7 Analytics from numerics: five-point QCD amplitudes at two loops

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7.1 Introduction

The operation of the Large Hadron Collider (LHC) has been a great success, with Run 1 culminating in the discovery of the Higgs boson by the ATLAS and CMS experiments in 2012. In Run 2, the LHC experiments have moved towards performing high-precision measurements with uncertainties reaching below the percentage level for certain observables. Looking forward to the Future Circular Collider with electron beams (FCC-ee), which will operate in the experimentally much cleaner environment of electron–positron initial states, there will be an even more dramatic increase in experimental precision. To exploit the precision measurements, the theory community will need to provide high-precision predictions that match the experimental uncertainties. This requires the development of efficient ways to compute these corrections, breaking through the current computational bottlenecks.

In this section, we discuss the calculation of a key component in making such predictions—the loop amplitude. Specifically, we discuss the computation of an independent set of analytical two-loop five-gluon helicity amplitudes in the leading-colour approximation. These amplitudes are an ingredient for the phenomenologically relevant description of three-jet production at next-to-next-to-leading order (NNLO) for hadron colliders. Nonetheless, the methods we present are completely general and can also be applied to predictions for electron–positron collisions.

The first two-loop five-gluon amplitude to be computed was the one with all helicities positive in the leading-colour approximation, initially numerically [1] and subsequently analytically [2, 3]. In the last few years, a flurry of activity in this field led to the numerical calculation of all five-gluon [4, 5], and then all five-parton [6, 7] amplitudes in the leading-colour approximation. The combination of numerical frameworks with finite-field techniques, with a view to the reconstruction of the rational functions appearing in the final results, was first introduced to our field in Ref. [8], and an algorithm applicable to multiscale calculations was presented in Ref. [9]. Inspired by these ideas, the four-gluon amplitudes were analytically reconstructed from floating-point evaluations [10]. The first application involving multiple scales was the single-minus two-loop five-gluon amplitude [11]. In this section, we describe the calculation of the full set of independent five-gluon amplitudes in the leading-colour approximation [12]. These results were obtained using analytical reconstruction techniques, starting from numerical results obtained in the framework of two-loop numerical unitarity [5, 7, 10, 13]. Recently, the remaining five-parton amplitudes have also become available [14], and all two-loop amplitudes for three-jet production at NNLO in QCD are now known analytically in the leading-colour approximation.†

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†The approach taken in Ref. [14] is very similar to that described here; we refer the reader to the results presented in Ref. [14] for a more compact expression for the five-gluon amplitudes and further improvements in

This section is organised as follows. In Section 7.2, we describe the amplitudes under consideration and the numerical unitarity framework employed for their evaluation. Section 7.3 describes the objects we will be computing and the simplifications that are made to allow for an efficient functional reconstruction. The implementation and the results are presented in Section 7.4 and we conclude in Section 7.5.

7.2 Amplitudes

We discuss the computation of the two-loop five-gluon amplitudes in QCD. The calculation is performed in the leading-colour approximation where there is a single partial amplitude. The bare amplitude can be perturbatively expanded as

$$\begin{aligned}\mathcal{A}(\{p_i, h_i\}_{i=1,\dots,5})\Big|_{\text{leading colour}} \\ = \sum_{\sigma\in S_5/Z_5} \mathrm{Tr}\left(T^{a_{\sigma(1)}}T^{a_{\sigma(2)}}T^{a_{\sigma(3)}}T^{a_{\sigma(4)}}T^{a_{\sigma(5)}}\right) g_0^3 \left(\mathcal{A}^{(0)} + \lambda\mathcal{A}^{(1)} + \lambda^2\mathcal{A}^{(2)} + \mathcal{O}(\lambda^3)\right). \quad (7.1)\end{aligned}$$

Here, $\lambda = N_c g_0^2/(4\pi)^2$, g_0 is the bare QCD coupling and S_5/Z_5 is the set of all non-cyclic permutations of five indices. The amplitudes $\mathcal{A}^{(k)}$ appearing in the expansion of Eq. (7.1) depend on the momenta $p_{\sigma(i)}$ and the helicities $h_{\sigma(i)}$ and these proceedings focus on the calculation of $\mathcal{A}^{(2)}$ in the 't Hooft–Veltman scheme of dimensional regularisation, with $D = 4 - 2\epsilon$.

