

Advancements in the Theory of QCD Amplitudes and Their Application to Photon-Pair Production at the LHC at Next-to-Next-to-Next-to-Leading Order

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Abstract

At the Large Hadron Collider (LHC), protons are collided at very high center-of-mass energies of up to 13.6 TeV. The resulting final states are reconstructed and counted, enabling the measurement of production cross sections. Comparing these cross sections with theoretical predictions allows for precise tests of the Standard Model of particle physics, a fundamental theory describing all known physical interactions except for gravity.

Theoretical calculations of cross sections at hadron colliders rely on Quantum Chromodynamics (QCD), the theory of the strong interaction, in particular through perturbation theory, where one tries to calculate as many orders as possible in the perturbative expansion in the strong coupling constant α_s .

In this thesis, we present the first calculation of a hadron-collider cross section at next-to-next-to-next-to-leading order (N³LO) in QCD for a $2 \rightarrow 2$ process, that is a process where from the two initial-state protons two particles are produced within the initial hard interaction. Specifically, we calculate the production cross section of a photon pair, $pp \rightarrow \gamma\gamma$, at N³LO. To this end, we use the q_T -slicing method combined with a next-to-next-to-leading-order (NNLO) subtraction scheme at very high numerical precision. To achieve this precision, we perform an analytic calculation of the necessary six-point one-loop scattering amplitudes using state-of-the-art techniques. These techniques include rational reconstruction of the results from numerical finite-field probes and the construction of compact ansätze using phase-space points on singular varieties expressed through p -adic numbers. We obtain a fiducial cross section with a total uncertainty of 3 %, compared to 8 % of previous NNLO calculations. The result agrees with a measurement at the LHC by the ATLAS Collaboration. Furthermore, we for the first time observe perturbative convergence for this process. We also show a differential result in form of the invariant-mass distribution of the photon pair.

Additionally, we present theoretical insights into general QCD scattering amplitudes by studying their behavior in infrared limits. This leads to process-independent next-to-leading-power expansions of tree-level amplitudes in collinear limits, and of one-loop amplitudes in the soft-gluon limit. These expansions are valid for amplitudes containing any number of massless or massive particles. They have a multitude of potential future applications, including numerical stabilization of amplitude evaluations, the inclusion of power corrections in slicing methods, or next-to-leading-power resummation.

Zusammenfassung

Am Large Hadron Collider (LHC) werden Protonen mit sehr hohen Schwerpunktsenergien von bis zu 13.6 TeV kollidiert. Die entstehenden Endzustände werden rekonstruiert und gezählt, was die Messung von Wirkungsquerschnitten ermöglicht. Durch Vergleich dieser Wirkungsquerschnitte mit theoretischen Vorhersagen kann das Standardmodell der Teilchenphysik, eine fundamentale Theorie die alle bekannten Wechselwirkungen außer Gravitation beschreibt, getestet werden.

Theoretische Berechnungen von Wirkungsquerschnitten an Hadronenbeschleunigern beruhen auf Quantenchromodynamik (QCD), der Theorie der starken Wechselwirkung, insbesondere durch Verwendung von Störungstheorie, innerhalb der man versucht so viele Ordnungen der Störungsreihe in der starken Kopplungskonstante α_s wie möglich zu berechnen.

In dieser Dissertation präsentieren wir die erste Berechnung eines Hadronenbeschleuniger-Wirkungsquerschnitts für einen $2 \rightarrow 2$ Prozess – d.h. für einen Prozess, bei dem die zwei Protonen des Ausgangszustands zwei Teilchen innerhalb der initialen hochenergetischen Interaktion produzieren – in vierter Ordnung (next-to-next-to-next-to-leading order, $N^3\text{LO}$) der Störungstheorie. Genauer gesagt berechnen wir den Wirkungsquerschnitt zur Produktion eines Photonpaares, $pp \rightarrow \gamma\gamma$, in $N^3\text{LO}$. Dazu verwenden wir die q_T -Slicing-Methode in Kombination mit einem Subtraktionsschema dritter Ordnung (next-to-next-to-leading order, NNLO), das sehr hohe numerische Präzision liefert. Um diese Präzision zu erreichen, führen wir eine analytische Berechnung der benötigten Sechs-Teilchen-Ein-Schleifen-Streuamplitude mit modernen Methoden durch. Diese Methoden beinhalten eine rationale Rekonstruktion der Ergebnisse ausgehend von numerischen Evaluierungen auf endlichen Körpern. Außerdem konstruieren wir kompakte Ansätze mithilfe von Phasenraumpunkten auf singulären Varietäten, ausgedrückt durch p -adische Zahlen. Wir erhalten einen Wirkungsquerschnitt bezogen auf einen Referenz-Phasenraum („fiducial cross section“) mit einer Unsicherheit von 3 %, im Vergleich zu 8 % von vorherigen NNLO Berechnungen. Die Ergebnisse stimmen mit experimentellen Messungen am LHC durch das ATLAS-Experiment innerhalb der Unsicherheiten überein. Außerdem beobachten wir, zum ersten Mal für diesen Prozess, eine Konvergenz der Störungsreihe. Schließlich präsentieren wir mit der Verteilung in der invarianten Masse ein differentielles Ergebnis.

Zusätzlich erlangen wir neue theoretische Einblicke in allgemeine QCD Streuamplituden, indem wir ihr Verhalten in infraroten Limites studieren. Wir erhalten eine prozessunabhängige, subleitende (next-to-leading power, NLP) Entwicklung von Baumdiagramm-Amplituden in kollinearen Limites und von Ein-Schleifen-Amplituden in niederenergetischen („soften“) Limites. Diese Entwicklungen gelten für Amplituden mit einer beliebigen Anzahl masseloser oder massiver Teilchen. Sie haben eine Vielzahl von möglichen zukünftigen Anwendungen, unter anderem die numerische Stabilisierung von Amplituden, die Einbeziehung von NLP-Korrekturen in Slicing-Methoden oder NLP Resummation.

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Eidesstattliche Versicherung

Ich, Felix Eschment, erkläre, dass diese Dissertation und die darin dargelegten Inhalte die eigenen sind und selbstständig, als Ergebnis der eigenen originären Forschung, generiert wurden.

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- [1] M. Czakon, F. Eschment, and T. Schellenberger. “Subleading effects in soft-gluon emission at one-loop in massless QCD.” In: *JHEP* 12 (2023), p. 126. DOI: 10.1007/JHEP12(2023)126. arXiv: 2307.02286 [hep-ph]
- [2] M. Czakon, K. Erhard Minguez, and F. Eschment. “Subleading Effects in Soft-Gluon Emission at One-Loop in Massive QCD.” In: *JHEP* 02 (2026), p. 110. DOI: 10.1007/JHEP02(2026)110. arXiv: 2510.21655 [hep-ph]
- [3] M. Czakon, F. Eschment, T. Generet, and R. Poncelet. *Next-to-next-to-next-to-leading order QCD corrections to photon-pair production*. Apr. 2026. arXiv: 2604.12613 [hep-ph]

Aachen, den 22. Juli 2026

Felix Eschment

List of Publications

This thesis is based on my research conducted at the Institute for Theoretical Particle Physics and Cosmology of the RWTH Aachen University. Of the resulting publications, the following are relevant to this thesis:

- [1] M. Czakon, F. Schment, and T. Schellenberger. “Subleading effects in soft-gluon emission at one-loop in massless QCD.” In: *JHEP* 12 (2023), p. 126. DOI: 10.1007/JHEP12(2023)126. arXiv: 2307.02286 [hep-ph]
- [2] M. Czakon, K. Erhard Minguez, and F. Schment. “Subleading Effects in Soft-Gluon Emission at One-Loop in Massive QCD.” In: *JHEP* 02 (2026), p. 110. DOI: 10.1007/JHEP02(2026)110. arXiv: 2510.21655 [hep-ph]
- [3] M. Czakon, F. Schment, T. Generet, and R. Poncelet. *Next-to-next-to-next-to-leading order QCD corrections to photon-pair production*. Apr. 2026. arXiv: 2604.12613 [hep-ph]

While Chapters 1 and 2 introduce and discuss known textbook and literature results, research from Refs. [1, 2] is contained in Chapter 3 and research from Ref. [3] in Chapters 4 and 5. My personal contributions to each publication are discussed at the beginning of the relevant chapters.

Furthermore, my research contributed to the following publications not directly relevant to this thesis:

- [4] M. Czakon, F. Schment, and T. Schellenberger. “Revisiting the double-soft asymptotics of one-loop amplitudes in massless QCD.” In: *JHEP* 04 (2023), p. 065. DOI: 10.1007/JHEP04(2023)065. arXiv: 2211.06465 [hep-ph]
- [5] M. Czakon, F. Schment, M. Niggetiedt, R. Poncelet, and T. Schellenberger. “Top-Bottom Interference Contribution to Fully Inclusive Higgs Production.” In: *Phys. Rev. Lett.* 132.21 (2024), p. 211902. DOI: 10.1103/PhysRevLett.132.211902. arXiv: 2312.09896 [hep-ph]
- [6] M. Czakon, F. Schment, M. Niggetiedt, R. Poncelet, and T. Schellenberger. “Quark mass effects in Higgs production.” In: *JHEP* 10 (2024), p. 210. DOI: 10.1007/JHEP10(2024)210. arXiv: 2407.12413 [hep-ph]

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Chapter 1

Introduction

1.1 The Standard Model of Particle Physics

Research in fundamental physics aims to identify rules that can, in principle, explain all observed phenomena in nature. While many phenomena observed in everyday life can be explained by Newtonian mechanics, research has shown that it is only an approximation of an underlying, more fundamental, theory. While a more fundamental theory is not necessarily more useful than previously known approximations because it might be too complicated to solve for the problem at hand, the curiosity of humankind has driven the search for more and more fundamental explanations. Historically, previously unknown physics has been observed by studying nature at smaller length scales or, equivalently, higher energy scales. The current frontier of high-energy experiments is the *Large Hadron Collider (LHC)*, which currently operates at a center-of-mass energy of 13.6 TeV, corresponding to a length scale of

$$\frac{\hbar c}{13.6 \text{ TeV}} \sim 10^{-20} \text{ m}, \quad (1.1)$$

with the Planck constant $\hbar$ and the speed of light c as natural scales.¹ On the theory side, research has culminated in the *Standard Model of Particle Physics (SM)*. We refrain from giving a detailed introduction and instead refer to textbooks, e.g. Ref. [7], for a pedagogical treatment. Let us only state that the SM is a quantum field theory (QFT), in particular a gauge theory of the $\text{SU}(3)_C \times \text{SU}(2)_L \times \text{U}(1)_Y$ group. Its Lagrangian has the schematic form

$$\mathcal{L}_{\text{SM}} = \underbrace{-\frac{1}{4}F_{\mu\nu}F^{\mu\nu}}_{\text{gauge fields}} + \underbrace{i\bar{\psi}\not{D}\psi}_{\text{fermions}} + \underbrace{(\psi_i y_{ij} \psi_j \phi + \text{h.c.})}_{\text{Yukawa interactions}} + \underbrace{(D_\mu \phi)^\dagger (D^\mu \phi) - V(\phi)}_{\text{Higgs sector}}. \quad (1.2)$$

It governs the dynamics of and interactions between all types of elementary particles occurring in the SM, namely spin-1 gauge fields, spin- $\frac{1}{2}$ fermions, and the scalar Higgs boson. In addition to this schematic form of the Lagrangian, let us specify the particle content of the SM. Figure 1.1 shows all known fermions, which form the ordinary matter, as well as the gauge bosons with which they interact. Finally, the Higgs mechanism generates the masses of the particles through spontaneous symmetry breaking and the Yukawa terms in the Lagrangian. Additionally, it gives rise to one scalar boson, the Higgs boson. Its discovery in 2012 [8, 9] completed the particle content of the SM.

¹For the remainder of this thesis, we work in a natural unit system with $\hbar = c = 1$.

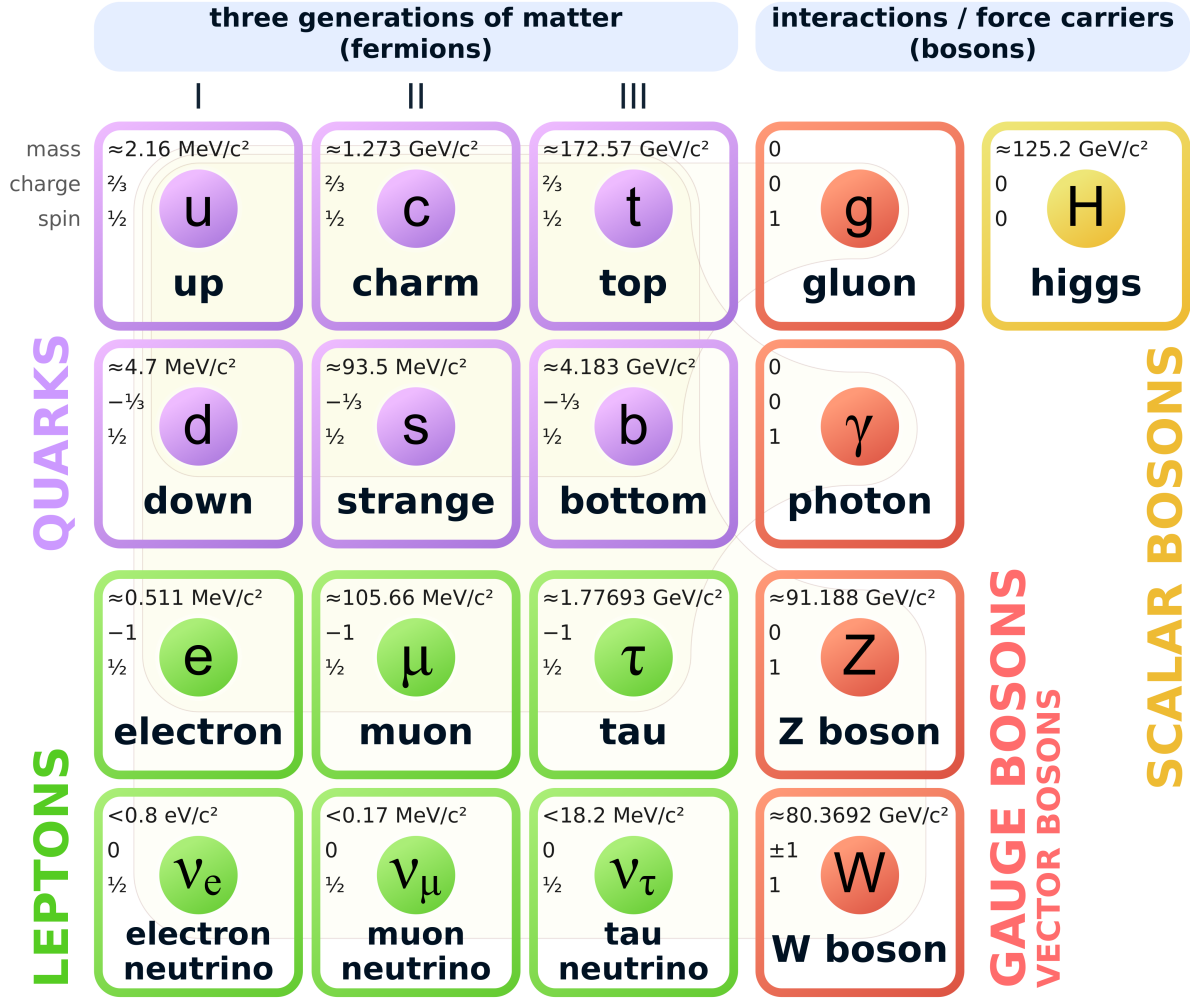


Figure 1.1: Schematic of the particle content of the Standard Model after electroweak symmetry breaking. The three loops in the background indicate which particles participate in the strong, electromagnetic, and weak interactions, respectively. Figure taken from https://upload.wikimedia.org/wikipedia/commons/0/00/Standard_Model_of_Elementary_Particles.svg.

The SM is very successful and no experiment has shown a clear deviation from its predictions so far.² While it is no candidate for a “theory of everything”—a hypothetical fundamental theory of nature from which all other fields of physics could be derived as approximations, so-called effective theories—because it does not include gravity, testing such a theory is expected to require probing length scales of the order 10^{-35} m, 15 orders of magnitude beyond what we can currently achieve at the LHC. It also cannot explain all cosmological observations, most prominently the existence of dark matter. However, it is unclear if and how a hypothetical dark matter particle can be detected. Still, continued research in high-energy physics is justified. While the concrete path the observation of physics beyond the SM is unclear, research on the SM itself is far from finished. As the most fundamental theory available, it is desirable to at least in principle know how to make predictions at arbitrary precision, with the only limitation being computation power. However, the current cutting-edge predictions rely on *perturbation theory*, which we introduce in Chapter 2 and use throughout this thesis. As outlined there, perturbation theory is expected to break down at some level of precision, while there also exist phenomena which cannot be explained by it at all. On the path to exploring the limitations of perturbation theory, we try to push it to higher and higher orders, which is also the objective of this thesis. This also leads to phenomenological results of higher and higher precision which can be tested experimentally at the LHC, increasing the confidence we can have in our most fundamental theory so far.

