4 Unsubtractions at NNLO

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4.1 Introduction

Computations in perturbative quantum field theory (pQFT) feature several aspects that, although intrinsically non-physical, are traditionally successfully eluded by modifying the dimensions of space–time. Closed loops in pQFT implicitly extrapolate the validity of the Standard Model (SM) to infinite energies—equivalent to zero distance—much above the Planck scale. We should expect this to be a legitimate procedure if the loop scattering amplitudes that contribute to the physical observables are either suppressed at very high energies, or if there is a way to suppress or renormalise their contribution in this limit. In gauge theories like QCD, massless particles can be emitted with zero energy, and pQFT treats the quantum state with N external partons as different from the quantum state with emission of extra massless particles at zero energy, while these two states are physically identical. In addition, partons can be emitted in exactly the same direction, or, in other words, at zero distance. All these unphysical features have a price and lead to the emergence of infinities in the four dimensions of space–time.

In dimensional regularisation (DREG) [1–5], the infinities are replaced by explicit poles in $1/\varepsilon$, with $d = 4 - 2\varepsilon$, through integration of the loop momenta and the phase space of real radiation. Then, the $1/\varepsilon$ ultraviolet (UV) singularities of the virtual contributions are removed by renormalization, and the infrared (IR) soft and collinear singularities are subtracted. The general idea of subtraction [6–18] involves introducing counterterms that mimic the local IR behaviour of the real components and that can easily be integrated analytically in d dimensions. In this way, the integrated form is combined with the virtual component, while the unintegrated counterterm cancels the IR poles originated from the phase space integration of the real-radiation contribution.

Although this procedure efficiently transforms the theory into a calculable and well-defined mathematical framework, a big effort needs to be invested in evaluating loop and phase space integrals in arbitrary space–time dimensions, which are particularly difficult at higher perturbative orders. In view of the highly challenging demands imposed by the expected accuracy attainable at the LHC and future colliders, like the FCC, there has been a recent interest in the community to define perturbative methods directly in $d = 4$ space–time dimensions in order to avoid the complexity of working in a non-physical multidimensional space [19]. Examples of these methods are the four-dimensional formulation (FDF) [20] of the four-dimensional helicity scheme, the six-dimensional formalism (SDF) [21], implicit regularisation (IREG) [22, 23], and four-dimensional regularisation or renormalization (FDR) [24, 25].[†] In this section, we review the four-dimensional unsubtraction (FDU) [26–28] method, which is based on loop-tree duality

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[†]See Section C.3 in this report.

(LTD) [29–36]. The idea behind FDU is to exploit a suitable mapping of momenta between the virtual and real kinematics in such a way that the summation over the degenerate soft and collinear quantum states is performed locally at integrand level without the necessity of introducing IR subtractions, whereas the UV singularities are locally suppressed at very high energies, e.g., at two loops [35]. The method should improve the efficiency of Monte Carlo event generators because it simultaneously describes real and virtual contributions.

Finally, LTD is also a powerful framework to analyse the singular structure of scattering amplitudes directly in the loop momentum space, which is particularly interesting for characterizing unitarity thresholds and anomalous thresholds for specific kinematic configurations [36].

4.2 Loop-tree duality

The LTD representation of a one-loop scattering amplitude is given by

$$\mathcal{A}^{(1)}(\{p_n\}_N) = -\int_\ell \mathcal{N}(\ell, \{p_n\}_N) \otimes G_D(\alpha) \; , \tag{4.1}$$

where $G_D(\alpha) = \sum_{i\in\alpha} \tilde{\delta}\,(q_i) \prod_{j\neq i} G_D(q_i; q_j)$, and $\mathcal{N}(\ell, \{p_n\}_N)$ is the numerator of the integrand, which depends on the loop momentum ℓ and the external momenta $\{p_n\}_N$. The delta function $\tilde{\delta}\,(q_i) = \mathrm{i}2\pi\,\theta(q_{i,0})\,\delta(q_i^2 - m_i^2)$ sets on-shell the internal propagator with momentum $q_i = \ell + k_i$ and selects its positive energy mode, $q_{i,0} > 0$. At one loop, $\alpha = \{1, \ldots, N\}$ labels all the internal momenta, and Eq. (4.1) is the sum of N single-cut dual amplitudes. The dual propagators,

$$G_D(q_i; q_j) = \frac{1}{q_j^2 - m_j^2 - \mathrm{i}0\,\eta \cdot k_{ji}} \; , \tag{4.2}$$

differ from the usual Feynman propagators only by the imaginary prescription, which now depends on $\eta \cdot k_{ji}$, with $k_{ji} = q_j - q_i$. The dual propagators are implicitly linear in the loop momentum, owing to the on-shell conditions. With $\eta = (1, \mathbf{0})$, which is equivalent to integrating out the energy component of the loop momentum, the remaining integration domain is Euclidean.