The first step in the analytic reconstruction procedure is the numerical evaluation of the amplitude. We evaluate the amplitudes in the framework of two-loop numerical unitarity [5, 7, 10, 13]. The integrands of the amplitudes $\mathcal{A}^{(2)}$ are parametrized with a decomposition in terms of master integrands and surface terms. On integration, the former yield the master integrals, while the latter vanish. Labelling the loop momenta ℓ_l, the parametrization we use is given by

$$\mathcal{A}^{(2)}(\ell_l) = \sum_{\Gamma\in\Delta}\sum_{i\in M_\Gamma\cup S_\Gamma} c_{\Gamma,i}\frac{m_{\Gamma,i}(\ell_l)}{\prod_{j\in P_\Gamma}\rho_j}, \quad (7.2)$$

with Δ being the set of all propagator structures Γ, P_Γ the associated set of propagators, and M_Γ and S_Γ denoting the corresponding sets of master integrands and surface terms, respectively. If the master integrals are known, the evaluation of the amplitude reduces to the determination of master coefficients $c_{\Gamma,i}$ with $i \in M_\Gamma$. In numerical unitarity, this is achieved by solving a linear system, which is generated by sampling on-shell values of the loop momenta ℓ_l^Γ belonging to the algebraic variety of P_Γ. In this limit, the leading contribution to Eq. (7.1) factorises into products of tree amplitudes

$$\sum_{\text{states}}\prod_{i\in T_\Gamma}\mathcal{A}_i^{\text{tree}}(\ell_l^\Gamma) = \sum_{\substack{\Gamma'\geq\Gamma,\\ i\in M_{\Gamma'}\cup S_{\Gamma'}}} \frac{c_{\Gamma',i}\, m_{\Gamma',i}(\ell_l^\Gamma)}{\prod_{j\in(P_{\Gamma'}\setminus P_\Gamma)}\rho_j(\ell_l^\Gamma)}. \quad (7.3)$$

The tree amplitudes associated with vertices in the diagram corresponding to Γ are denoted T_Γ and the sum is over the physical states of each internal line of Γ. On the right-hand side, the sum is performed over all propagator structures Γ', such that $P_\Gamma \subseteq P_{\Gamma'}$. At two loops, subleading contributions appear, which cannot be described by a factorisation theorem in the on-shell limit. In practice, this complication is eliminated by constructing a larger system of equations, as described, for instance, in Ref. [15]. For a given (rational) phase space point, we

the methodology.

solve the linear system in Eq. (7.3) using finite-field arithmetic. This allows us to obtain exact results for the master integral coefficients in a very efficient manner.

Once the coefficients $c_{\Gamma,i}$ are known, the amplitude can be decomposed into a linear combination of master integrals $\mathcal{I}_{\Gamma,i}$, according to

$$\mathcal{A}^{(2)} = \sum_{\Gamma\in\Delta} \sum_{i\in M_\Gamma} c_{\Gamma,i}\mathcal{I}_{\Gamma,i}\,, \tag{7.4}$$

with

$$\mathcal{I}_{\Gamma,i} = \int \mathrm{d}^D l_l \frac{m_{\Gamma,i}(l_l)}{\prod_{j\in P_\Gamma}\rho_j}\,. \tag{7.5}$$

For planar massless five-point scattering at two loops, the basis of master integrals is known in analytical form [16, 17].