The calculation of predictions within the SM is a broad field, implying that we can only cover a small part of it in this thesis. In particular, we do not include any effects related to the weak interaction and to the Higgs boson, limiting ourselves to the theories of *Quantum Chromodynamics (QCD)* and *Quantum Electrodynamics (QED)*. This means that we work in the $SU(3)_C \times SU(1)_Q$ gauge groups, $SU(3)_C$ corresponding to interactions of particles which carry a *color charge*, and $SU(1)_Q$ corresponding to interactions of electrically charged particles. Furthermore, we consider only quarks as matter, neglecting leptons, and treat all quarks except for the top quark as massless because their masses are usually much smaller than the energies relevant at the LHC. In this effective QCD+QED description after electroweak symmetry breaking, the top-quark mass is included as an explicit mass term. Therefore, instead of working with the full SM Lagrangian (1.2), we consider

$$\mathcal{L}_{\text{QCD+QED}} = -\frac{1}{4}G_{\mu\nu}^a G^{a,\mu\nu} - \frac{1}{4}F_{\mu\nu} F^{\mu\nu} + \sum_{i=1}^5 \bar{\psi}_i i \not{D} \psi_i + \bar{\psi}_t (i \not{D} - m_t) \psi_t, \quad (1.3)$$

$$G_{\mu\nu}^a \equiv \partial_\mu A_\nu^a - \partial_\nu A_\mu^a + g_s f^{abc} A_\mu^b A_\nu^c, \quad (1.4)$$

$$F_{\mu\nu} \equiv \partial_\mu A_\nu^{\text{em}} - \partial_\nu A_\mu^{\text{em}}, \quad (1.5)$$

$$D_\mu \equiv \partial_\mu - i g_s T^a A_\mu^a - i Q_i e A_\mu^{\text{em}}, \quad (1.6)$$

where A_μ^a and A_μ^{em} are the gluon and photon fields, g_s and e the strong and electromagnetic gauge coupling parameters, and m_t the top-quark mass. Furthermore, T^a are the generators of the color group $SU(3)$ with $[T^a, T^b] = i f^{abc} T^c$. The algebra of the group $SU(N_c)$, $N_c = 3$ the number of colors, has the Casimir invariants $C_A = 2T_F N_c = 3$ and $C_F = T_F(N_c^2 - 1)/N_c = 4/3$, with $T_F = 1/2$ defined through $\text{Tr}(T^a T^b) = T_F \delta^{ab}$. Q_i are the fractional charges of the quarks as shown in Fig. 1.1. Except for Chapter 3, we work in fully massless QCD with $n_f = 5$ quark

²In the original formulation of the SM, neutrinos were assumed to be massless particles. Since then, the observation of neutrino oscillations has shown that this assumption is not correct. However, neutrino masses can be introduced in analogy to the other fermion masses, which is why we do not treat them as physics beyond the SM here.

flavors, neglecting the contribution of the top quark. This implies the omission of the last term in Eq. (1.3).

In essence, the majority of measurements conducted at the LHC are counting experiments, where one measures the rate that a certain set of particles in a final state X , is produced in proton-proton collisions. This rate can be expressed as

$$\frac{dN_{pp \rightarrow X}}{dt} = L \times \sigma_{pp \rightarrow X}, \quad (1.7)$$

where the *instantaneous luminosity* L with dimensions $\text{Length}^{-2} \times \text{Time}^{-1}$ depends on the specific experimental setup of the collider experiment and will not be further discussed in this thesis, whereas the *cross section* $\sigma_{pp \rightarrow X}$ is accessible through theory calculations in a QFT given a Lagrangian such as Eq. (1.3). Besides the particle content X of the final state, experiments can also measure kinematic properties, e.g. the solid angle Ω in which (combinations of) particles are detected. This is encoded in *differential* cross sections, e.g. $d\sigma_{pp \rightarrow X}/d\Omega$. While the notation should not be mistaken as a derivative—after all, the total cross section $\sigma_{pp \rightarrow X}$ does not contain a functional dependence on kinematic parameters—it is intuitive when considering integrals over the parameters:

$$\sigma_{pp \rightarrow X} = \int d\Omega \frac{d\sigma_{pp \rightarrow X}}{d\Omega}. \quad (1.8)$$

Fully differential cross sections can be conveniently denoted as the infinitesimal quantity $d\sigma_{pp \rightarrow X}$. If the integral in Eq. (1.8) is performed over the full phase space, one obtains the *total inclusive* cross section. On the other hand, it is often useful to impose requirements on the kinematic variables of final-state particles, so-called *phase-space cuts*. The *fiducial* cross sections obtained this way are oftentimes more useful than inclusive cross sections because one can incorporate experimental constraints due to which certain areas of the phase space are inaccessible for measurements. On the other hand, their theoretical calculation tends to be more difficult. Overall, the calculation of total or differential cross sections, either inclusive or fiducial, is the main objective of most high-energy phenomenology for collider physics, including this thesis.

1.2 Outline of the Thesis

The main phenomenological result of this thesis is the calculation of the fiducial cross section for the production of a photon pair at the LHC at next-to-next-to-next-to leading order in QCD. Theoretical background and methodology regarding higher-order cross section calculations is discussed in Chapter 2. A major ingredient of cross section calculations is given by *scattering amplitudes*. In Chapter 3, we present a theoretical study of such amplitudes through one-loop order in QCD, investigating their general behavior in infrared limits at next-to-leading power. In particular, we present process-independent formulae for the collinear limit of tree-level amplitudes and the soft limit of one-loop amplitudes. Then, in Chapter 4, we turn our attention to specific amplitudes, namely six-point amplitudes including two photons at one-loop order. We discuss modern methods relevant for amplitude calculations and apply them to obtain analytic results for the amplitudes. Finally, these amplitudes are used to obtain the photon-pair production cross section presented in Chapter 5, which contains the phenomenological background, details of the calculation, and the results. We conclude in Chapter 6, including a discussion of potential future directions of higher-order QCD calculations.

Chapter 2

Cross Sections at Higher Order in QCD

As discussed in Chapter 1, the most relevant observables at colliders are cross sections. In this chapter, we start by recalling basic textbook material regarding the calculation of cross sections in QCD. Again, we refer to standard textbooks like Ref. [7] for a more comprehensive, pedagogical introduction. In Sections 2.1 and 2.2, we give an overview over *subtraction* and *slicing* schemes, two methods used in state-of-the-art calculations of cross sections, including this thesis.¹

In a QFT, the infinitesimal cross section for the production of a final state X containing $m \equiv n - 2$ particles with momenta $p_3, \dots, p_n$ from two massless elementary particles i and j with momenta p_1 and p_2 is given by

$$d\sigma_{ij \rightarrow X} = \frac{1}{F} d\Phi_m |M_{ij \rightarrow X}|^2, \quad (2.1)$$

with the *flux factor* $F \equiv 4p_1 \cdot p_2$, the Lorentz-invariant *phase-space measure*

$$d\Phi_m \equiv \left[\prod_{i=3}^n \frac{d^3 \vec{p}_i}{(2\pi)^3 2p_i^0} \right] (2\pi)^4 \delta^{(4)}(p_1 + p_2 - \sum_{i=3}^n p_i), \quad (2.2)$$

and the *squared scattering amplitude* $|M_{ij \rightarrow X}|^2$. The squaring implicitly contains a summation over color and helicity indices of the involved particles. While color indices are fundamentally unmeasurable, summation over helicity is included because it is usually unresolved at the LHC:

$$|M_{ij \rightarrow X}|^2 \equiv \sum_{\{\sigma_i\}, \{c_i\}} M_{ij \rightarrow X}^*(p_1, \dots, p_n, \sigma_1, \dots, \sigma_n, c_1 \dots c_n) M_{ij \rightarrow X}(p_1, \dots, p_n, \sigma_1, \dots, \sigma_n, c_1 \dots c_n), \quad (2.3)$$

with the shorthand notation $\{a_i\} \equiv \{a_i\}_{i=1}^n$, which is used through this thesis. Given a Lagrangian, e.g. Eq. (1.3), there exists a prescription to obtain the scattering amplitude in *perturbation theory*, where interactions between particles are viewed as a small perturbation from states of free, uninteracting particles, for which the theory is solvable exactly and which the initial and final states of scattering experiments are defined to form. Hence, we write the scattering

¹Note that because the foundations of slicing methods and the current state of N³LO calculations are also discussed in our publication, Ref. [3], to which my personal contributions are described in the beginning of Chapters 4 and 5, parts of their treatment in this chapter are parallel to the one of Ref. [3].

amplitude as a perturbative series in the *coupling constants*,

$$\alpha_s \equiv \frac{g_s}{4\pi}, \quad \alpha \equiv \frac{e^2}{4\pi}, \quad (2.4)$$

of the strong and electromagnetic interaction. At hadron colliders, the effects of the strong interaction are usually much more important than electroweak effects. Therefore, we always truncate the expansion in α at leading order and expand the scattering amplitude only in *orders in QCD*. In particular, having neglected all leptons in our Lagrangian (1.3), the only QED effects we take into account are the couplings of external photons to quarks. Then,

$$M_{ij \rightarrow X} \equiv \alpha^{n_\gamma/2} \alpha_s^{(n-n_\gamma-2)/2} \left(M_{ij \rightarrow X}^{(0)} + \frac{\alpha_s}{4\pi} M_{ij \rightarrow X}^{(1)} + \frac{\alpha_s^2}{(4\pi)^2} M_{ij \rightarrow X}^{(2)} + \dots \right), \quad (2.5)$$

where n_γ is the number of external photons, and we call $M_{ij \rightarrow X}^{(L)}$ the L -loop amplitude, with the special case of the *tree-level* amplitude for $L = 0$. The naming makes sense from the perspective of the calculation method to obtain scattering amplitudes. One draws all possible *Feynman diagrams*, where the external particles are connected with lines and vertices, taking into account the fundamental properties of the theory like flavor and charge conservation. The resulting contribution to the scattering amplitude is then obtained by means of *Feynman rules*, which associate a factor to every internal line or vertex. The Feynman rules can be derived from the Lagrangian, and we summarize them in Appendix A.1. The scattering amplitude is then given by the sum of all possible diagrams. Since the power of couplings corresponds to the number of vertices, tree diagrams have the smallest possible power—ergo the name *tree level*—and every loop within the diagram corresponds to two additional QCD vertices, increasing the order in α_s by one. Due to the correspondence between number of loops and α_s order, the number of corresponding diagrams to a specific order is always finite, a necessary condition for concrete calculations. Besides Feynman rules, external states correspond to appropriate *wave functions*, which can be found in Appendix A.2.

At tree level, every leg has a defined momentum according to momentum conservation at all vertices and fixed external momenta. Different methods to parametrize the external phase-space points with (ideally independent) variables exist, as is described for the example of six massless momenta in Section 4.1. If loops are introduced, this is no longer sufficient and unconfined *loop momenta* are introduced, over which the loop integral

$$\int \frac{d^4 l_1}{(2\pi)^4} \dots \frac{d^4 l_L}{(2\pi)^4} \quad (2.6)$$

is taken. This unconfined integration can lead to divergent integrals, where the problematic regions can be *ultraviolet*, where $l^\mu \rightarrow \infty$, or *infrared*, where $l^2 \rightarrow 0$.² First, such divergences are treated within *dimensional regularization*, where one replaces

$$\frac{d^4 l}{(2\pi)^4} \mapsto \bar{\mu}^{2\epsilon} \frac{d^d l}{(2\pi)^d}, \quad (2.7)$$

with the spacetime dimension $d \equiv 4 - 2\epsilon$ and a mass scale $\bar{\mu}$. The physical four dimensions are recovered in the limit $\epsilon \rightarrow 0$, where also the dependence on $\bar{\mu}$ disappears in principle. Accordingly, divergences appear as poles in ϵ . Of course, predictions of physical observables

²Within infrared divergences, one differentiates between soft and collinear divergences as discussed below. Thus, an infrared limit need not necessarily correspond to $l^\mu \rightarrow 0$.

need to be finite in order for the theory to be useful, implying that all poles in ϵ should cancel when calculating final results.

In the case of ultraviolet divergences, the cancellation of ϵ poles can be achieved by means of *renormalization*. In essence, this means that the fields, couplings, and masses in the Lagrangian are expressed through renormalized quantities which are related to the unrenormalized, *bare* quantities through multiplication with renormalization constants. For example,

$$g_s \mapsto g_s^B = Z_g g_s^R, \quad (2.8)$$

where g_s^B and g_s^R are the bare and renormalized QCD coupling parameters, respectively. The Lagrangian then has the form

$$\mathcal{L} \mapsto \mathcal{L}^B = \mathcal{L}^R + \mathcal{L}^{CT}, \quad (2.9)$$

where the renormalized Lagrangian $\mathcal{L}^R$ is identical to the bare Lagrangian $\mathcal{L}^B$ with all bare quantities replaced by renormalized ones, and there is the additional *counterterm* Lagrangian $\mathcal{L}^{CT}$. It introduces additional Feynman rules which lead to the cancellation of all ultraviolet divergences, which was shown for QCD in Ref. [10]. While the definition of renormalized quantities is not unique, we exclusively work in $\overline{MS}$ *renormalization*, which defines them such that only the ultraviolet ϵ poles and the inconvenient quantities $\log(4\pi)$ and the Euler-Mascheroni constant γ_E are removed from scattering amplitudes. This, however, leads to renormalized quantities depending on the mass scale $\bar{\mu}$ or, alternatively, on

$$\mu^2 \equiv \frac{4\pi}{e^{\gamma_E}} \bar{\mu}^2, \quad (2.10)$$

which we also call *renormalization scale*. For example, the dependence of the strong coupling $\alpha_s(\mu)$ is governed by the *QCD beta function* [11, 12]

$$\beta(\alpha_s) \equiv \frac{1}{4\pi} \frac{\partial \alpha_s}{\partial \log(\mu)} = -2 \left(\frac{\alpha_s}{4\pi} \right)^2 \left(\frac{11}{3} C_A - \frac{4}{3} T_F n_f + \mathcal{O}(\alpha_s) \right), \quad (2.11)$$

with the QCD parameters $C_A = 3$, $T_F = \frac{1}{2}$, and the number of quark flavors $n_f \leq 6$. Solving the truncated differential equation for α_s yields

$$\frac{\alpha_s(\mu)}{4\pi} = \frac{1}{\left(\frac{11}{3} C_A - \frac{4}{3} T_F n_f \right) \log\left(\frac{\mu^2}{\Lambda^2} \right)}, \quad (2.12)$$

with an integration constant Λ . On the one hand, this implies that $\alpha_s(\mu) \rightarrow 0$ as $\mu \rightarrow \infty$. On the other hand, Eq. (2.12) indicates $\alpha_s(\mu) \rightarrow \infty$ as $\mu \rightarrow \Lambda$. However, Eq. (2.11) was derived within perturbation theory, which assumes $\alpha_s \ll 1$. Thus, perturbation theory breaks down for small values of μ . While μ was introduced as an arbitrary parameter, it turns out that such an energy dependence of the strong coupling constant is also observed experimentally. In particular, particles behave *asymptotically free* at very large energies, while they are *confined* at low energies. This confinement implies that the colored particles, quarks and gluons, cannot be observed directly but only within composite particles like the proton. Thus, it seems natural to set μ to a physical scale related to the problem at hand. Furthermore, the structure of the proton cannot be calculated within perturbation theory, and other methods, like *lattice QCD*, have to be employed. While we do not discuss lattice QCD in this thesis, let us mention that it can be used to show that a scale Λ for which the strong coupling diverges indeed exists, and calculate this *QCD scale* to be approximately $\Lambda_{\text{QCD}} \approx 300$ MeV. The appearance of a

dimensionful quantity even within massless QCD, which does not contain any free dimensionful parameters, is called *dimensional transmutation*, a remarkable feature of QCD.