At two loops, the corresponding dual representation is [31, 35]

$$\begin{aligned}\mathcal{A}^{(2)}(\{p_n\}_N) = \int_{\ell_1}\int_{\ell_2} \mathcal{N}(\ell_1, \ell_2, \{p_n\}_N) \otimes [G_D(\alpha_1)\, G_D(\alpha_2 \cup \alpha_3) + G_D(-\alpha_2 \cup \alpha_1) G_D(\alpha_3) \\ - G_D(\alpha_1)\, G_F(\alpha_2)\, G_D(\alpha_3)] \; .\end{aligned} \tag{4.3}$$

Now, the internal momenta are $q_i = \ell_1 + k_i$, $q_j = \ell_2 + k_j$, and $q_k = \ell_1 + \ell_2 + k_k$, and are classified into three different sets, with $i \in \alpha_1$, $j \in \alpha_2$, and $k \in \alpha_3$ (see Fig. C.4.1). The minus sign in front of α_2 indicates that the momenta in α_2 are reversed to hold a momentum flow consistent with α_1. The dual representation in Eq. (4.3) spans over the sum of all possible double-cut contributions, with each of the two cuts belonging to a different set. In general, at higher orders, LTD transforms any loop integral or loop scattering amplitude into a sum of tree-level-like objects that are constructed by setting on-shell a number of internal loop propagators equal to the number of loops.

Explicit LTD representations of the scattering amplitude describing the decay $\mathrm{H} \to \gamma\gamma$ have been presented at one [34] and two loops [35].

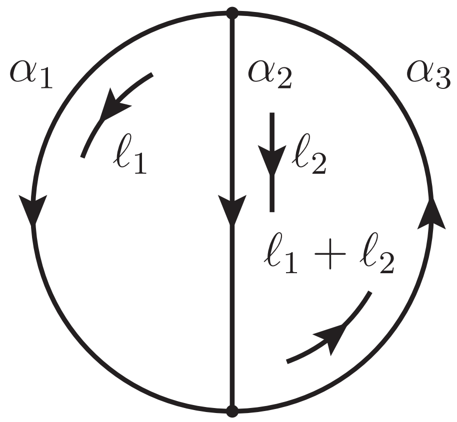

Fig. C.4.1: Momentum flow of a two-loop Feynman diagram

4.3 Four-dimensional unsubtraction

It is interesting to note that although in Eqs. (4.1) and (4.3) the on-shell loop three-momenta are unrestricted, all the IR and physical threshold singularities of the dual amplitudes are restricted to a compact region [32, 36], as discussed in Section 4.4. This is essential to define the four-dimensional unsubtraction (FDU) [26–28] algorithm, namely, to establish a mapping between the real and virtual kinematics in order to locally cancel the IR singularities without the need for subtraction counterterms.

In the FDU approach, the cross-section at next-to-leading order (NLO) is constructed, as usual, from the renormalised one-loop virtual correction with N external partons and the exclusive real cross-section with $N+1$ partons

$$\sigma^{\rm NLO} = \int_N d\sigma_{\rm V}^{(1,{\rm R})} + \int_{N+1} d\sigma_{\rm R}^{(1)} \;, \tag{4.4}$$

integrated over the corresponding phase space, $\int_N$ and $\int_{N+1}$. The virtual contribution is obtained from its LTD representation

$$\int_N d\sigma_{\rm V}^{(1,{\rm R})} = \int_{(N,\vec{\ell})} 2\,{\rm Re}\,\langle \mathcal{M}_N^{(0)} | \left(\sum_i \mathcal{M}_N^{(1)}(\tilde{\delta}(q_i)) \right) - \mathcal{M}_{\rm UV}^{(1)}(\tilde{\delta}(q_{\rm UV}))\rangle \, \hat{\mathcal{O}}(\{p_n\}_N) \;, \tag{4.5}$$