7.3 Simplifications for functional reconstruction

Functional reconstruction techniques allow one to reconstruct rational functions from numerical data, preferably in a finite field to avoid issues related to loss of precision [8, 9]. By choosing an appropriate set of variables, such as momentum twistors [18], we can guarantee that the coefficients $c_{\Gamma,i}$ in Eq. (7.4) are rational. The specific parametrization we use is [9]

$$\begin{aligned}
&s_{12} = x_4, \qquad s_{23} = x_2x_4, \qquad s_{34} = x_4\left(\frac{(1+x_1)x_2}{x_0} + x_1(x_3-1)\right),\\
&s_{45} = x_3x_4, \qquad s_{51} = x_1x_4(x_0 - x_2 + x_3)\,,\\
&\mathrm{tr}_5 = 4\,\mathrm{i}\,\varepsilon(p_1,p_2,p_3,p_4)\\
&\quad\;= x_4^2\left(x_2(1+2x_1) + x_0x_1(x_3-1) - \frac{x_2(1+x_1)(x_2-x_3)}{x_0}\right),
\end{aligned} \tag{7.6}$$

where $s_{ij} = (p_i+p_j)^2$, with the indices defined cyclically. One could, in principle, reconstruct the rational master integral coefficients. However, the difficulty of the reconstruction is governed by the complexity of the function under consideration. The amplitude $\mathcal{A}^{(2)}$ of Eq. (7.4) contains a lot of redundant information; to improve the efficiency of the reconstruction, it is thus beneficial to remove this redundancy. Furthermore, while Eq. (7.4) provides a decomposition in terms of master integrals in dimensional regularisation, after expanding the master integrals in ϵ there can be new linear relations between the different terms in the Laurent expansion in ϵ. We thus expect cancellations between the different coefficients $c_{\Gamma,i}$. In this section, we discuss how we address these issues and define the object we reconstruct.

We start by expressing the Laurent expansion of the master integrals in Eq. (7.5) in terms of a basis B of so-called pentagon functions $h_i \in B$ [17]. That is, we rewrite the amplitudes as

$$\mathcal{A}^{(2)} = \sum_{i\in B}\sum_{k=-4}^{0} \epsilon^k\, \tilde{c}_{k,i}(\vec{x})h_i(\vec{x}) \,+\mathcal{O}(\epsilon), \tag{7.7}$$

where $\vec{x} = \{x_0, x_1, x_2, x_3, x_4\}$ and the $\tilde{c}_{k,i}(\vec{x})$ are rational functions of the twistor variables. All linear relations between master integrals that appear after expansion in ϵ are resolved in such a decomposition.

Next, we recall that the singularity structure of two-loop amplitudes is governed by lower-loop amplitudes [19–22]. One can thus exploit this knowledge to subtract the pole structure from the amplitudes in order to obtain a finite remainder that contains the new two-loop information. There is freedom in how to define the remainders, as they are only constrained by removing the poles of the amplitudes. For helicity amplitudes that vanish at tree level, $\mathcal{A}^{(k)}_{\pm++++}$, we use

$$\mathcal{R}^{(2)}_{\pm++++} = \bar{\mathcal{A}}^{(2)}_{\pm++++} + S_\epsilon \bar{\mathcal{A}}^{(1)}_{\pm++++} \sum_{i=1}^{5} \frac{(-s_{i,i+1})^{-\epsilon}}{\epsilon^2} + \mathcal{O}(\epsilon), \tag{7.8}$$

where $S_\epsilon = (4\pi)^\epsilon e^{-\epsilon\gamma_E}$. The $\bar{\mathcal{A}}^{(k)}$ denote amplitudes normalised to remove any ambiguity related to overall phases. In the case of amplitudes that vanish at tree level, we normalise to the leading order in ϵ of the (finite) one-loop amplitude. For the maximally helicity violating (MHV) amplitudes, $\mathcal{A}^{(k)}_{-\mp\pm++}$, which we normalise to the corresponding tree amplitude, we define