Even though we discuss cross sections for colliders operating at very high energies, confinement is of direct relevance for cross section calculations. The assumption in Eq. (2.1) that particles i and j are elementary particles is not fulfilled at the LHC, where composite protons are collided. To obtain a cross section for proton-proton collisions, one has to perform a convolution with the non-perturbative *parton distribution functions (PDFs)* f_i , which describe the proton structure:

$$d\sigma_{pp \rightarrow X} = \sum_{i,j} \int_0^1 dx_1 \int_0^1 dx_2 f_i(x_1, \mu_F) f_j(x_2, \mu_F) d\sigma_{ij \rightarrow X}(x_1, x_2, \mu_F), \quad (2.13)$$

where the sums over i and j run over the particle flavors that are considered to exist within the proton. These constituents, namely gluons and massless quarks, are also called *partons*. They are approximated to be exactly collinear to the protons and carry the fractions x_1 and x_2 of the proton momenta. Finally, μ_F is called *factorization scale* and separates the non-perturbative physics treated by the PDFs from perturbative physics which is used to calculate the *partonic cross section* $d\sigma_{ij \rightarrow X}$. This introduces a dependence of $d\sigma_{ij \rightarrow X}$ on μ_F due to *collinear counterterms*, which absorb some infrared divergences into the PDFs, namely those that stem from momentum regions collinear to the initial-state partons i and j . For details on collinear divergences, see below. Due to their non-perturbative nature, PDFs are in practice obtained from experimental data. Despite this, one can make predictive cross section calculations because the PDFs do not depend on the final state X .

Renormalization and the introduction of PDFs have introduced two scale parameters, the renormalization scale μ , which we also call μ_R to distinguish it from the second parameter, the factorization scale μ_F . Since these parameters are arbitrary, the prediction for the cross section $d\sigma_{pp \rightarrow X}$ should not depend on them. However, this would only be true if we were able to calculate the cross section exactly to all orders in the coupling constant α_s . Because we work in perturbation theory and truncate the α_s expansion at a finite order, there remains a residual dependence on μ_R and μ_F . For example, there might appear logarithms of the form $\log(\mu^2/Q^2)$ with some physical scale Q related to the studied process. In order to obtain reliable predictions within perturbation theory, it is usually necessary to choose $\mu_F \sim \mu_R \sim Q$. On the one hand, this necessity complicates calculations of cross sections. On the other hand, the scale dependence can be leveraged as a tool to estimate the theoretical uncertainty that stems from the truncation of the perturbative series. In general, less dependence on the scale parameters indicates a more reliable result. A standard procedure is *seven-point scale variation*, where after calculating the cross section at the chosen central scale (μ_R, μ_F) , the calculation is redone with the values

$$(\mu_R/2, \mu_F), (\mu_R, \mu_F/2), (\mu_R/2, \mu_F/2), (2\mu_R, \mu_F), (\mu_R, 2\mu_F), (2\mu_R, 2\mu_F). \quad (2.14)$$

The envelope of results is then quoted as the *scale uncertainty*, which is expected to decrease when increasing the perturbative order.

In principle, one might expect that the precision of predictions can be increased arbitrarily by going higher and higher in perturbation theory. However, it turns out that the expansion in α_s is only an asymptotic, not a convergent expansion [13]. That is, while predictions in perturbation theory approach the correct value as $\alpha_s \rightarrow 0$, the series does not converge if the order N of the expansion approaches infinity. Instead, one expects to observe divergent behavior at some

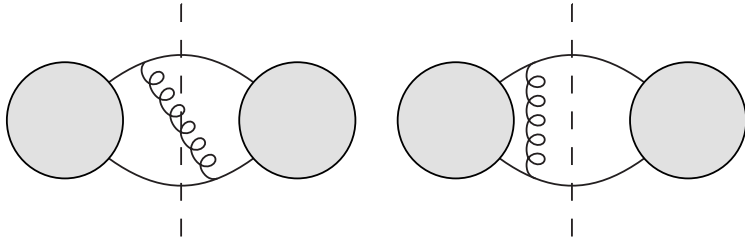


Figure 2.1: Schematic of squared amplitudes contributing to NLO cross sections. Particles which are cut by the dashed line correspond to final state particles. In particular, there is the real-radiation contribution $|M_{ij \rightarrow Xg}^{(0)}|$ (left) and the virtual correction $|M_{ij \rightarrow X}^{(1)}|$ (right). The diagrams, as well as all further Feynman diagrams in this thesis, were produced with JaxoDraw [21–23].

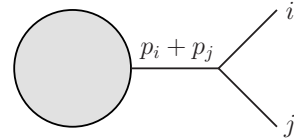


Figure 2.2: Momentum routing for radiation off an external leg that can lead to infrared divergences.

order in perturbation theory, even if $\alpha_s \ll 1$. This divergence can be related to non-perturbative effects like instantons [14, 15] or infrared renormalons [16, 17]. While we do not study such non-perturbative effects in this thesis, it has been shown that the behavior of amplitudes in infrared limits at next-to-leading power, which we discuss at length in Chapter 3, can be helpful for renormalon calculus [18]. Additionally, specific calculations at high perturbative orders are necessary in order to explore the convergence behavior of cross section calculations, which is one motivation for the research presented in this thesis. Another potential problem regarding the current treatment of non-perturbative effects is that the strict PDF factorization (2.13) might be violated starting from next-to-next-to-next-to-leading order ($N^3\text{LO}$) in perturbation theory if colored particles are included in the final state [19, 20]. On the way to such a calculation, the first computation of a $pp \rightarrow X$ cross section at $N^3\text{LO}$ where X consists of 2 particles directly coupling to colored particles, presented in Ref. [3] and Chapter 5 of this thesis, is a major milestone.

So far, divergences discussed in this thesis have been cancelled by counterterms stemming either directly from the Lagrangian after renormalization or from the introduction of PDFs. The remaining infrared (IR) divergences can unfortunately not be removed by renormalization. Instead, one has to be more sensible in the definition of physical observables. As discussed when discussing confinement and PDFs, quarks and gluons are not directly observable in experiment. Instead, one observes hadrons that are formed out of these partons. As a low-energy process, this *hadronization* cannot be calculated within perturbation theory, in analogy to PDFs. Therefore, it is useful to define *jets* as final-state objects, which consist of colored particles and correspond to partons produced in the high-energy, perturbatively calculable process. Ideally, one would want each jet to correspond to exactly one produced parton. However, this is not a sensible definition due to infrared radiation. To be specific, there might be *soft* partons with momenta $p^\mu/Q \ll 1$, Q corresponding to a typical scale of the process, or two *collinear* massless partons i and j with $p_i \cdot p_j/Q^2 \ll 1$, which travel in the same direction due to $p_i \cdot p_j = E_i E_j (1 - \cos \theta_{ij})$, where E_i and E_j are the energies of the partons and θ_{ij} the angle between them. In such cases, one cannot assume that each parton forms its own, visible jet. Only if the final-state observables are chosen correctly and the possibility of soft or collinear radiation is accounted for, one can expect a quantity free from divergences. Indeed, the Kinoshita-Lee-Nauenberg (KLN) theorem [24, 25] shows that all IR divergences cancel if such *real radiation* is taken into account. Therefore, higher orders in cross section calculations not only include more loops in

the expansion (2.5) of scattering amplitudes, but also scattering amplitudes with additional particles in the final state. Thus, in contrast to the nomenclature of L -loop amplitudes, one refers to cross sections calculated to different orders as leading order (LO), next-to-leading order (NLO), next-to-next-to-leading order (NNLO), and so on. The LO cross section is also called the *Born approximation*, and the tree-level amplitude without any additional real radiation is referred to as *Born amplitude*. Figure 2.1 schematically shows real corrections from radiation and *virtual* corrections from higher loop orders for the NLO case. One can immediately see that both corrections increase the order of α_s by one. In order for the divergent contributions from virtual corrections stemming from loop integrals to cancel, real radiation also needs to be associated with divergent behavior. Indeed, a propagator connected to the external legs i and j , as shown in Fig. 2.2, contributes the factor

$$\frac{1}{(p_i + p_j)^2 - m^2} \quad (2.15)$$

to the scattering amplitude, where m is the mass of the intermediate state formed from i and j . The two cases discussed above from an experimental perspective indeed lead to a divergence of this factor: If particle j is massless, $m_j = 0$ and thus $m = m_i$, the soft limit $p_j^\mu \rightarrow 0$ corresponds to a pole of Eq. (2.15), analogously for $i \leftrightarrow j$. Furthermore, if both i and j are massless, the collinear limit $(p_i + p_j)^2 = 2p_i \cdot p_j \rightarrow 0$ implies a divergent scattering amplitude. These divergences are regulated by dimensional regularization of the phase-space integral, in analogy to loop integrals:

$$\frac{d^3 \vec{p}_i}{(2\pi)^3 2p_i^0} \mapsto \bar{\mu}^{2\epsilon} \frac{d^{d-1} \vec{p}_i}{(2\pi)^{d-1} 2p_i^0}. \quad (2.16)$$

Then, all remaining ϵ poles cancel between real and virtual contributions as advertised above.

IR divergences are the ones most relevant to this thesis. While the KLN theorem proves their cancellation, the specific organization of the calculation is still plagued by many difficulties, especially at high orders. Calculation methods include *subtraction schemes*, discussed in Section 2.1, and *slicing methods*, discussed in Section 2.2. As discussed there, they have enabled calculations of cross sections for hadron colliders up to N³LO in QCD, including the calculation presented in this thesis. Another method with less direct relevance for this thesis is *reverse unitarity* [26, 27], where inclusive cross sections can be calculated analytically by converting the phase-space integral (2.2) to loop integrals. It has enabled the first N³LO calculations for cross sections at hadron colliders. Specifically, it was used to calculate predictions for $2 \rightarrow 1$ processes, that is processes where a single particle is produced from the two protons in the initial state. In Refs. [28–31], Higgs production is discussed at N³LO, whereas Refs. [32, 33] contain predictions for Drell Yan, that is the production of a single vector boson. The software package **n3loxs** [34] is a numerical implementation of these results. To obtain differential cross sections from inclusive N³LO results, one can use the *projection-to-Born* method [35], which has been done for Higgs production [36]. The reason why we do not employ reverse unitarity in this thesis is that it is difficult to apply to processes with higher multiplicity, and that fiducial phase-space cuts cannot be easily incorporated. Since our objective is the calculation of the fiducial cross section of a $2 \rightarrow 2$ process at N³LO, we resort to other methods discussed in the remainder of this chapter.

2.1 Subtraction Schemes

The main motivation for subtraction schemes is the desire to perform the phase-space integration with numerical Monte Carlo methods. In such methods, one generates random phase-space configurations called *events*. This is typically done by expressing an m -particle final-state phase space in terms of $3m-4$ parameters $x_k \in [0, 1]$. This is possible due to the finite size of the final-state phase space for a fixed energy of the initial state. An example for such a parametrization is given by the **RAMBO** algorithm [37]. One then has to perform an integral over

$$dx_1 dx_2 d\Phi_m = J(\vec{x}) d^{3m-2}x, \quad (2.17)$$

where x_1 and x_2 are the integration variables for the convolution with the PDFs, see Eq. (2.13), and $J(\vec{x})$ is the Jacobian of the transformation. The integral can then be approximated by taking the average over all generated events.

$$\int d^{3m-2}x |M_{ij \rightarrow X}(\vec{x})|^2 \approx \frac{1}{N} \sum_{k=1}^N |M_{ij \rightarrow X}(\vec{x}_k)|^2, \quad (2.18)$$

with N events drawn from the uniform distribution $U([0, 1]^{3m-2})$. The statistical uncertainty is determined by the variance of the sampled results and decreases with $\sqrt{N}$. It can be reduced by invoking *importance sampling*, where the $\vec{x}$ values are not drawn from a uniform distribution but optimized to approximate the shape of the integrand, e.g. with the **VEGAS** algorithm [38].

The usage of Monte Carlo integration solves multiple problems. First, phase-space integrals are oftentimes not solvable analytically, especially for high-multiplicity final states. An exception is the aforementioned method of reverse unitarity. However, the calculation of fiducial cross sections is difficult when using this method because the integration is performed over the full phase space by default. On the other hand, the full phase-space information is available in generated events, and phase-space cuts can easily be implemented by discarding all phase-space points that do not fulfill the imposed conditions.

The problem when trying to apply Monte Carlo integration to higher-order cross sections is that the phase-space integrals needed to calculate contributions from real and virtual corrections are different. This is obvious because the number of particles in the phase space is different in both cases. However, since both contributions are separately divergent, they cannot be treated on their own in numerical implementations. To illustrate the basic idea of subtraction schemes, let us introduce the following simplified notation for an NLO cross section:

$$\sigma^{\text{NLO}} - \sigma^{\text{LO}} = \int_{m+1} d\sigma^R + \int_m d\sigma^V, \quad (2.19)$$

where $d\sigma^R$ and $d\sigma^V$ are the infinitesimal contributions from real and virtual corrections, respectively, and the subscript of the integral denotes the number of final-state particles over which a phase-space integration has to be performed. Subtraction schemes can then separately perform the integrals in the following way:

$$\sigma^{\text{NLO}} - \sigma^{\text{LO}} = \int_{m+1} \left[d\sigma^R - d\sigma^A \right] + \int_m \left[d\sigma^V + \int_1 d\sigma^A \right], \quad (2.20)$$

where the *subtraction term* $-d\sigma^A$ subtracts an approximation of the real-radiation cross section which has the same behavior in soft and collinear limits. This way, the left integral is finite,

which implies that the right integral also has to be finite, except for the integral in the *integrated subtraction term* $\int_1 d\sigma^A$. If $d\sigma^A$ can be chosen simple enough that this integration over the phase space of a single, so-called *unresolved* particle can be performed analytically in dimensional regularization, the ϵ poles of $d\sigma^V$ are cancelled analytically. Luckily, the construction of such subtraction terms is made feasible due to *hard-soft-collinear factorization* [39] (see also Ref. [40] for a pedagogical treatment) which states that infrared radiation can be described independently of the specific hard process.³ Such process-independent descriptions of infrared radiation will be studied in detail in Chapter 3. Still, the fact that we use a simplified notation for illustration purposes already hints at the fact that the detailed definition is far from straightforward. In particular, it is not unique and many different subtraction schemes have been proposed. Since the real-radiation cross section $d\sigma^R$ can contain singularities at many different phase-space points, an important question in the construction of subtraction schemes is how to isolate the different soft and collinear limits that can occur, so that the corresponding approximation can be subtracted. Furthermore, one has to find mappings between the corresponding m -particle and $(m+1)$ -particle phase-space points to parametrize the limits and keep on-shellness and momentum conservation fulfilled.

The first subtraction scheme applicable to arbitrary processes at hadron colliders was constructed by Catani and Seymour [41]. In essence, it leverages the fact that at NLO, every $(m+1)$ -particle phase-space point corresponds to only a single particle being soft or collinear. It then builds a sum of subtraction terms made purely from Lorentz-invariant quantities, while mapping the generated $(m+1)$ -particle phase-space point to a different m -particle phase-space point for each subtraction term. Other subtraction schemes which are, to some extent, related to the Catani-Seymour subtraction scheme could be extended to NNLO, namely antenna subtraction [42–44] and CoLoRFulNNLO [45–47], whose implementations in the software packages NNLOJET [48] and NNLOCAL [49] have recently been made publicly available.

A contrasting approach has been taken in the subtraction scheme developed by Frizzone, Kunszt, and Signer (FKS) [50]. There, specific infrared limits are isolated with the introduction of *selector functions* $\mathcal{S}_{ij}$ which fulfill

$$\sum_{i,j} \mathcal{S}_{ij} = 1, \quad (2.21)$$

where the sum runs over the external particles of the process. The integrand can therefore be multiplied with this sum without altering the result. The isolation of infrared limits where i becomes unresolved can then be achieved by constructing selector functions which behave in these limits as follows:

$$\mathcal{S}_{ij} \rightarrow 1, \quad \mathcal{S}_{kl} \rightarrow 0, \quad \text{for all } k, l \notin \{i, j\}. \quad (2.22)$$

A possible set of selector functions shown in Ref. [51], where a slightly adapted implementation of the FKS scheme is discussed, reads

$$\mathcal{S}_{ij} = \frac{1}{\mathcal{D}} \frac{1}{d_{ij}} h\left(\frac{E_i}{E_i + E_j}\right), \quad d_{ij} = (E_i E_j)^a (1 - \cos(\theta_{ij}))^b, \quad \mathcal{D} = \sum_{i,j} \frac{1}{d_{ij}},$$

$$h(z) = \frac{(1-z)^c}{z^c + (1-z)^c}, \quad (2.23)$$

for E_i , E_j the energies of particles i and j , θ_{ij} the angle between them, and the in principle arbitrary parameters $a, b, c > 0$. It is immediately clear that in contrast to the Catani-Seymour

³This independence can be violated with factorization-breaking effects already mentioned above. They appear starting from N³LO in collinear limits when particles of both initial and final state are involved.

scheme, the construction is not Lorentz invariant but requires the choice of a specific reference frame, typically the center-of-mass frame of the partonic collision. This, however, makes the correspondence of variables and infrared limits more transparent. In particular, it is convenient to split the integration over the $(m+1)$ -particle phase space into one over an m -particle Born phase space and frame-dependent variables directly parametrizing the infrared limits. Thus, for each term of the selector function, a specific mapping from the m -particle phase space to the $(m+1)$ -particle phase space is employed. The subtraction terms corresponding to an integration variable ξ which parametrizes a singularity are then generated with the identity

$$\frac{1}{\xi^{1+a\epsilon}} = -\frac{\delta(\xi)}{a\epsilon} + \left[\frac{1}{\xi^{1+a\epsilon}} \right]_+, \quad (2.24)$$

where the first term becomes the integrated subtraction term and the second term is integrable with the *plus distribution* defined by

$$\int_0^1 d\xi \left[\frac{1}{\xi^{1+a\epsilon}} \right]_+ f(\xi) = \int_0^1 d\xi \frac{f(\xi) - f(0)}{x^{1+a\epsilon}}. \quad (2.25)$$

The specific choice of selector functions and phase-space mappings is not straightforward, especially when extending the scheme to NNLO calculations. A first such extension has been presented in form of the sector-improved residue subtraction scheme introduced in Ref. [52]. The complicated nature of the problem is underlined by the fact that the scheme has been refined multiple times [53, 54]. Besides the choice of selector functions and phase-space mappings, the possibility of two unresolved particles complicates the construction of subtraction terms according to Eq. (2.24). This is solved by incorporating the concept of *sector decomposition* [55–57] to further divide each sector into subsectors. The sector-improved residue subtraction scheme is implemented in the private software package **STRIPPER**, which has been used to produce the cross section results of this thesis. It aims at implementing as many integrals as possible with numerical integration techniques in order to simplify the construction. Other NNLO extensions of the FKS scheme aim at implementations where more process-independent integrals have been performed analytically, namely the nested soft-collinear subtraction scheme [58, 59] with a publicly available software implementation **history** [60], as well as the local analytic sector subtraction scheme [61].