where $\mathcal{M}_N^{(0)}$ is the N-leg scattering amplitude at leading order (LO), and $\mathcal{M}_N^{(1)}(\tilde{\delta}(q_i))$ is the dual representation of the unrenormalised one-loop scattering amplitude with the internal momentum q_i set on-shell. The integral is weighted with the explicit observable function $\hat{\mathcal{O}}(\{p_n\}_N)$. The expression includes appropriate counterterms, $\mathcal{M}_{\rm UV}^{(1)}(\tilde{\delta}(q_{\rm UV}))$, that implement renormalization by subtracting the UV singularities locally, as discussed in Refs. [27, 28], including UV singularities of degree higher than logarithmic that integrate to zero.

By means of an appropriate mapping between the real and virtual kinematics [27, 28],

$$\{p'_r\}_{N+1} \to (q_i, \{p_n\}_N) \;, \tag{4.6}$$

the real phase space is rewritten in terms of the virtual phase space and the loop three-momentum

$$\int_{N+1} = \int_{(N,\vec{\ell})} \sum_i \mathcal{J}_i(q_i)\, \mathcal{R}_i(\{p'_r\}_{N+1}) \;, \tag{4.7}$$

where $\mathcal{J}_i(q_i)$ is the Jacobian of the transformation with q_i on-shell, and $\mathcal{R}_i(\{p'_j\}_{N+1})$ defines a complete partition of the real phase space

$$\sum_i \mathcal{R}_i(\{p'_r\}_{N+1}) = 1 \ . \tag{4.8}$$

As a result, the NLO cross-section is cast into a single integral in the Born or virtual phase space and the loop three-momentum

$$\sigma^{\mathrm{NLO}} = \int_{(N,\vec{\ell})} \Bigg[2\,\mathrm{Re}\,\langle \mathcal{M}_N^{(0)} | \Bigg(\sum_i \mathcal{M}_N^{(1)}(\tilde{\delta}(q_i)) \Bigg) - \mathcal{M}_{\mathrm{UV}}^{(1)}(\tilde{\delta}(q_{\mathrm{UV}})) \rangle \, \hat{\mathcal{O}}(\{p_n\}_N) \\ + \sum_i \mathcal{J}_i(q_i)\, \mathcal{R}_i(\{p'_r\}_{N+1})\, |\mathcal{M}_{N+1}^{(0)}(\{p'_r\}_{N+1})|^2\, \hat{\mathcal{O}}(\{p'_r\}_{N+1}) \Bigg] \ , \tag{4.9}$$

and exhibits a smooth four-dimensional limit in such a way that it can be evaluated directly in four space–time dimensions. Explicit computations are presented in Refs. [27, 28] with both massless and massive final-state quarks. More importantly, with suitable mappings in Eq. (4.6) conveniently describing the quasi-collinear configurations, the transition from the massive [28] to the massless configuration [27] is also smooth.

The extension of FDU to next-to-next-to-leading order (NNLO) is obvious; the total cross-section consists of three contributions

$$\sigma^{\mathrm{NNLO}} = \int_N \mathrm{d}\sigma_{\mathrm{VV}}^{(2,\mathrm{R})} + \int_{N+1} \mathrm{d}\sigma_{\mathrm{VR}}^{(2,\mathrm{R})} + \int_{N+2} \mathrm{d}\sigma_{\mathrm{RR}}^{(2)} \ , \tag{4.10}$$

where the double virtual cross-section $\mathrm{d}\sigma_{\mathrm{VV}}^{(2,\mathrm{R})}$ receives contributions from the interference of the two-loop with the Born scattering amplitudes, the square of the one-loop scattering amplitude with N external partons, the virtual-real cross-section $\mathrm{d}\sigma_{\mathrm{VR}}^{(2,\mathrm{R})}$ includes the contributions from the interference of one-loop and tree-level scattering amplitudes with one extra external particle, and the double real cross-section $\mathrm{d}\sigma_{\mathrm{RR}}^{(2)}$ comprises tree-level contributions with the emission of two extra particles. The LTD representation of the two-loop scattering amplitude, $\langle \mathcal{M}_N^{(0)} | \mathcal{M}_N^{(2)}(\tilde{\delta}(q_i, q_j))\rangle$, is obtained from Eq. (4.3), while the two-loop momenta of the squared one-loop amplitude are independent and generate dual contributions of the type $\langle \mathcal{M}_N^{(1)}(\tilde{\delta}(q_i)) | \mathcal{M}_N^{(1)}(\tilde{\delta}(q_j))\rangle$. In both cases, there are two independent loop three-momenta and N external momenta with which to reconstruct the kinematics of the tree-level corrections entering $\mathrm{d}\sigma_{\mathrm{RR}}^{(2)}$ and the one-loop corrections in $\mathrm{d}\sigma_{\mathrm{VR}}^{(2,\mathrm{R})}$:

$$\{p''_r\}_{N+2} \to (q_i, q_j, \{p_n\}_N) \ , \qquad (q'_k, \{p'_s\}_{N+1}) \to (q_i, q_j, \{p_n\}_N) \ , \tag{4.11}$$

in such a way that all the contributions to the NNLO cross-section are cast into a single phase space integral

$$\sigma^{\mathrm{NNLO}} = \int_{(N,\vec{\ell}_1,\vec{\ell}_2)} \mathrm{d}\sigma^{\mathrm{NNLO}} \ . \tag{4.12}$$

Explicit applications of FDU at NNLO are currently under investigation.

4.4 Unitarity thresholds and anomalous thresholds

An essential requirement for FDU to work is to prove that all the IR singularities of the dual amplitudes are restricted to a compact region of the loop three-momenta. This has recently been proven at higher orders [36], thus extending the one-loop analysis of Ref. [32], as well as analysing the case of anomalous thresholds. The location of the singularities of the dual amplitudes in the loop three-momentum space are encoded at one loop through the set of conditions

$$\lambda_{ij}^{\pm\pm} = \pm q_{i,0}^{(+)} \pm q_{j,0}^{(+)} + k_{ji,0} \to 0 \ , \tag{4.13}$$

where $q_{r,0}^{(+)} = \sqrt{\vec{q}_r^{\,2} + m_r^2}$, with $r \in \{i,j\}$, are the on-shell loop energies. There are, indeed, only two independent solutions. The limit $\lambda_{ij}^{++} \to 0$ describes the causal unitarity threshold, and determines that $q_{r,0}^{(+)} < |k_{ji,0}|$, where $k_{ji,0}$ depends on the external momenta only and is therefore bounded. For massless partons, it also describes soft and collinear singularities. The other potential singularity occurs for $\lambda_{ij}^{+-} \to 0$, but this is a non-causal or unphysical threshold and it cancels locally in the forest defined by the sum of all the on-shell dual contributions. For this to happen, the dual prescription of the dual propagators plays a central role. Finally, anomalous thresholds are determined by overlapping causal unitarity thresholds, e.g., λ_{ij}^{++} and $\lambda_{ik}^{++} \to 0$ simultaneously.

At two loops, the location of the singularities is determined by the set of conditions

$$\lambda_{ijk}^{\pm\pm\pm} = \pm q_{i,0}^{(+)} \pm q_{j,0}^{(+)} \pm q_{k,0}^{(+)} + k_{k(ij),0} \to 0 \ , \tag{4.14}$$

where $k_{k(ij)} = q_k - q_i - q_j$ depends on external momenta only, with $i \in \alpha_1$, $j \in \alpha_2$, and $k \in \alpha_3$. Now, the unitarity threshold is defined by the limit $\lambda_{ijk}^{+++} \to 0$ (or $\lambda_{ijk}^{---} \to 0$) with $q_{r,0}^{(+)} \leq |k_{k(ij),0}|$ and $r \in \{i,j,k\}$, and the potential singularities at $\lambda_{ijk}^{++-} \to 0$ and $\lambda_{ijk}^{+--} \to 0$ cancel locally in the forest of all the dual contributions. Again, the anomalous thresholds are determined by the simultaneous contribution of unitarity thresholds. The generalisation of Eq. (4.14) to higher orders is straightforward.

4.5 Conclusions

The bottleneck in higher-order perturbative calculations is not only the evaluation of multiloop Feynman diagrams, but also the gathering of all the quantum corrections from different loop orders (and thus different numbers of final-state partons). To match the expected experimental accuracy at the LHC, particularly in the high-luminosity phase, and at future colliders, new theoretical efforts are still needed to overcome the current precision frontier. LTD is also a powerful framework to analyse, comprehensively, the emergence of anomalous thresholds at higher orders.

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