$$\mathcal{R}^{(2)}_{-\mp\pm++} = \bar{\mathcal{A}}^{(2)}_{-\mp\pm++} - \left(\frac{5\,\tilde{\beta}_0}{2\epsilon} + \mathbf{I}^{(1)}\right) S_\epsilon \bar{\mathcal{A}}^{(1)}_{-\mp\pm++} + \left(\frac{15\,\tilde{\beta}_0^2}{8\epsilon^2} + \frac{3}{2\epsilon}\left(\tilde{\beta}_0 \mathbf{I}^{(1)} - \tilde{\beta}_1\right) - \mathbf{I}^{(2)}\right) S_\epsilon^2 + \mathcal{O}(\epsilon)\,, \tag{7.9}$$

where $\tilde{\beta}_i$ are the coefficients of the QCD β function divided by N_c^{i+1} and $\mathbf{I}^{(1)}$ and $\mathbf{I}^{(2)}$ are the standard Catani operators at leading colour. Precise expressions for the operators in our conventions can be found in Appendix B of Ref. [7]. We note that for both Eq. (7.8) and Eq. (7.9) we require one-loop amplitudes expanded up to order ϵ^2. By expressing the one-loop amplitudes and the Catani operators in the basis of pentagon functions, the remainder can be expressed in the same way,

$$\mathcal{R}^{(2)} = \sum_{i\in B} r_i(\vec{x})\, h_i(\vec{x})\,. \tag{7.10}$$

We observe that the coefficients $r_i(\vec{x})$ are rational functions of lower total degree than the $\tilde{c}_{k,i}(\vec{x})$ of Eq. (7.7).

As a further simplification, we investigate the pole structure of the coefficients $r_i(\vec{x})$. The alphabet determines the points in phase space where the pentagon functions have logarithmic singularities, and as such provides a natural candidate to describe the pole structure of the coefficients. We use the alphabet A determined in Ref. [17] to build an ansatz for the denominator structure of the $r_i(\vec{x})$,

$$r_i(\vec{x}) = \frac{n_i(\vec{x})}{\prod_{j\in A} w_j(\vec{x})^{q_{ij}}}\,. \tag{7.11}$$

We then reconstruct the remainder on a slice $\vec{x}(t) = \vec{a}\cdot t + \vec{b}$, where all the twistor variables depend on a single parameter t and $\vec{a}$ and $\vec{b}$ are random vectors of finite-field values. This reconstruction in one variable is drastically simpler than the full multivariate reconstruction. In addition, the maximal degree in t on the slice corresponds to the total degree in $\vec{x}$. We determine the exponents q_{ij} by matching the ansatz on the univariate slice and check its validity on a second slice. Having determined the denominators of the rational coefficients r_i, the reconstruction reduces to the much simpler polynomial reconstruction of the numerators $n_i(\vec{x})$.

The last simplification we implement is a change of basis in the space of pentagon functions. Amplitudes are expected to simplify in specific kinematic configurations where the pentagon functions degenerate into a smaller basis, which requires relations between the different coefficients. This motivates the search for (helicity-dependent) bases with coefficients of lower

Table C.7.1: Each t^n/t^d denotes the total degree of numerator (n) and denominator (d) of the most complex coefficient for each helicity amplitude in the decomposition of Eq. (7.7) (second column) or Eq. (7.10) (third column). The fourth column lists the highest polynomial we reconstruct. The final column lists the number of letters $w_j(\vec{x})$ that contribute in the denominator of Eq. (7.11).

Helicity	$\tilde{c}_{k,i}(t)$	$r_i(t)$	$n'_i(t)$	w_js in denominator
$+++++$	t^{34}/t^{28}	t^{10}/t^{4}	t^{10}	3
$-++++$	t^{50}/t^{42}	t^{35}/t^{28}	t^{35}	14
$--+++$	t^{70}/t^{65}	t^{50}/t^{45}	t^{40}	17
$-+-++$	t^{84}/t^{82}	t^{68}/t^{66}	t^{53}	20

total degree. To find them, we construct linear combinations of coefficients

$$\sum_{i\in B} a_{i,k} r_i(\vec{x}) = \frac{N_k(\vec{x}, a_{i,k})}{\prod_{j\in A} w_j(\vec{x})^{q'_{kj}}}\,, \tag{7.12}$$