While a complete description of the **STRIPPER** framework is beyond the scope of this thesis, we instead refer the reader to Refs. [52–54], let us list the contributions which occur when using it to calculate a cross section at NNLO. At LO, no subtraction is necessary to calculate the Born cross section

$$\sigma^{\text{LO}} = \sigma^B. \quad (2.26)$$

At NLO, the contributions are

$$\sigma^{\text{NLO}} = \sigma^{\text{LO}} + \sigma^R + \sigma^V + \sigma^C, \quad (2.27)$$

including real (R) and virtual (V) corrections, analogously to Eq. (2.19), and additionally the contribution σ^C including collinear counterterms due to PDF factorization discussed above. Following Eq. (2.20), the real contributions are further decomposed as

$$\sigma^R = \sigma_F^R + \sigma_U^R, \quad (2.28)$$

where σ_F^R is the finite (F) first integral of Eq. (2.20), and σ_U^R contains the integrated subtraction term, where the unresolved (U) momentum is integrated out, regulated by the phase-space measure in dimensional regularization. As it still contains ϵ poles, it is numerically integrated order by order up to $\mathcal{O}(\epsilon^0)$. The virtual (V) corrections σ^V is also decomposed into the $\mathcal{O}(\epsilon^0)$, finite (F) part, and its ϵ poles, which can be obtained from the action of a process-independent operator acting on leading-order amplitudes as explained in Section 3.4.5:

$$\sigma^V = \sigma_F^V + \sigma_U^V. \quad (2.29)$$

By adding the numerical results of the ϵ poles of σ_U^R , σ_U^V , and σ^C , pole cancellation can be explicitly verified.

At NNLO, double-virtual (VV) two-loop corrections start to contribute, and to cancel their divergences, double-real (RR) corrections with two real emissions need to be included. There can also be mixed real-virtual corrections (RV) with one-loop amplitudes containing a single real radiation. Finally, the collinear counterterms have a more complicated form. Overall, there is

$$\sigma^{\text{NNLO}} = \sigma^{\text{NLO}} + \sigma^{RR} + \sigma^{RV} + \sigma^{VV} + \sigma^{C1} + \sigma^{C2}. \quad (2.30)$$

In analogy to the NLO case, we further decompose each contribution into finite terms and terms containing ϵ poles. However, the latter can now either be single-unresolved (SU) or double-unresolved (DU), with one or two divergent phase-space integrations expanded in ϵ , respectively. Therefore,

$$\begin{aligned} \sigma^{RR} &= \sigma_F^{RR} + \sigma_{SU}^{RR} + \sigma_{DU}^{RR}, \\ \sigma^{RV} &= \sigma_F^{RV} + \sigma_{SU}^{RV} + \sigma_{DU}^{RV} + \sigma_{FR}^{RV}, \\ \sigma^{VV} &= \sigma_F^{VV} + \sigma_{DU}^{VV} + \sigma_{FR}^{VV}, \\ \sigma^{C1} &= \sigma_{SU}^{C1} + \sigma_{DU}^{C1}, \\ \sigma^{C2} &= \sigma_{FR}^{C2} + \sigma_{DU}^{C2}. \end{aligned} \quad (2.31)$$

The contributions labeled FR are the *finite-remainder* contributions and need to be introduced when formulating the subtraction scheme such that scattering amplitudes with four-dimensional external momenta (in the so-called *'t Hooft-Veltman scheme*) can be used. See Ref. [54] for details on this reduction to four dimensions.

The progress in the construction of subtraction schemes have led to remarkable results in fixed-order QCD calculations for hadron colliders. For example, calculations for $2 \rightarrow 3$ processes are now routinely performed using the software packages **STRIPPER** and **NNLOJET** [62–70]. Besides going to even higher multiplicities, a natural next step is the construction of an N^3LO subtraction scheme. While such an extension applicable to e^+e^- collisions has been performed for antenna subtraction, leading to a calculation of $\sigma_{e^+e^- \rightarrow jj}^{\text{N}^3\text{LO}}$ [71], a generalization applicable to hadron colliders is highly challenging and remains out of reach. Since the goal of this thesis is the calculation of an N^3LO cross section, we therefore resort to the alternative given by *slicing methods* presented in the following section.

2.2 Slicing Methods

As discussed in the previous section, the construction of subtraction schemes is a very difficult task and no subtraction scheme for the calculation of N^3LO cross sections at hadron colliders is currently available. A conceptually simpler method for numerical higher-order cross section

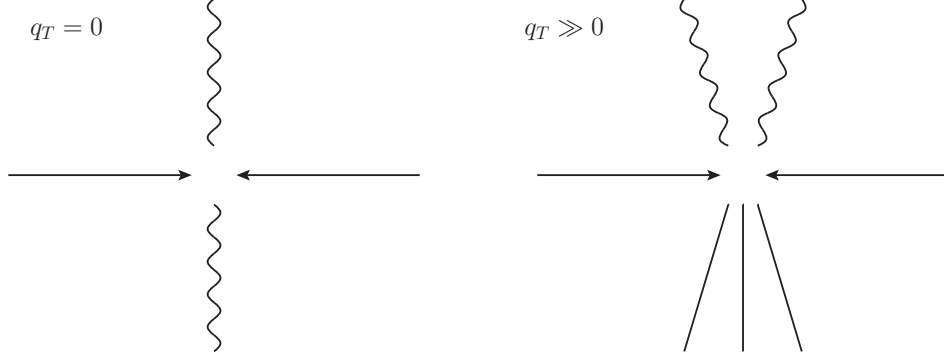


Figure 2.3: Illustration of the spatial distribution of two contributions to a cross section within q_T slicing for the case of the production of a photon pair. While on the left-hand side, the q_T of the photon pair is zero, for a large q_T displayed on the right-hand side, additional jet radiation is required to fulfill momentum conservation.

calculations is given by *slicing methods*. Their basic idea is a decomposition of the cross section as follows:

$$\sigma_{pp \rightarrow X}^{\text{N}^m \text{LO}} = \int_0^{\tau_{\text{cut}}} d\tau \frac{d\sigma_{pp \rightarrow X}^{\text{N}^m \text{LO}}}{d\tau} + \int_{\tau_{\text{cut}}}^{\infty} d\tau \frac{d\sigma_{pp \rightarrow X+\text{jet}}^{\text{N}^{m-1} \text{LO}}}{d\tau}. \quad (2.32)$$

This equation is correct if the *slicing parameter* τ is a variable which implies jet radiation additionally to the production of X unless τ is zero. An illustrative example is q_T slicing proposed in Ref. [72]. There, X is required to be a final state which does not contain jets, and $\tau = q_T \equiv |\vec{q}_T|$ is the transverse momentum of the particles in this final state. As sketched in Fig. 2.3, a finite $q_T > 0$ clearly requires resolved jet radiation, implying that $d\sigma_{pp \rightarrow X}^{\text{N}^m \text{LO}}$ is equivalent to $d\sigma_{pp \rightarrow X+\text{jet}}^{\text{N}^{m-1} \text{LO}}$, which can be calculated if an $\text{N}^{m-1} \text{LO}$ subtraction scheme is available. The key ingredient to slicing methods is given by an approximation of the first term of Eq. (2.32) which holds for small τ and does not require the full calculation of the $\text{N}^m \text{LO}$ cross section. By choosing τ_{cut} sufficiently small but non-zero, we can therefore obtain a very good approximation of $\sigma_{pp \rightarrow X}^{\text{N}^m \text{LO}}$. However, decreasing τ_{cut} imposes problems because both terms of Eq. (2.32) individually diverge as $\tau_{\text{cut}} \rightarrow 0$. Given that our objective is a numerical calculation with in principle full differential information, very high numerical precision is necessary to obtain reliable results.

In the case of q_T slicing, the approximation of the first term of Eq. (2.32) is achieved through the factorization theorem [73–77]

$$\begin{aligned} \frac{d\sigma_{pp \rightarrow X}}{dQ^2 dy} &= \sum_{a,b} H_{a,b}(Q^2, \mu) \\ &\times \int d^2 \vec{q}_T \int \frac{d^2 \vec{b}_T}{(2\pi)^2} e^{i\vec{q}_T \cdot \vec{b}_T} B_a(x_1, b_T, \mu, \frac{\nu}{\omega_a}) B_b(x_2, b_T, \mu, \frac{\nu}{\omega_b}) S(b_T, \mu, \nu) + \mathcal{O}(q_T/Q), \end{aligned} \quad (2.33)$$

$|\vec{q}_T| < q_{T,\text{cut}}$

where we have used the notation of Ref. [78]. We have included additional differential dependence on the center-of-mass energy Q and the rapidity y of the final state X . The sum over a, b runs over the partonic flavors which are contained in the initial-state protons, and the functions $H_{a,b}$, B_a , and S are the *hard*, *beam*, and *soft* functions, respectively. As the naming suggests, the hard function contains the Born cross section and the finite part of virtual corrections to the hard process $ab \rightarrow X$, the beam function contains collinear radiation off the proton beams,

and the soft function soft radiation off them.⁴ The Fourier conjugate of $\vec{q}_T$ is labeled $\vec{b}_T$ with $b_T \equiv |\vec{b}_T|$ and called *impact parameter*. Only in b_T space, the beam functions B_a and B_b enter multiplicatively into the factorization theorem. Finally, we have introduced the variables

$$\omega_a \equiv Q^{+y} \propto x_1, \quad \omega_b \equiv Q^{-y} \propto x_2, \quad (2.34)$$

which contain the energies of the partons a and b , and two scale parameters μ and ν . The dependence on ν cancels exactly, as can be made explicit with the introduction of the *transverse-momentum-dependent (TMD)* parton distribution functions

$$\tilde{f}_a(x, b_T, \mu) \equiv B_a(x_1, b_T, \mu, \frac{\nu}{\omega_a}) \sqrt{S(b_T, \mu, \nu)}. \quad (2.35)$$

They can be written as convolutions with regular PDFs:

$$\tilde{f}_a(x, b_T, \mu) = \sum_i \int_x^1 \frac{dz}{z} f_i(\frac{x}{z}, \mu) \tilde{I}_{a,i}^{\text{TMD}}(z, b_T, \mu) + \mathcal{O}(b_T \Lambda_{\text{QCD}}), \quad (2.36)$$

with the matching kernel $\tilde{I}_{a,i}^{\text{TMD}}(z, b_T, \mu)$, and where power corrections in the QCD scale are neglected as usual when working with standard PDF factorization. Putting everything together, Eq. (2.33) can be written as

$$\begin{aligned} \frac{d\sigma_{pp \rightarrow X}}{dQ^2 dy} &= \sum_{a,b} H_{a,b}(Q^2, \mu) \sum_{i,j} \int_{x_1}^1 \frac{dz_1}{z_1} f_i(\frac{x_1}{z_1}, \mu) \int_{x_2}^1 \frac{dz_2}{z_2} f_j(\frac{x_2}{z_2}, \mu) \\ &\times \int_{|\vec{q}_T| < q_{T,\text{cut}}} d^2 \vec{q}_T \int \frac{d^2 \vec{b}_T}{(2\pi)^2} e^{i\vec{q}_T \cdot \vec{b}_T} \tilde{I}_{a,i}^{\text{TMD}}(z, b_T, \mu) \tilde{I}_{b,j}^{\text{TMD}}(z, b_T, \mu) + \mathcal{O}(q_T/Q). \end{aligned} \quad (2.37)$$

For the case of massless final states X , $\tilde{I}_{b,j}^{\text{TMD}}(z, b_T, \mu)$ has been calculated through N³LO in Refs. [78, 79]. Because they are only given as functions of a single scale μ , care has to be taken when the renormalization scale μ_R and the factorization scale μ_F are not identical. To be explicit, one has to first insert $\mu = \mu_R$ and then run the result to the desired μ_F using DGLAP evolution [80–82] with three-loop splitting functions [83, 84]. After this, the $\vec{q}_T$ and $\vec{b}_T$ integrations can be performed analytically for every a, b pair. This is particularly convenient when using the solution of $\tilde{I}_{b,j}^{\text{TMD}}(z, b_T, \mu)$ in electronic format provided in the ancillary files of Ref. [79]. Because the remaining steps, convolutions and phase-space integration, are also present in contributions of the sector-improved residue subtraction scheme, see Section 2.1, and implemented as efficient numerical integrations in STRIPPER, it is straightforward to implement Eq. (2.37) at N³LO as well. As STRIPPER also has the functionality to calculate NNLO cross sections, this enables it to calculate N³LO cross sections for processes with colorless final state, as has been done for the calculation presented in Ref. [3] and Chapter 5. Before this, q_T slicing had been used to calculate differential cross sections for $2 \rightarrow 1$ processes at N³LO, namely Higgs production, $pp \rightarrow H$, and Drell-Yan production, $pp \rightarrow V$, where V is a vector boson, see Refs. [85, 86] and [87–93], respectively.

An obvious drawback of q_T slicing is the limitation to colorless final states. Massive colored particles can in principle be included by adapting the soft function, which has been done for top-quark pair production at NNLO [94]. However, no such calculation is available at N³LO.

⁴If the final state X contains massive colored particles—massless partons are excluded by definition—soft radiation off them needs to be included as well.

Including jets is conceptually impossible when the usual q_T as the slicing variable. While there have been attempts to calculate cross sections at hadron colliders with resolved jets using an adapted version of q_T slicing [95–98], none of them has exceeded NNLO. A different solution in order to include resolved jets is N -jettiness slicing [99, 100], where N is the number of resolved jets and the slicing parameter τ is set to the N -jettiness [101]

$$\mathcal{T}_N = \sum_k \min_i \left(\frac{p_i \cdot p_k}{E_i} \right), \quad (2.38)$$

where i includes the resolved jets with momenta p_i and energy E_i , and the sum runs over all other, unresolved jets. A factorization theorem similar to Eq. (2.33) can be employed. While the necessary beam [102, 103] and jet [104, 105] functions are known at N³LO, the soft function is only known for the zero-jettiness case at this order [106, 107], again leading to the requirement of colorless final states. Thus, the inclusion of colored particles in the final state of N³LO cross sections for hadron colliders remains out of reach.

Chapter 3

QCD Amplitudes at Next-to-Leading Power in Infrared Limits

As discussed in the previous chapter, a process-independent description of infrared radiation is paramount for the calculation of higher-order cross section. In this chapter, we study this behavior of QCD amplitudes with $n + 1$ external, all outgoing particles, where particle $n + 1$ is the massless unresolved particle.¹ Infrared limits always involve some momentum invariants becoming “small”. Throughout this chapter, we will use λ as a small quantity, i.e. the infrared limit corresponds to taking the limit $\lambda \rightarrow 0$. The kinematics of the studied amplitudes are defined by the momenta $\{p_k\}_{k=1}^{n+1}$. Momentum p_{n+1} can either become soft,

$$p_{n+1}^\mu = \mathcal{O}(\lambda), \quad (3.1)$$

or collinear to the massless momentum p_i , which can be parametrized in the *Sudakov parametrization* [108]

$$p_{n+1} = xp'_i + l_\perp - \frac{l_\perp^2}{2x} \frac{q}{p'_i \cdot q}, \quad p_i = (1-x)p'_i - l_\perp - \frac{l_\perp^2}{2(1-x)} \frac{q}{p'_i \cdot q}, \quad (3.2)$$

with the light-like reference momentum q and the perpendicular momentum $l_\perp$, which becomes small in the collinear limit, $l_\perp^\mu = \mathcal{O}(\sqrt{\lambda})$. The momenta $\{p'_k\}_{k=1}^n$ correspond to the n -particle Born phase space. Explicitly, there is

$$l_\perp \cdot p'_i = l_\perp \cdot q = q^2 = 0, \quad p_j = p'_j + \mathcal{O}(l_\perp^2) = p'_j + \mathcal{O}(\lambda) \quad \text{for } j \in \{1, \dots, n\} \setminus \{i\}. \quad (3.3)$$

Note that we use the shorthand notations $\{p_k\} \equiv \{p_k\}_{k=1}^{n+1}$ and $\{p'_k\} \equiv \{p'_k\}_{k=1}^n$ throughout the chapter.²

Hard-soft-collinear factorization [39], already mentioned in Chapter 2, ensures that we can write amplitudes in the schematic form

$$|M_{n+1}(\{p_k\})\rangle = \mathbf{IR} \, |M_n(\{p'_k\})\rangle + \mathcal{O}(\lambda^0), \quad (3.4)$$

¹In Chapter 2, we have considered the Born amplitude to have two incoming and $m = n - 2$ outgoing particles. Here, we treat all particles as outgoing for simplicity. The case of incoming particles can be recovered by crossing symmetry.

