lists obtained from primary MIs by changing (up to two) of their unit indices to two for subsequent use in finding additional relations among MIs.
- ‘Finding additional relations and the list of 62 MIs’ describes IBP reductions of sample integrals obtained in the previous step to MIs and derivation of additional two relations among them.
- ‘Analysis of bad denominators and preferential set of integrals’ uses the package from ref. [21] for the detection of ‘bad’ denominators in IBPs.
- ‘Choosing 62 improved (@ level 5) MIs’ describes the elimination of bad denominator using a basis transformation.
- ‘Deriving DEs’ demonstrates the use of `LiteRed` for the derivation of differential equations for 62 primary MIs in the Mandelstam variables and the off-shellness.
- ‘Leading singularities with Baikov and UT: A2Z for the ice cream cone’ provides a thorough analysis of the ‘ice cream cone’ graph (which represents a subsector for the double box) making use of the software from ref. [41] for derivation of MIs of uniform transcendentality (UT).
- ‘Finding canonical basis’ gives sample calculations for the derivation of UT MIs and their complete final list.
- ‘Canonical DEs: matrices and plots’ presents canonical A-matrices for all differential equations and their sparsity plots for visualization purposes.

A.2 `AsySolCdbox.nb`

This notebook quotes solutions to the canonical differential equations deduced in `A2Zdbox.nb` in the limit $\mu \to 0$ to order $O(\mu^0)$ and obtained as a Laurent expansion in the parameter of dimensional regularization ε up to finite terms.

A.3 `AsyClevel6.nb`

Here, we provide a sample derivation of the asymptotically canonical elements for the non-planar box integral in the level-6 sector $\{111101100\}$.

A.4 `AsyCnbox.nb`

We give level-by-level transformation (split in 14 steps) of the primary set of MIs for the non-planar box to the asymptotically canonical form by using two public codes `Canonica.m` and `Libra.m` from refs. [46–48] and [50], respectively. The result for the canonical A-matrices is obtained there as well.

A.5 AsySolCnbox.nb

The notebook contains detailed solutions of differential equations for the nonplanar box. In particular,

- 'Data, routines, substitutions' folder starts by providing a glossary of the nomenclature used in the file.
  - 'Numerical results for MIs and finite integrals from FIESTA' contains tables of numerical input values for MIs for subsequent determination of integration constants.
  - 'A-matrices and the Integrator' quotes the A-matrices for differential equations in Mandelstam variables and provides a routine `Integrator` for their automatic integration.
  - 'Lists of polylog substitutions' gives a comprehensive list of relations among classical polylogarithms up to level four as well as the MPL $\mathrm{Li}_{2,2}$. These are used in the rest of the notebook for analytical simplification of integration constants.
  - 'PSLQ' provides a one-line code making use of the built-in Mathematica command `FindIntegerNullVector`.
- 'Ep^0' to 'Ep^5' describe the step-by-step determination of integration constants of the Laurent expansion in the parameter of dimensional regularization ε at orders from zero to four based on criteria outlined in section 6 of the main body of this paper. They contain all numerical cross checks against `FIESTA` data making use of the `GiNaC` integrator [60] implemented in the `PolyLogTools.m` package [61].

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