and solve for phase space independent $a_{i,k}$ such that the numerators $N_k(\vec{x}, a_{i,k})$ factorise a subset of the $w_j \in A$. This can be performed on univariate slices by only accepting solutions that are invariant over a number of slices. The matrix $a_{i,k}$ allows us to change to a new basis B' in the space of special functions, in which remainders can be decomposed as in Eq. (7.10), with coefficients $r'_i(\vec{x})$ whose numerators $n'_i(\vec{x})$ are polynomials of lower total degree than those of Eq. (7.11).

7.4 Implementation and results

The master integral coefficients of the one- and two-loop amplitudes are computed using numerical unitarity in a finite field. They are combined with the corresponding master integrals, expressed in terms of pentagon functions, and the known pole structure is subtracted to obtain the finite remainders as a linear combination of pentagon functions. After a rotation in the space of pentagon functions and multiplication by the predetermined denominator factors, we obtain numerical samples for the numerators $n'_i(\vec{x})$ in a finite field. These samples are used to analytically reconstruct the $n'_i(\vec{x})$ with the algorithm of Ref. [9], which we slightly modified to allow a more efficient parallelization. These steps were implemented in a flexible C++ framework, which was used to reconstruct the analytical form of the two-loop remainders of a basis of five-gluon helicity amplitudes (the other helicities can be obtained by parity and charge conjugation). Two finite fields of cardinality $O(2^{31})$ were necessary for the rational reconstruction by means of the Chinese remainder theorem.

Table C.7.1 shows the impact of the simplifications discussed in the previous section for each helicity. In the most complicated case, the $\mathrm{g}^-\mathrm{g}^+\mathrm{g}^-\mathrm{g}^+\mathrm{g}^+$ helicity amplitude, we must reconstruct a polynomial of degree 53. This required 250 000 numerical evaluations, with 4.5 min per evaluation.

The results that we provide contain the one-loop amplitudes in terms of master integrals and the two-loop remainders in terms of pentagon functions. The one-loop master integrals are provided in terms of pentagon functions up to order ϵ^2. The combined size of the expressions amounts to 45 MB without attempting any simplification (we refer the reader to Ref. [14]

for more compact expressions). These expressions can be combined to construct the full analytical expression for the two-loop five-gluon leading-colour amplitudes in the Euclidean region. We validated our expressions by reproducing all the target benchmark values available in the literature [1–5, 7, 11].

7.5 Conclusion

In this section, we have presented the recent computation of the analytical form of the leading-colour contributions to the two-loop five-gluon scattering amplitudes in pure Yang–Mills theory. This computation was undertaken in a novel way, made possible by a collection of mature tools. The amplitude is first numerically reduced to a basis of master integrals with the two-loop numerical unitarity approach, where the coefficients take finite-field values [5,7,10,13]. This allows us to numerically calculate a finite remainder, expressed in terms of pentagon functions [17]. The generation of these numerical samples is driven by a functional reconstruction algorithm [9], which determines the analytical form of the pentagon-function coefficients from a series of evaluations. A key step in efficiently implementing this strategy was to utilise physical information to simplify the analytical form of the objects we reconstruct, and hence reduce the required number of evaluations. First, we reconstruct the finite remainder, which removes redundant information related to lower-loop contributions. Second, we decompose the remainder in terms of pentagon functions to account for relations between different master integrals after expansion in the dimensional regulator. Next, we exploit the knowledge of the singularity structure of the pentagon functions to efficiently establish the denominators of the coefficient functions. Finally, we find a basis of pentagon functions with coefficients of lower degree by exploiting their reconstruction on a univariate slice.

These techniques show a great deal of potential for future calculations. Indeed, they have very recently been used to obtain the full set of leading-colour contributions to the five-parton scattering amplitudes [14]. We foresee further applications to processes with a higher number of scales and loops, such as those required for a future lepton collider in the near future.

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