²This extends the shorthand notation introduced in Chapter 2, where the set always had n entries. Analogously, we use this notation not only for momenta but also for helicity and color indices.

where a process-independent operator $\mathbf{IR}$ acting on the Born amplitude yields the correct divergent terms of the full amplitude. For a rigorous definition of the notation used for the amplitudes, see Section 3.1. In this chapter, the *power* in λ is of particular importance. We call the poles in λ *leading-power* (LP) terms. The behavior at $\mathcal{O}(\lambda^0)$ is then at *next-to-leading power* (NLP). This nomenclature is used to differentiate from the *order* in the strong coupling constant α_s . We also use the term *subleading* behavior as a synonym to behavior at NLP.

While the knowledge of infrared limits at LP is sufficient for the construction of subtraction schemes, also the study of the NLP behavior has seen attention for a long time. In QED, the NLP soft expansion for single-gluon emission at tree level is called the Low-Burnett-Kroll (LBK) theorem [109, 110], which was later generalized to QCD [111, 112]. Violations of hard-soft-collinear factorization at NLP complicate the discussion at higher loop orders, as was first understood in Ref. [113] and we will see later in this chapter. The mixing of collinear and soft effects can be avoided by studying the soft limit in massive QED, where collinear radiation is regularized and the LBK theorem can be generalized to all orders [114–116]. In massless theories, NLP effects that are unrelated to collinear regions have been described with the help of the Feynman rules of *next-to-eikonal* lines [117, 118]. They are a generalization of *eikonal* lines, defined as lines from which only soft gluons can be radiated and which are frequently used in the context of LP soft factorization [39, 40]. The inclusion of collinear effects has been performed for scalar theories [119], and necessary ingredients have been identified for QED and QCD [120, 121]. For the QED case, these ingredients have been calculated through two-loop order in Refs. [122, 123]. In our study in Ref. [1], we build on Ref. [122] and provide a process-independent expression for the soft expansion of one-loop amplitudes in massless QCD. Besides a generalization to QCD, our result provides desirable simplifications compared to Ref. [122]. For massive QCD, we provide a non-abelian generalization of Ref. [114] in Ref. [2]. Taken together, the results of Refs. [1, 2] can be applied to any one-loop QCD amplitude containing any number of massive and massless particles.

Besides the radiation of a soft photon or gluon in QED and QCD, process-independent theorems for infrared behavior at NLP have also been proposed for the radiation of a soft graviton [124–127], as well as within *soft-collinear effective theory* (SCET) [128–130]. Furthermore, soft radiation in QED and QCD is still seeing recent attention at tree level, e.g. by considering soft-quark radiation [131–133]. The surging interest in NLP effects can be explained by the multitude of available applications. For example, slicing methods discussed in Section 2.2 can be improved by using a better approximation of the cross section below the cut parameter. This can be achieved by including NLP effects, see Ref. [134] and references therein. Furthermore, there has been recent interest in how well fixed-order distributions can be approximated when calculated in the soft approximation at NLP, as was done in Refs. [135, 136] and references therein. Another application of NLP factorization is *resummation*, where infrared effects can be included to all orders in α_s . For the inclusion of NLP effects in resummation, see e.g. Refs. [137–141]. Finally, NLP expansions can simply be used as approximations to the full amplitude for highly infrared phase-space points, where numerical implementations of the full amplitude might be plagued by instabilities, as was done in Refs. [142, 143].

In contrast to the enormous research results considering soft emission at NLP, little had been known about subleading effects in collinear radiation. In Ref. [1], we fill this gap by providing a general formula for tree-level amplitudes at NLP in collinear limits, with one missing piece later provided in Ref. [2]. Besides the theoretical insights gained by this formulation, it can directly be used in the description of collinear regions appearing in the subleading soft expansion at

one-loop order mentioned above. Only then a truly general solution can be achieved, another achievement of Ref. [1].

In this chapter, we reproduce the work of Refs. [1, 2] by deriving universal expressions for the collinear expansion of tree-level amplitudes and for the soft expansion of one-loop amplitudes in QCD. While the derivation is oftentimes identical or closely related to Refs. [1, 2], we adapt the description of collinear radiation by the introduction of purely leading-power splitting operators in Eq. (3.64), which we believe leads to results with more intuitive expressions.³

3.1 Notation

In this chapter, we study QCD amplitudes containing $n + 1$ outgoing particles as mentioned above. We mostly follow the notation of Ref. [1, 2], which we recall in this section. For simplicity, we consider all particles to be either (anti-)quarks or gluons, even though uncolored particles may easily be added as they do not contribute to QCD radiation. Therefore, instead of using the $M_{ij \rightarrow X}$ notation from Chapter 2, we denote the full amplitude as M_{n+1} . Because particle $n + 1$ is the unresolved particle, the Born amplitude, where it is removed, is denoted as M_n . To be explicit about the renormalization, we work with the bare coupling constant α_s^B but include mass counterterms whenever working with massive particles. However, we neglect any closed fermion loops containing massive quarks.

All amplitudes are written as vectors in color and spin space. This space is spanned by the orthonormal basis vectors

$$|c_1, \dots, c_l; \sigma_1, \dots, \sigma_m\rangle \equiv |c_1, \dots, c_l\rangle \otimes |\sigma_1, \dots, \sigma_m\rangle \equiv |c_1\rangle \otimes \dots \otimes |c_l\rangle \otimes |\sigma_1\rangle \otimes \dots \otimes |\sigma_m\rangle, \quad (3.5)$$

where c_i are the color indices of l particles and σ_i the helicity indices of m particles. For the special cases $l = m = n + 1$ and $l = m = n$, we use the shorthand notations

$$|\{c_k\}, \{\sigma_k\}\rangle \equiv |c_1, \dots, c_{n+1}; \sigma_1, \dots, \sigma_{n+1}\rangle, \quad |\{c'_k\}, \{\sigma'_k\}\rangle \equiv |c'_1, \dots, c'_n; \sigma'_1, \dots, \sigma'_n\rangle. \quad (3.6)$$

The components of a vector representing a scattering amplitude are then the amplitude values for the corresponding spin and color configurations, for example

$$|M_{n+1}\rangle \equiv \sum_{\substack{\text{color} \\ \text{spin}}} M_{n+1}(\{c_k\}, \{\sigma_k\}) |\{c_k\}, \{\sigma_k\}\rangle, \quad (3.7)$$

where the sum runs over all possible index combinations. As indicated in Eq. (3.4), we aim at expressing the infrared behavior as an operator that acts on vectors in color and spin space. For example, some expressions will depend on generators of the color algebra, whose form furthermore depends on the flavor of a particle i , which we denote as a_i throughout this chapter:

$$M_{n+1}(\{c_k\}) \supset \sum_{c'_i} (T_{a_i})_{c_i, c'_i}^{c_{n+1}} M_n(\{c'_k\}) \quad (3.8)$$

³A note on the author's personal contribution to Refs. [1, 2]: I performed the analytical derivation of the expressions in Ref. [1] as well as an independent numerical implementation of the numerical checks, which were also performed by T. Schellenberger. A less compact expression describing the soft region of one-loop massless amplitudes as well as an analysis of the collinear region for specific processes was already performed for my Master's thesis [144]. M. Czakon contributed supervision and simplification of results to both Refs. [1, 2]. To the latter, I contributed cross checks of intermediate results, as well as co-supervision of the calculation mainly performed by K. Erhard.

with

$$(T_{a_i})_{c_i, c'_i}^{c_{n+1}} = \begin{cases} T_{c_i c'_i}^{c_{n+1}}, & a_i = q, \\ -T_{c'_i c_i}^{c_{n+1}}, & a_i = \bar{q}, \\ -i f^{c_{n+1} c_i c'_i}, & a_i = g. \end{cases} \quad (3.9)$$

By introducing the operator $\mathbf{T}_i$ defined by

$$\mathbf{T}_i |c'_i\rangle \equiv \sum_{c_i, c_{n+1}} (T_{a_i})_{c_i, c'_i}^{c_{n+1}} |c_i, c_{n+1}\rangle, \quad (3.10)$$

Eq. (3.8) reduces to the convenient form

$$|M_{n+1}\rangle \supset \mathbf{T}_i |M_n\rangle. \quad (3.11)$$

Note that applying $\mathbf{T}_i$ implies that the vector's dimension increases by one. In other words, the operator “adds another particle”, a convenient property when constructing operators relating amplitudes whose particle number differs by one. Still, sometimes we employ the operator $\mathbf{T}_i^{c_{n+1}} \equiv \langle c_{n+1} | \mathbf{T}_i$ which keeps the dimension fixed:

$$\mathbf{T}_i^c |c'_i\rangle = \sum_{c_i} (T_{a_i})_{c_i, c'_i}^c |c_i\rangle. \quad (3.12)$$

In spin space, we also introduce operators that change the dimension of a vector, namely $\bar{\mathbf{u}}_i$, $\mathbf{v}_i$, and $\varepsilon_{i,\mu}^*$, in relation to spinors and polarization vectors. In the gluon case, they act as

$$\varepsilon_{n+1,\mu}^* |\sigma_1, \dots, \sigma'_n\rangle \equiv \sum_{\sigma_{n+1}} \varepsilon_\mu^*(p_{n+1}, \sigma_{n+1}) |\sigma_1, \dots, \sigma'_n, \sigma_{n+1}\rangle, \quad (3.13)$$

and analogously in the (anti-)quark case. Note that we also use the shorthand notation $\varepsilon_{n+1,\mu}^* \equiv \varepsilon_\mu^*(p_{n+1}, \sigma_{n+1})$ for polarization vectors and analogously for spinors. We also employ operators acting in the opposite way, removing the wave function and therefore one spin-space dimension from an amplitude. In the gluon case,

$$\partial_{\varepsilon_i^*}^\mu |M\rangle \equiv \sum_{\substack{\text{color} \\ \text{spin}}} \frac{\partial M(\dots, \sigma_i, \dots)}{\partial \varepsilon_\mu^*(p_i, \sigma_i)} |\dots, \sigma_{i-1}, \sigma_{i+1}, \dots\rangle. \quad (3.14)$$

The degree of freedom is therefore moved from spin space to Lorentz space. The analogous definition for (anti-)quarks moves the degree of freedom into Dirac space. Also with these definitions available, it is still sometimes useful to directly access the indices. This can be done by means of the surjection operator $\mathbf{P}_i$ defined by

$$\mathbf{P}_i(\sigma, c) |\dots, c_{i-1}, c_i, c_{i+1}, \dots; \dots, \sigma_{i-1}, \sigma_i, \sigma_{i+1}, \dots\rangle \equiv \delta_{\sigma\sigma_i} \delta_{cc_i} |\dots, c_{i-1}, c_{i+1}, \dots; \dots, \sigma_{i-1}, \sigma_{i+1}, \dots\rangle. \quad (3.15)$$

We also use the shorthand notation $\mathbf{P}_i \equiv \mathbf{P}_i(\sigma_i, c_i)$ and sometimes employ a surjection operator $\mathbf{P}_i(c)$, which only acts in color space and leaves the spin space unchanged. Finally, let us define an operator to exchange both color and spin indices between two particles:

$$\mathbf{E}_{i,j} |\dots, c_i, \dots, c_j, \dots; \dots, \sigma_i, \dots, \sigma_j, \dots\rangle \equiv |\dots, c_j, \dots, c_i, \dots; \dots, \sigma_j, \dots, \sigma_i, \dots\rangle. \quad (3.16)$$

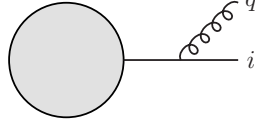


Figure 3.1: Radiation of a soft photon at tree level. Particle i can be either an (anti-)quark or a gluon.

3.2 Soft Limit of Tree-Level Amplitudes

Let us start with the well-known [145] leading behavior of tree-level amplitudes when radiating a soft gluon. We use the standard notation $q \equiv p_{n+1}$ to denote the soft momentum. Note that this momentum has in principle nothing to do with the reference momentum q used in the Sudakov parametrization (3.2), as two completely different infrared limits are described. However, choosing the same symbol will turn out to be convenient in Section 3.4.3.

Fig. 3.1 shows the diagram that leads to a soft divergence at tree-level when $q^\mu \rightarrow 0$. It exists for all external partons in the amplitude, so we have to perform a sum:

$$|M_{n+1}^{(0)}(\{p_k\})\rangle = \sum_i \mathcal{S}_{\text{LP},i}^{(0)}(p_i, q) |M_n^{(0)}(\{p'_k\})\rangle + \mathcal{O}(\lambda^0), \quad (3.17)$$

where we denote the leading-power contribution from soft radiation off particle i as $\mathcal{S}_{\text{LP},i}^{(0)}(p_i, q)$. Let us calculate it by inserting simple Feynman rules, assuming that particle i is a massless quark:

$$\begin{aligned} \mathcal{S}_{\text{LP},i}^{(0)}(p_i, q) |M_n^{(0)}(\{p'_k\})\rangle &= \epsilon_{n+1,\mu}^* \bar{u}_i i \mathbf{T}_i \gamma^\mu i \frac{\not{p}_i + \not{q}}{(p_i + q)^2} \partial_{\bar{u}_i'} |M_n^{(0)}(\{p'_k\})\rangle \\ &= -\epsilon_{n+1,\mu}^* \mathbf{T}_i \frac{1}{2p_i \cdot q} \bar{u}_i \gamma^\mu \not{p}_i \partial_{\bar{u}_i'} |M_n^{(0)}(\{p'_k\})\rangle + \mathcal{O}(\lambda^0) \\ &= -\epsilon_{n+1,\mu}^* \mathbf{T}_i \frac{p_i^\mu}{p_i \cdot q} |M_n^{(0)}(\{p'_k\})\rangle + \mathcal{O}(\lambda^0), \end{aligned} \quad (3.18)$$

where we have used $\gamma^\mu \not{p}_i = -\not{p}_i \gamma^\mu + 2p_i^\mu$ and $\bar{u}_i \not{p}_i = 0$. It is easy to perform a similar calculation in the case of the radiating particle being a massive (anti-)quark or a gluon. Then, one obtains the same result as in the massless quark case. Hence, the soft limit at leading power is independent of type and spin of the radiating particle. This independence can be formalized with the notion of eikonal lines up to a general proof of soft factorization [39]. However, since we want to generalize soft factorization to subleading power, where spin independence breaks down, we do not go into details in this work. Back to leading power, we use the notation

$$\begin{aligned} |M_{n+1}^{(0)}(\{p_k\})\rangle &\equiv \mathcal{S}_{\text{LP}}^{(0)}(\{p_k\}, q) |M_n^{(0)}(\{p'_k\})\rangle + \mathcal{O}(\lambda^0) \\ &\equiv \epsilon_{n+1,\mu}^* \mathcal{S}_{\text{LP}}^{(0),\mu}(\{p_k\}, q) |M_n^{(0)}(\{p'_k\})\rangle + \mathcal{O}(\lambda^0), \end{aligned} \quad (3.19)$$

with the leading-power *soft current*

$$\mathcal{S}_{\text{LP}}^{(0),\mu}(\{p_k\}, q) = - \sum_i \mathbf{T}_i \frac{p_i^\mu}{p_i \cdot q}. \quad (3.20)$$

Note that if one wants the current to be strictly leading power, one has to use $\mathbf{S}_{\text{LP}}^{(0),\mu}(\{p'_k\}, q)$ instead of $\mathbf{S}_{\text{LP}}^{(0),\mu}(\{p_k\}, q)$ since $\{p_k\}$ contains a λ dependence when expressed through the Born momenta $\{p'_k\}$. The soft current fulfills the Ward identity (c.f. Eq. (A.47))

$$q_\mu \mathbf{S}_{\text{LP}}^{(0),\mu}(\{p_k\}, q) |M_n^{(0)}(\{p'_k\})\rangle = - \sum_i \mathbf{T}_i |M_n^{(0)}(\{p'_k\})\rangle = 0 \quad (3.21)$$

due to color conservation.

Let us now move to subleading terms in the soft expansion, i.e. let us try to compute the terms of order $\mathcal{O}(\lambda^0)$. As mentioned above, this corresponds to the QCD generalization of the classic LBK theorem. Subleading corrections stem from

1. terms of order $\mathcal{O}(\lambda^0)$ neglected in Eq. (3.18),
2. the difference between the momentum configuration $\{p_k\}|_{p_i \mapsto p_i + q}$, which is carried by the shaded circle in Fig. 3.1, and $\{p'_k\}$, which has to be used for calculating the Born amplitude due to on-shellness,
3. radiation off internal legs without a divergent propagator.

Addressing these contributions, we start by writing for the quark case

$$|M_{n+1}^{(0)}(\{p_k\})\rangle = -\varepsilon_{n+1,\mu}^* \sum_i \mathbf{T}_i \bar{\mathbf{u}}_i \left[\frac{p_i^\mu}{p_i \cdot q} \left(1 + \sum_j (p_j - p'_j) \cdot \partial_j + q \cdot \partial_i \right) + \frac{\gamma^\mu \not{q}}{2p_i \cdot q} \right] \partial_{\bar{\mathbf{u}}_i'} |M_n^{(0)}(\{p'_k\})\rangle \\ + |M_{n+1}^{\text{int}}(\{p_k\})\rangle + \mathcal{O}(\lambda), \quad (3.22)$$

where we have included the previously neglected spin-dependent terms and the corrections to the momentum configuration as a Taylor expansion to first order. Note that the latter is only necessary for all terms that also contribute at leading power because if a term already is of order $\mathcal{O}(\lambda^0)$, any additional expansion in λ will contribute only at order $\mathcal{O}(\lambda)$, which is neglected. Finally, we introduced $|M_{n+1}^{\text{int}}(\{p_k\})\rangle$ as a placeholder for internal radiation at order $\mathcal{O}(\lambda^0)$.

The crucial observation of the LBK theorem is that NLP internal-emission contributions $|M_{n+1}^{\text{int}}(\{p_k\})\rangle \equiv \varepsilon_{n+1,\mu}^* |M_{n+1}^{\text{int},\mu}(\{p_k\})\rangle$ can be fully derived from the gauge-invariance condition that the amplitude fulfill the Ward identity:

$$0 = - \sum_i \mathbf{T}_i \bar{\mathbf{u}}_i q \cdot \partial_i \partial_{\bar{\mathbf{u}}_i'} |M_n^{(0)}(\{p'_k\})\rangle + q_\mu |M_{n+1}^{\text{int},\mu}(\{p_k\})\rangle, \quad (3.23)$$

where we have used color conservation for all terms that do not explicitly depend on i , as well as $q \not{q} = 0$. This implies

$$|M_{n+1}^{\text{int},\mu}(\{p_k\})\rangle = \sum_i \mathbf{T}_i \bar{\mathbf{u}}_i \partial_i^\mu \partial_{\bar{\mathbf{u}}_i'} |M_n^{(0)}(\{p'_k\})\rangle + \text{terms proportional to } q^\mu. \quad (3.24)$$

Since internal emissions cannot give rise to propagators divergent in q , any terms proportional to q^μ would be beyond order $\mathcal{O}(\lambda^0)$ and can therefore not be part of $|M_{n+1}^{\text{int},\mu}(\{p_k\})\rangle$. Inserting

this into Eq. (3.22) yields

$$|M_{n+1}^{(0)}(\{p_k\})\rangle = -\varepsilon_{n+1,\mu}^* \sum_i \mathbf{T}_i \left[\frac{p_i^\mu}{p_i \cdot q} \left(1 + \sum_j (p_j - p'_j) \cdot \partial_j \right) |M_n^{(0)}(\{p'_k\})\rangle \right. \\ \left. + \bar{\mathbf{u}}_i \left(\frac{p_i^\mu}{p_i \cdot q} q \cdot \partial_i - \partial_i^\mu + \frac{\gamma^\mu \not{q}}{2p_i \cdot q} \right) \partial_{\bar{\mathbf{u}}_i} |M_n^{(0)}(\{p'_k\})\rangle \right] + \mathcal{O}(\lambda), \quad (3.25)$$

where we have divided the current into the parts where we can straightforwardly recover $|M_n^{(0)}(\{p'_k\})\rangle = \bar{\mathbf{u}}_i \partial_{\bar{\mathbf{u}}_i} |M_n^{(0)}(\{p'_k\})\rangle + \mathcal{O}(\lambda)$ and the parts where derivatives and Dirac matrices render this non-trivial. Let us first bring Eq. (3.25) into a more compact form by introducing the abelian field-strength tensor

$$F_{\mu\nu} \equiv i(q_\mu \varepsilon_{n+1,\nu}^* - q_\nu \varepsilon_{n+1,\mu}^*), \quad (3.26)$$

which we use in the operator version $\mathbf{F}_{\mu\nu}$ with $\varepsilon_{n+1}^* \mapsto \varepsilon_{n+1}^*$, as well as the four-dimensional angular-momentum tensor operator

$$J_i^{\mu\nu} \equiv i(p_i^\mu \partial_i^\nu - p_i^\nu \partial_i^\mu), \quad (3.27)$$

and the standard notation for the commutator of Dirac matrices,

$$\sigma^{\mu\nu} \equiv \frac{i}{2}[\gamma^\mu, \gamma^\nu], \quad (3.28)$$

analogously to Refs. [1, 2]:

$$|M_{n+1}^{(0)}(\{p_k\})\rangle = - \sum_i \mathbf{T}_i \left[\frac{p_i \cdot \varepsilon_{n+1}^*}{p_i \cdot q} \left(1 + \sum_j (p_j - p'_j) \cdot \partial_j \right) |M_n^{(0)}(\{p'_k\})\rangle \right. \\ \left. + \frac{1}{2p_i \cdot q} \mathbf{F}_{\mu\nu} \bar{\mathbf{u}}_i \left(J_i^{\mu\nu} + \frac{1}{2} \sigma^{\mu\nu} \right) \partial_{\bar{\mathbf{u}}_i} |M_n^{(0)}(\{p'_k\})\rangle \right] + \mathcal{O}(\lambda). \quad (3.29)$$

Due to Lorentz invariance, one can expect that it is possible to eliminate the explicit dependence on $\partial_{\bar{\mathbf{u}}_i} |M_n^{(0)}(\{p'_k\})\rangle$ and to write the soft current as an operator acting on $|M_n^{(0)}(\{p'_k\})\rangle$ with no bispinors removed. Indeed, considering a Lorentz transformation generated by the antisymmetric generator $\omega^{\mu\nu}$ which acts in momentum space as

$$p'_i \equiv \Lambda p_i = e^{\omega} p_i \quad (3.30)$$

and in spinor space as

$$\bar{u}'(p_i, \sigma) \equiv \bar{u}(p_i, \sigma) S^{-1}(\Lambda) = \bar{u}(p_i, \sigma) e^{\frac{i}{4} \omega_{\mu\nu} \sigma^{\mu\nu}}, \quad (3.31)$$

there is

$$\bar{u}'(p_i, \sigma) - \bar{u}(p'_i, \sigma) = \bar{u}(p_i, \sigma) \left(1 + \frac{i}{4} \omega_{\mu\nu} \sigma^{\mu\nu} \right) - (1 + \omega_{\mu\nu} p_i^\nu \partial_i^\mu) \bar{u}(p_i, \sigma) + \mathcal{O}(\omega^2) \\ = \frac{i}{2} \omega_{\mu\nu} \left(\bar{u}(p_i, \sigma) \frac{1}{2} \sigma^{\mu\nu} - J_i^{\mu\nu} \bar{u}(p_i, \sigma) \right) + \mathcal{O}(\omega^2). \quad (3.32)$$

On the other hand, Lorentz transformations of spinors are, as described in Appendix A.2, given by

$$\bar{u}(p_i, \sigma) S^{-1}(\Lambda) = \sum_{\sigma'} [\mathcal{D}_{\sigma'\sigma}^{(1/2)}(U)]^* \bar{u}(p'_i, \sigma') \quad (3.33)$$

in the massive case and

$$\bar{u}(p_i, \sigma) S^{-1}(\Lambda) = e^{i\theta\sigma} \bar{u}(p'_i, \sigma) \quad (3.34)$$

in the massless case. Hence, we can equate the right-hand side of Eq. (3.32) with

$$\begin{aligned} \bar{u}'(p_i, \sigma) - \bar{u}(p'_i, \sigma) &= \sum_{\sigma'} \left\{ ([\mathcal{D}_{\sigma'\sigma}^{(1/2)}(U)]^* - \delta_{\sigma'\sigma}) \bar{u}(p'_i, \sigma'), \quad p_i \text{ massive}, \right. \\ &\quad \left. (e^{i\theta\sigma} - 1) \delta_{\sigma'\sigma} \bar{u}(p'_i, \sigma'), \quad p_i \text{ massless}, \right. \\ &\equiv -\frac{i}{2} \omega_{\mu\nu} \sum_{\sigma'} K_{q,\sigma\sigma'}^{\mu\nu} \bar{u}(p_i, \sigma') + \mathcal{O}(\omega^2), \end{aligned} \quad (3.35)$$

where we have used $p'_i = p_i + \mathcal{O}(\omega)$, as well as that at $\omega = 0$, the Wigner rotation matrix equals $\delta_{\sigma'\sigma}$ and θ becomes zero. We therefore know that there exists a $K_{q,\sigma\sigma'}^{\mu\nu}$ such that

$$\sum_{\sigma'} K_{q,\sigma\sigma'}^{\mu\nu} \bar{u}(p_i, \sigma') = J_i^{\mu\nu} \bar{u}(p_i, \sigma) - \bar{u}(p_i, \sigma) \frac{1}{2} \sigma^{\mu\nu}, \quad (3.36)$$

which enables us to rewrite Eq. (3.29) without relying on $\partial_{\bar{u}_i}$. Values for $K_{q,\sigma\sigma'}^{\mu\nu}$ can be obtained by multiplying Eq. (3.36) with $\gamma^0 u(p_i, \sigma'')$ from the right. This projects out $K_{q,\sigma\sigma''}^{\mu\nu}$ due to $\bar{u}(p_i, \sigma) \gamma^0 u(p_i, \sigma'') = 2p_i^0 \delta_{\sigma\sigma''}$. On the other hand, after defining $\bar{u}(p_i, \sigma)$ in an explicit convention, a simpler form of $K_{q,\sigma\sigma'}^{\mu\nu}$ can be derived. For our definition outlined in Appendix A.2, it follows from Eqs. (A.34) and (A.42) that

$$A_{\Lambda p}^{-1} A(\omega) A_p - 1 = \frac{i}{2} \omega_{\mu\nu} K_q^{\mu\nu} + \mathcal{O}(\omega^2). \quad (3.37)$$

This yields for massless spinors

$$K_{q,\sigma\sigma'}^{\mu\nu} = \sigma \delta_{\sigma\sigma'} \frac{\epsilon^{\mu\nu\alpha\beta} p_\alpha \bar{p}_{0,\beta}}{p \cdot \bar{p}_0}, \quad (3.38)$$

with $\bar{p}_0 \equiv (E, 0, 0, -E)$, where the dependence on E cancels. For massive spinors, one obtains

$$K_{q,\sigma\sigma'}^{\mu\nu} = \frac{\epsilon^{\mu\nu\alpha i} (p + p_0)_\alpha \sigma_{\sigma\sigma'}^i}{(p + p_0)^0} \frac{1}{2}, \quad (3.39)$$

with $p_0 = (m, 0, 0, 0)$ and the Pauli matrices σ^i given in Eq. (A.14). $\epsilon^{\mu\nu\alpha\beta}$ is the Levi-Civita tensor with $\epsilon_{0123} = +1$.

The calculation of the subleading soft current can be performed in complete analogy for other flavors of the emitting particle, namely (massive or massless) antiquarks or gluons. This leads to the general formula

$$|M_{n+1}^{(0)}(\{p_k\})\rangle = \mathbf{S}_{\text{NLP}}^{(0)}(\{p_k\}, \{p'_k\}, q) |M_n^{(0)}(\{p'_k\})\rangle + \mathcal{O}(\lambda), \quad (3.40)$$

with

$$\mathbf{S}_{\text{NLP}}^{(0)}(\{p_k\}, \{p'_k\}, q) = - \sum_i \mathbf{T}_i \left[\frac{p_i \cdot \boldsymbol{\varepsilon}_{n+1}^*}{p_i \cdot q} \left(1 + \sum_j (p_j - p'_j) \cdot \partial_j \right) + \frac{1}{2p_i \cdot q} \mathbf{F}_{\mu\nu} \left(J_i^{\mu\nu} - \mathbf{K}_i^{\mu\nu} \right) \right], \quad (3.41)$$

where the flavor dependence is solely contained in the spin-space operator $\mathbf{K}_i^{\mu\nu}$, which acts as

$$\mathbf{K}_i^{\mu\nu} |\dots, \sigma'_i, \dots\rangle \equiv \sum_{\sigma_i} K_{a_i, \sigma_i \sigma'_i}^{\mu\nu} |\dots, \sigma_i, \dots\rangle. \quad (3.42)$$

Similarly to the quark case defined in Eq. (3.36), there is

$$K_{\bar{q}, \sigma \sigma'}^{\mu\nu} = K_{q, \sigma \sigma'}^{\mu\nu}, \quad (3.43)$$

$$\sum_{\sigma'} K_{g, \sigma \sigma'}^{\mu\nu} \varepsilon_\alpha^*(p_i, \sigma') = \left(J_i^{\mu\nu} g_{\alpha\beta} + i(\delta_\alpha^\mu \delta_\beta^\nu - \delta_\alpha^\nu \delta_\beta^\mu) \right) \varepsilon^{*\beta}(p_i, \sigma) + \text{terms proportional to } p_{i,\alpha}, \quad (3.44)$$

for antiquarks and gluons. For gluons, terms proportional to $p_{i,\alpha}$ are irrelevant since they vanish when either contracted with $\varepsilon(p_i, \sigma'')^\alpha$ or with transverse amplitudes. Furthermore, one can again derive a convention-dependent simple formula. If the polarization vectors are defined as in the spinor-helicity formalism, see Eq. (A.49), one finds that the formula for quarks, Eq. (3.38), is also valid for gluons.⁴

While this concludes the derivation of a universal subleading soft operator at tree level, let us finally remark that the occurrence of $J_i^{\mu\nu} - \mathbf{K}_i^{\mu\nu}$ is not random. On the one hand, one expects the soft operator, including $F_{\mu\nu} J_i^{\mu\nu}$, to act on the complete Born amplitude including its spinors or polarization vectors. On the other hand, the full amplitude should not actually contain a dependence on e.g. $F_{\mu\nu} J_i^{\mu\nu} \bar{u}(p_i, \sigma)$, since the soft radiation should not alter the external spinor. Thus, we need to subtract the spin-space operator $\mathbf{K}_i^{\mu\nu}$ which exactly cancels the derivatives acting on the external wave functions. We will see the same pattern when discussing the soft momentum region at one-loop order in Section 3.4.2.

3.3 Collinear Limit of Tree-Level Amplitudes

The universal leading behavior of tree-level amplitudes in a single-collinear limit is well-known. For squared amplitudes, it is described by the *Altarelli-Parisi splitting functions*, which were calculated a long time ago [82]. We use the even simpler collinear operators which encapsulate the collinear behavior of non-squared amplitudes. We follow the notation from Ref. [1]:

$$|M_{n+1}^{(0)}(\{p_k\})\rangle = \mathbf{Split}_{i, n+1 \leftarrow i}^{(0)}(p_i, p_{n+1}, p'_i) |M_n^{(0)}(\{p'_k\})\rangle + \mathcal{O}(\lambda^0), \quad (3.45)$$

where $\mathbf{Split}_{i, n+1 \leftarrow i}^{(0)}$ is an operator that increases the dimension in color and spin space:

$$\begin{aligned} \mathbf{Split}_{i, n+1 \leftarrow i}^{(0)}(p_i, p_{n+1}, p'_i) |\dots c'_i \dots; \dots \sigma'_i \dots\rangle \equiv \\ \sum_{\sigma_i, c_i, \sigma_{n+1}, c_{n+1}} \langle c_i, c_{n+1}; \sigma_i, \sigma_{n+1} | \mathbf{Split}_{a_i, a_{n+1} \leftarrow a'_i}^{(0)}(p_i, p_{n+1}, p'_i) | c'_i; \sigma'_i \rangle \\ \times |\dots c_i \dots, c_{n+1}; \dots \sigma_i \dots, \sigma_{n+1}\rangle. \end{aligned} \quad (3.46)$$

⁴Note, however, that one has to substitute $\sigma = \pm 1$ in the gluon case, whereas $\sigma = \pm \frac{1}{2}$ in the quark case.

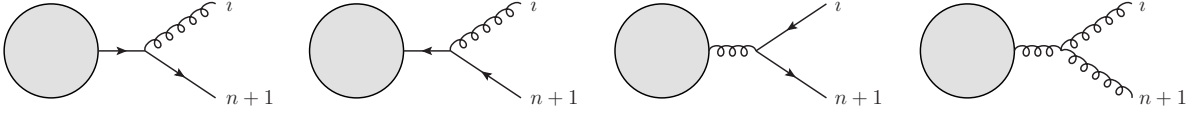


Figure 3.2: Tree-level splittings that lead to collinear divergences in massless QCD.

To simplify notation, we write

$$\text{Split}_{a_i, a_{n+1} \leftarrow a'_i}^{(0)}(i, n+1, i') \equiv \langle c_i, c_{n+1}; \sigma_i, \sigma_{n+1} | \mathbf{Split}_{a_i, a_{n+1} \leftarrow a'_i}^{(0)}(p_i, p_{n+1}, p'_i) | c'_i; \sigma'_i \rangle, \quad (3.47)$$

which takes a different form depending on the flavors a_i , a_{n+1} , and a'_i , corresponding to the four possible single-collinear splittings that can occur in QCD:

$$\text{Split}_{qg \leftarrow q}^{(0)}(i, n+1, i') = -\frac{1}{s_{i,n+1}} T_{c_i c'_i}^{c_{n+1}} \bar{u}_i \not{\epsilon}_{n+1}^* u_{i'}, \quad (3.48)$$

$$\text{Split}_{\bar{q}g \leftarrow \bar{q}}^{(0)}(i, n+1, i') = +\frac{1}{s_{i,n+1}} T_{c'_i c_i}^{c_{n+1}} \bar{v}_{i'} \not{\epsilon}_{n+1}^* v_i, \quad (3.49)$$

$$\text{Split}_{q\bar{q} \leftarrow g}^{(0)}(i, n+1, i') = -\frac{1}{s_{i,n+1}} T_{c_i c_{n+1}}^{c'_i} \bar{u}_i \not{\epsilon}_{i'} v_{n+1}, \quad (3.50)$$

$$\begin{aligned} \text{Split}_{g\bar{g} \leftarrow g}^{(0)}(i, n+1, i') &= -\frac{1}{s_{i,n+1}} i f^{c_i c'_i c_{n+1}} \\ &\times ([\varepsilon_i^* \cdot \varepsilon_{i'}] [2p_i \cdot \varepsilon_{n+1}^*] - [\varepsilon_{n+1}^* \cdot \varepsilon_{i'}] [2p_{n+1} \cdot \varepsilon_i^*] + [\varepsilon_i^* \cdot \varepsilon_{n+1}^*] [(p_{n+1} - p_i) \cdot \varepsilon_{i'}]), \end{aligned} \quad (3.51)$$

with the Mandelstam variable $s_{i,n+1} = 2p_i \cdot p_{n+1}$. These splitting operators follow directly from applying Feynman rules to the diagrams depicted in Fig. 3.2. For example, in the case of a splitting quark, corresponding to the leftmost diagram, one obtains

$$\begin{aligned} &\mathbf{P}_i \mathbf{P}_{n+1} |M_{n+1}^{(0)}(\{p_k\})\rangle \\ &= \sum_{c'_i} \varepsilon_{n+1}^{*\mu} \bar{u}_i i T_{c_i c'_i}^{c_{n+1}} \gamma_\mu i \frac{\not{p}_i + \not{p}_{n+1}}{(p_i + p_{n+1})^2} \mathbf{P}_i(c'_i) \partial_{\bar{u}_{i'}} |M_n^{(0)}(\{p'_k\})\rangle + \mathcal{O}(\lambda^0) \\ &= -\sum_{c'_i} \frac{1}{s_{i,n+1}} T_{c_i c'_i}^{c_{n+1}} \bar{u}_i \not{\epsilon}_{n+1}^* \left(\not{p}'_i - \frac{l_\perp^2}{2x(1-x)} \frac{\not{q}}{p'_i \cdot q} \right) \mathbf{P}_i(c'_i) \partial_{\bar{u}_{i'}} |M_n^{(0)}(\{p'_k\})\rangle + \mathcal{O}(\lambda^0) \\ &= -\sum_{\sigma'_i, c'_i} \frac{1}{s_{i,n+1}} T_{c_i c'_i}^{c_{n+1}} \bar{u}_i \not{\epsilon}_{n+1}^* u_{i'} \bar{u}_{i'} \mathbf{P}_i(\sigma'_i) \partial_{\bar{u}_{i'}} |M_n^{(0)}(\{p'_k\})\rangle + \mathcal{O}(\lambda^0) \\ &= \sum_{\sigma'_i, c'_i} \text{Split}_{qg \leftarrow q}^{(0)}(i, n+1, i') \mathbf{P}_i(\sigma'_i, c'_i) |M_n^{(0)}(\{p'_k\})\rangle + \mathcal{O}(\lambda^0), \end{aligned} \quad (3.52)$$

where we have neglected terms of order $\mathcal{O}(\lambda^0)$ and used $\not{p} = \sum_\sigma u(p, \sigma) \bar{u}(p, \sigma)$. Of course, there are additional diagrams to the one from Fig. 3.2 contributing to the full amplitude $|M_{n+1}^{(0)}\rangle$. However, any internal radiation or radiation off a non-collinear leg does not lead to a divergent propagator, and is therefore of order $\mathcal{O}(\lambda^0)$.

Note that despite the $s_{i,n+1} = -l_\perp^2/(x(1-x)) = \mathcal{O}(\lambda)$ factor in the denominator, the operators carry only a $\mathcal{O}(1/\sqrt{\lambda})$ divergence. For a precise analysis of the λ dependence, it is useful to express the splitting operators in spinor-helicity formalism, see Section 4.1. Let us, as

an example, consider quark splitting and a specific helicity configuration:

$$\begin{aligned} \text{Split}_{qg \leftarrow q}^{(0)}(i, n+1, i') \Big|_{\sigma_i=\sigma'_i=+\frac{1}{2}, \sigma_{n+1}=+1} &= -\frac{1}{s_{i,n+1}} T_{c_i c'_i}^{c_{n+1}} \bar{u}(p_i, +\frac{1}{2}) \not{\epsilon}^*(p_{n+1}, +1) u(p'_i, +\frac{1}{2}) \\ &= T_{c_i c'_i}^{c_{n+1}} \frac{\sqrt{2} \langle r|i' \rangle}{\langle i|n+1 \rangle \langle r|n+1 \rangle}, \end{aligned} \quad (3.53)$$

where we chose r as the reference momentum in the definition of polarization vectors, which can in principle be different from the Sudakov reference momentum q . Since Weyl spinors are two-dimensional objects, one can choose two spinors with independent momenta as a basis. Since p_i and p_{n+1} depend on $k_\perp$ when expressed through the Born momentum p'_i and the Sudakov reference momentum q , we use the latter two for the basis. Then,

$$|n+1\rangle = a|i'\rangle + b|q\rangle, \quad |n+1] = a^*|i'] + b^*|q] \quad (3.54)$$

with some complex coefficients a and b . To identify them, we can use

$$\begin{aligned} |n+1\rangle [n+1] &= |a|^2 |i'\rangle [i'] + ab^* |i'\rangle [q] + a^* b |q\rangle [i'] + |b|^2 |q\rangle [q] \\ &\stackrel{!}{=} x |i'\rangle [i'] + |l_\perp\rangle [l_\perp] - \frac{l_\perp^2}{2xp'_i \cdot q} |q\rangle [q]. \end{aligned} \quad (3.55)$$

Note that while we use the notation $|l_\perp\rangle [l_\perp]$ for an operator that can act on spinors, it does not mean that the spinor $|l_\perp\rangle$ exists, as Weyl spinors are only defined for massless momenta. Due to the transversality conditions

$$2p'_i \cdot l_\perp = \langle i'|l_\perp|i'\rangle = 0, \quad 2p'_{n+1} \cdot l_\perp = \langle n+1|l_\perp|n+1\rangle = 0, \quad (3.56)$$

we can infer

$$|l_\perp\rangle [l_\perp] = ab^* |i'\rangle [q] + a^* b |q\rangle [i'] \quad (3.57)$$

without any $|i'\rangle [i']$ or $|q\rangle [q]$ contribution. Hence, $|a|^2 = x$, and since the global phase of spinors can be chosen arbitrarily we choose $a = \sqrt{x}$ for simplicity. Eq. (3.57) now directly yields

$$\langle i'|l_\perp|q\rangle = \sqrt{x} b \langle i'|q\rangle [i'|q] \implies b = -\frac{1}{\sqrt{x}} \frac{\langle i'|l_\perp|q\rangle}{2p'_i \cdot q}. \quad (3.58)$$

Indeed,

$$|b|^2 = \frac{\langle i'|l_\perp q l_\perp|i'\rangle}{4x(p'_i \cdot q)^2} = -\frac{l_\perp^2 \langle i'|q|i'\rangle}{4x(p'_i \cdot q)^2} = -\frac{l_\perp^2}{2xp'_i \cdot q}, \quad (3.59)$$

in agreement with Eq. (3.55). In summary, and after an analogous calculation for $|i\rangle$, there is

$$|n+1\rangle = \sqrt{x} |i'\rangle - \frac{1}{\sqrt{x}} \frac{\langle i'|l_\perp|q\rangle}{2p'_i \cdot q} |q\rangle, \quad |i\rangle = \sqrt{1-x} |i'\rangle + \frac{1}{\sqrt{1-x}} \frac{\langle i'|l_\perp|q\rangle}{2p'_i \cdot q} |q\rangle. \quad (3.60)$$

Inserting this into Eq. (3.53) yields

$$\text{Split}_{qg \leftarrow q}^{(0)}(i, n+1, i') \Big|_{\sigma_i=\sigma'_i=+\frac{1}{2}, \sigma_{n+1}=+1} = \sqrt{2} T_{c_i c'_i}^{c_{n+1}} \sqrt{1-x} \frac{[i'|q]}{\langle i'|l_\perp|q\rangle} \frac{1}{1 - \frac{1}{x} \frac{\langle i'|l_\perp|q\rangle \langle r|q\rangle}{2p'_i \cdot q} \frac{\langle r|i'\rangle}{\langle r|i'\rangle}}. \quad (3.61)$$

Expanding this in $l_\perp = \mathcal{O}(\sqrt{\lambda})$ yields

$$\text{Split}_{qg \leftarrow q}^{(0)}(i, n+1, i') \Big|_{\sigma_i = \sigma'_i = +\frac{1}{2}, \sigma_{n+1} = +1} = \sqrt{2} T_{c_i c'_i}^{c_{n+1}} \left(\sqrt{1-x} \frac{[i'|q]}{\langle i'|l_\perp|q \rangle} + \frac{\sqrt{1-x}}{x} \frac{\langle r|q \rangle}{\langle q|i' \rangle \langle r|i' \rangle} + \mathcal{O}(\sqrt{\lambda}) \right). \quad (3.62)$$

Thus, the leading power of the splitting function is $\mathcal{O}(1/\sqrt{\lambda})$. However, it also contains higher-power terms in λ when parametrized through the momenta p'_i and q . In the spinor-helicity literature, see e.g. Ref. [146] for a pedagogical treatment, it is customary to set $r \equiv q$, implying that all higher-power terms vanish. Also, one usually only substitutes $\langle r|n+1 \rangle$ in Eq. (3.53) and leaves $\langle i|n+1 \rangle$ untouched. The obtained formula

$$\text{Split}_{qg \leftarrow q}^{(0)}(i, n+1, i') \Big|_{\sigma_i = \sigma'_i = +\frac{1}{2}, \sigma_{n+1} = +1} = \sqrt{2} T_{c_i c'_i}^{c_{n+1}} \frac{1}{\sqrt{x} \langle i|n+1 \rangle} \quad (3.63)$$

is in agreement with well-known results in the spinor-helicity formalism [146].

On the other hand, our goal is to study the collinear limit beyond leading power. Also, we aim to achieve formulae that do not rely on a specific convention for polarization vectors. We therefore define the purely leading-power splitting operator

$$\widetilde{\text{Split}}_{i, n+1 \rightarrow i}^{(0)}(p_i, p_{n+1}, p'_i) \equiv \text{Split}_{i, n+1 \rightarrow i}^{(0)}(p_i, p_{n+1}, p'_i) \Big|_{\text{leading-}l_\perp \text{ terms}}. \quad (3.64)$$

Through order $\mathcal{O}(\lambda^0)$, it has the explicit form

$$\widetilde{\text{Split}}_{qg \leftarrow q}^{(0)}(i, n+1, i') = \text{Split}_{qg \leftarrow q}^{(0)}(i, n+1, i') + T_{c_i c'_i}^{c_{n+1}} \delta_{\sigma_i \sigma'_i} \sqrt{1-x} \frac{\varepsilon_{n+1}^* \cdot q}{p_{n+1} \cdot q} + \mathcal{O}(\sqrt{\lambda}), \quad (3.65)$$

$$\widetilde{\text{Split}}_{\bar{q}g \leftarrow \bar{q}}^{(0)}(i, n+1, i') = \text{Split}_{\bar{q}g \leftarrow \bar{q}}^{(0)}(i, n+1, i') - T_{c'_i c_i}^{c_{n+1}} \delta_{\sigma_i \sigma'_i} \sqrt{1-x} \frac{\varepsilon_{n+1}^* \cdot q}{p_{n+1} \cdot q} + \mathcal{O}(\sqrt{\lambda}), \quad (3.66)$$

$$\widetilde{\text{Split}}_{q\bar{q} \leftarrow g}^{(0)}(i, n+1, i') = \text{Split}_{q\bar{q} \leftarrow g}^{(0)}(i, n+1, i') + T_{c_i c_{n+1}}^{c'_i} \delta_{\sigma_i, -\sigma_{n+1}} \sqrt{x(1-x)} \frac{\varepsilon_{i'} \cdot q}{p'_i \cdot q}, \quad (3.67)$$

$$\begin{aligned} \widetilde{\text{Split}}_{gg \leftarrow g}^{(0)}(i, n+1, i') &= \text{Split}_{gg \leftarrow g}^{(0)}(i, n+1, i') \\ &+ i f^{c_i c'_i c_{n+1}} \left(\varepsilon_i^* \cdot \varepsilon_{i'} \frac{\varepsilon_{n+1}^* \cdot q}{p_{n+1} \cdot q} - \varepsilon_{n+1}^* \cdot \varepsilon_{i'} \frac{\varepsilon_i^* \cdot q}{p_i \cdot q} - \frac{x - (1-x)}{2} \varepsilon_i^* \cdot \varepsilon_{n+1} \frac{\varepsilon_{i'} \cdot q}{p'_i \cdot q} \right) + \mathcal{O}(\sqrt{\lambda}), \end{aligned} \quad (3.68)$$

where the additional term in Eq. (3.62) is exactly cancelled, and a similar cancellation can be observed when performing analogous calculations for all polarizations and flavors. This can be checked by insertion of Eq. (3.60) and subsequent series expansion, which can be conveniently done in an automatized way using a computer algebra system like **Mathematica**.

Note that the usage of $\widetilde{\text{Split}}_{i, n+1 \leftarrow i}^{(0)}$ over $\text{Split}_{i, n+1 \leftarrow i}^{(0)}$ is also relevant from the perspective of gauge invariance, specifically the Ward identity, at subleading power. For example,

$$\text{Split}_{qg \leftarrow q}^{(0)}(i, n+1, i') \Big|_{\varepsilon_{n+1}^* \mapsto p_{n+1}} = -\frac{1}{s_{i, n+1}} T_{c_i c'_i}^{c_{n+1}} \bar{u}_i \not{p}_{n+1} u_{i'}, \quad (3.69)$$

which can be simplified using

$$p_{n+1} = p'_i - p_i + \frac{s_{i, n+1}}{2} \frac{q}{p'_i \cdot q} \quad (3.70)$$

from the Sudakov parametrization (3.2), yielding

$$\text{Split}_{q\bar{q}\leftarrow q}^{(0)}(i, n+1, i') \Big|_{\varepsilon_{n+1}^* \mapsto p_{n+1}} = -T_{c_i c'_i}^{c_{n+1}} \frac{\bar{u}_i \not{q} u_{i'}}{2p'_i \cdot q} = -T_{c_i c'_i}^{c_{n+1}} \delta_{\sigma_i \sigma'_i} \sqrt{1-x} + \mathcal{O}(\lambda). \quad (3.71)$$

The remaining term gets exactly cancelled by the correction from Eq. (3.65). Analogously, in the case of a splitting gluon, there is

$$\text{Split}_{g\bar{g}\leftarrow g}^{(0)}(i, n+1, i') \Big|_{\varepsilon_{n+1}^* \mapsto p_{n+1}} = -i f^{c_i c'_i c_{n+1}} \varepsilon_i^* \cdot \varepsilon_{i'} + \mathcal{O}(\lambda), \quad (3.72)$$

$$\text{Split}_{g\bar{g}\leftarrow g}^{(0)}(i, n+1, i') \Big|_{\varepsilon_i^* \mapsto p_i} = i f^{c_i c'_i c_{n+1}} \varepsilon_{n+1}^* \cdot \varepsilon_{i'} + \mathcal{O}(\lambda), \quad (3.73)$$

which gets cancelled by the corresponding terms in Eq. (3.68).

After obtaining a purely leading-power splitting function, let us investigate the subleading behavior at order $\mathcal{O}(\lambda^0)$. Subleading corrections have origins similar to the soft case discussed in Section 3.2. Explicitly, there are

1. terms of order $\mathcal{O}(\lambda)^0$ neglected when calculating the splitting function, e.g. in Eq. (3.52),
2. non-divergent radiation from external legs other than i , as well as from internal lines.

Unlike in the soft case, we need not consider the correction in the momentum configuration because $p_i + p_{n+1} = p_{i'} + \mathcal{O}(\lambda)$, which leads to corrections starting at order $\mathcal{O}(\sqrt{\lambda})$, given the leading $1/\sqrt{\lambda}$ divergence. From Eq. (3.52), there follows for the quark case that

$$\begin{aligned} |M_{n+1}^{(0)}(\{p_k\})\rangle &= \mathbf{Split}_{i, n+1 \leftarrow i}^{(0)}(p_i, p_{n+1}, p'_i) |M_n^{(0)}(\{p'_k\})\rangle \\ &\quad - \mathbf{T}_i \bar{\mathbf{u}}_i \frac{\not{\varepsilon}_{n+1}^* \not{q}}{2p'_i \cdot q} \boldsymbol{\partial}_{\bar{\mathbf{u}}_{i'}} |M_n^{(0)}(\{p'_k\})\rangle + |M_{n+1}^{(0), \text{non-singular}}(\{p_k\})\rangle + \mathcal{O}(\sqrt{\lambda}). \end{aligned} \quad (3.74)$$

A similar calculation can be done for the $q\bar{q} \leftarrow g$ and $gg \leftarrow g$ cases, where we again use r as the reference vector for polarization vectors, such that⁵

$$\sum_{\sigma'_i} \varepsilon_\mu^*(p'_i, \sigma'_i) \varepsilon_\nu(p'_i, \sigma'_i) = -g_{\mu\nu} + \frac{p'_{i,\mu} r_\nu + p'_{i,\nu} r_\mu}{p'_i \cdot r}. \quad (3.75)$$

Then, we obtain for $q\bar{q} \leftarrow g$, that

$$\begin{aligned} \mathbf{P}_i \mathbf{P}_{n+1} |M_{n+1}^{(0)}(\{p_k\})\rangle &= \sum_{c'_i} \left[\sum_{\sigma'_i} \text{Split}_{q\bar{q}\leftarrow g}^{(0)}(i, n+1, i') \mathbf{P}_i(\sigma'_i, c'_i) |M_n^{(0)}(\{p'_k\})\rangle \right. \\ &\quad \left. - T_{c_i c_{n+1}}^{c'_i} \delta_{\sigma_{n+1}, -\sigma_i} \sqrt{x(1-x)} \left(\frac{q_\mu}{p'_i \cdot q} + \frac{r_\mu}{p'_i \cdot r} \right) \mathbf{P}_i(c'_i) \boldsymbol{\partial}_{\varepsilon_i^*}^\mu |M_n^{(0)}(\{p'_k\})\rangle \right] \\ &\quad + \mathbf{P}_i \mathbf{P}_{n+1} |M_{n+1}^{(0), \text{non-singular}}(\{p_k\})\rangle + \mathcal{O}(\sqrt{\lambda}), \end{aligned} \quad (3.76)$$

⁵While the results of this section will be reused in Section 3.4.3, where we work in a light-cone gauge with reference vector $\bar{n}$, the equations presented hereafter are independent of the gauge choice for the internal gluon propagator. Instead, the r dependence is only introduced through polarization vectors and furthermore cancels in the following steps.

while for $gg \leftarrow g$, there is

$$|M_{n+1}^{(0)}(\{p_k\})\rangle = \mathbf{Split}_{i,n+1 \leftarrow i}^{(0)}(p_i, p_{n+1}, p'_i) |M_n^{(0)}(\{p'_k\})\rangle \\ - \mathbf{T}_i \boldsymbol{\varepsilon}_{n+1}^* \cdot \boldsymbol{\varepsilon}_i^* \frac{x - (1-x)}{2} \left(\frac{q_\mu}{p'_i \cdot q} + \frac{r_\mu}{p'_i \cdot r} \right) \partial_{\varepsilon_i^*}^\mu |M_n^{(0)}(\{p'_k\})\rangle \\ + |M_{n+1}^{(0), \text{non-singular}}(\{p_k\})\rangle + \mathcal{O}(\sqrt{\lambda}). \quad (3.77)$$

In summary, let us define the subleading terms,

$$|\Delta M_{a_{n+1}, i}^{(0)}(x, \{p'_k\}, q)\rangle \equiv \lim_{l_\perp \rightarrow 0} \left[|M_{n+1}^{(0)}(\{p_k\})\rangle - \widetilde{\mathbf{Split}}_{i,n+1 \leftarrow i}^{(0)}(p_i, p_{n+1}, p'_i) |M_n^{(0)}(\{p'_k\})\rangle \right], \quad (3.78)$$

which, taking into account the difference between $\mathbf{Split}_{i,n+1 \leftarrow i}^{(0)}$ and $\widetilde{\mathbf{Split}}_{i,n+1 \leftarrow i}^{(0)}$, are given by

$$|\Delta M_{g,i}^{(0)}(x, \{p'_k\}, q)\rangle = \\ - \mathbf{T}_i \left\{ \begin{aligned} & \bar{\mathbf{u}}_i \left(\frac{\not{\varepsilon}_{n+1}^* q}{2p'_i \cdot q} + \frac{1}{x} \frac{\varepsilon_{n+1}^* \cdot q}{p'_i \cdot q} \right) \partial_{\bar{\mathbf{u}}_i}^\mu |M_n^{(0)}(\{p'_k\})\rangle, & a_i = q, \\ & |M_n^{(0)}(\{p'_k\})\rangle \partial_{v'_i}^\mu \left(\frac{\not{q} \not{\varepsilon}_{n+1}^*}{2p'_i \cdot q} + \frac{1}{x} \frac{\varepsilon_{n+1}^* \cdot q}{p'_i \cdot q} \right) \bar{v}_i, & a_i = \bar{q}, \\ & \left[-(x - (1-x)) \frac{(\varepsilon_{n+1}^* \cdot \varepsilon_i^*) q_\mu}{p'_i \cdot q} + \frac{1}{x} \frac{\varepsilon_{n+1}^* \cdot q}{p'_i \cdot q} \varepsilon_{i,\mu}^* - \frac{1}{1-x} \frac{\varepsilon_i^* \cdot q}{p'_i \cdot q} \varepsilon_{n+1,\mu}^* \right] \partial_{\varepsilon_i^*}^\mu |M_n^{(0)}(\{p'_k\})\rangle, & a_i = g \end{aligned} \right. \\ + |M_{n+1}^{(0), \text{non-singular}}(\{p_k\})\rangle \Big|_{l_\perp \rightarrow 0}. \quad (3.79)$$

for the case $a_{n+1} = g$ and

$$\mathbf{P}_i \mathbf{P}_{n+1} |\Delta M_{\bar{q}, i}^{(0)}(x, \{p'_k\}, q)\rangle = \\ - \sum_{c'_i} T_{c_i c_{n+1}}^{c'_i} \delta_{\sigma_i, -\sigma_{n+1}} \sqrt{x(1-x)} \frac{2q^\mu}{p'_i \cdot q} \mathbf{P}_i(c'_i) \partial_{\varepsilon_i^*}^\mu |M_n^{(0)}(\{p'_k\})\rangle, \\ + \mathbf{P}_i \mathbf{P}_{n+1} |M_{n+1}^{(0), \text{non-singular}}(\{p_k\})\rangle \Big|_{l_\perp \rightarrow 0} \quad (3.80)$$

for $a_{n+1} = \bar{q}$. Unfortunately, the contribution from non-singular diagrams cannot be inferred from general principles, in difference to the case of soft emission. Instead, we need to explicitly study those diagrams in the exact collinear limit $l_\perp \rightarrow 0$. While the specific structure of the diagrams are process-dependent, we can make general statements about the x dependence. First, depending on the flavors a_i and a_{n+1} , spinors $\bar{u}(p_i, \sigma) = \sqrt{1-x} \bar{u}(p'_i, \sigma) + \mathcal{O}(\lambda)$ and $v(p_{n+1}, \sigma) = \sqrt{x} v(p'_i, \sigma) + \mathcal{O}(\lambda)$ can introduce x dependence. Apart from that, notice that for any factor contributing an x to the numerator (a gluon vertex or the numerator of a quark propagator), there is a factor containing an x in the denominator (the denominator of a propagator).⁶ The only exception is if a gluon vertex connects the two external lines with momenta p_{n+1} and p_i , since then there is no propagator carrying a momentum depending on x . However, this can only occur in the singular collinear diagram. Indeed, there are terms linear in x for the gluon case in Eq. (3.79), but such terms are not contained in $|M_{n+1}^{(0), \text{non-singular}}(\{p_k\})\rangle$. By partial fractioning, the contribution can therefore be decomposed into terms independent of x and terms depending

⁶To analyze the x dependence of gluon propagators we work in Feynman gauge. Still, all final results are expressed through gauge-invariant quantities.

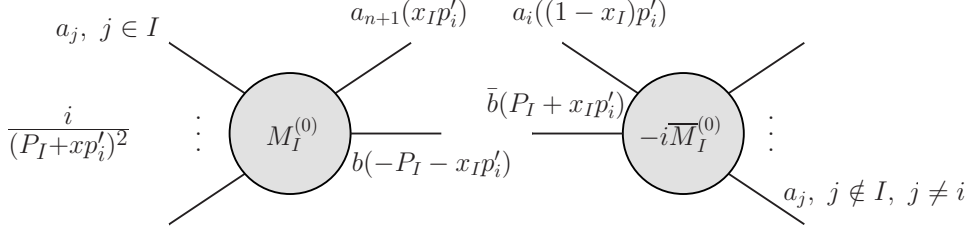


Figure 3.3: Depiction of contributions to the residue contribution $|R_{a_{n+1},i,I}^{(0)}(\{p'_k\})\rangle$ in the subleading collinear expansion of tree-level amplitudes. The details are described in the text following Eq. (3.85). Figure taken from Ref. [1].

on x through the propagators

$$\frac{1}{(P_{I_{\text{full}}} + x p'_i)^2 - m_{I_{\text{full}}}^2}, \quad P_{I_{\text{full}}} \equiv \sum_{j \in I_{\text{full}}} p_j, \quad I_{\text{full}} \subset \{1, \dots, n\} \setminus \{i\}, \quad |I_{\text{full}}| \leq n-2, \quad (3.81)$$

where $m_{I_{\text{full}}}$ is the mass of the particle of the propagator. This encapsulates all possible momentum combinations on internal propagators which lead to x dependence. These propagators lead to poles in x , which we write as

$$\frac{1}{x_{I_{\text{full}}} - x}, \quad x_{I_{\text{full}}} \equiv -\frac{P_{I_{\text{full}}}^2 - m_{I_{\text{full}}}^2}{2p'_i \cdot P_{I_{\text{full}}}}. \quad (3.82)$$

We separately treat the cases $|I_{\text{full}}| = 1$, where $x_{I_{\text{full}}} = 0$, and $|I_{\text{full}}| = n-2$, where momentum conservation implies

$$P_{I_{\text{full}}} = -(p_k + p'_i), \quad k \notin I_{\text{full}} \implies x_{I_{\text{full}}} = 1. \quad (3.83)$$

Thus, we write the x dependence of the subleading terms as

$$\begin{aligned} |\Delta M_{a_{n+1},i}^{(0)}(x, \{p'_k\}, q)\rangle &= x^{\dim(a_i)} (1-x)^{\dim(a_{n+1})} \left(\frac{1}{x} |S_{a_{n+1},i}^{(0)}(\{p'_k\}, q)\rangle \right. \\ &\quad + \frac{1}{1-x} |\bar{S}_{a_{n+1},i}^{(0)}(\{p'_k\}, q)\rangle + \sum_I \frac{1}{x_I - x} |R_{a_{n+1},i,I}^{(0)}(\{p'_k\})\rangle \\ &\quad \left. + |C_{a_{n+1},i}^{(0)}(\{p'_k\}, q)\rangle + x |L_{a_{n+1},i}^{(0)}(\{p'_k\}, q)\rangle \right), \quad (3.84) \end{aligned}$$

where $\dim(a_i)$ denotes the mass dimension of the wave function of particles of type a_i , namely $\dim(g) = 0$, $\dim(q) = \dim(\bar{q}) = \frac{1}{2}$. The sets

$$I \subset \{1, \dots, n\} \setminus \{i\}, \quad 2 \leq |I| < n-2 \quad (3.85)$$

are the ones that remain after removing the separately treated cases from I_{full} . This restriction enables the calculation of the *residue* contribution $|R_{a_{n+1},i,I}^{(0)}(\{p'_k\})\rangle$ through gauge-invariant amplitudes as shown in Fig. 3.3. The full amplitude is split into two separate amplitudes, each containing one of the collinear particles. This prevents the occurrence of divergent propagators and enables the insertion of exact-collinear kinematics. The propagator that would produce the $(x_I - x)$ pole in the full amplitude is split and added as external particles carrying the on-shell

momenta $\mp(P_I + x_I p'_i)$.⁷ Their flavors b and $\bar{b}$ are determined by flavor conservation. If no such b exists, we define the contribution to vanish for this I . To be explicit, the residue contribution has the value

$$\begin{aligned} \langle \{c_k\}, \{\sigma_k\} | R_{a_{n+1}, i, I}^{(0)}(\{p'_k\}) \rangle &= x_I^{-\dim(a_{n+1})} (1 - x_I)^{-\dim(a_i)} \\ &\times \frac{1}{2p'_i \cdot P_I} \sum_{\sigma c} M_I^{(0)}(\{p_k\}, \{\sigma_k\}, \{c_k\}, \sigma, c) \bar{M}_I^{(0)}(\{p_k\}, \{\sigma_k\}, \{c_k\}, \sigma, c), \end{aligned} \quad (3.86)$$

with the tree-level amplitudes M_I and $\bar{M}_I$ of the processes

$$0 \rightarrow \sum_{j \in I} a_j(p_j, \sigma_j, c_j) + a_{n+1}(x_I p'_i, \sigma_{n+1}, c_{n+1}) + b(-P_I - x_I p'_i, \sigma, c), \quad (3.87)$$

$$0 \rightarrow \sum_{\substack{j \notin I \\ j \neq i}} a_j(p_j, \sigma_j, c_j) + a_i((1 - x_I)p'_i, \sigma_i, c_i) + \bar{b}(P_I + x_I p'_i, -\sigma, c). \quad (3.88)$$

The *soft-pole* contribution $|S_{a_{n+1}, i}^{(0)}(\{p'_k\}, q)\rangle$, contains contributions from the singular diagram, which are given by the explicit $\frac{1}{x}$ terms in Eq. (3.79), and from the non-singular diagrams for the special case $|I_{\text{full}}| = 1$. In the case $a_{n+1} = g$, this corresponds to a gluon with momentum xp'_i being radiated off the legs $j \neq i$ of the Born amplitude. To obtain the leading $\frac{1}{x}$ behavior, we can thus use the leading-power soft limit discussed in Section 3.2. Altogether, there is⁸

$$\begin{aligned} |S_{g, i}^{(0)}(\{p'_k\}, q)\rangle &= - \left(\sum_{j \neq i} \mathbf{T}_j \frac{\varepsilon_{n+1}^* \cdot p_j}{p'_i \cdot p_j} + \mathbf{T}_i \frac{\varepsilon_{n+1}^* \cdot q}{p'_i \cdot q} \right) |M_n^{(0)}(\{p'_k\})\rangle \\ &= - \sum_{j \neq i} \mathbf{T}_j \left(\frac{\varepsilon_{n+1}^* \cdot p_j}{p'_i \cdot p_j} - \frac{\varepsilon_{n+1}^* \cdot q}{p'_i \cdot q} \right) |M_n^{(0)}(\{p'_k\})\rangle, \end{aligned} \quad (3.89)$$

where we have used color conservation. In the case $a_{n+1} = \bar{q}$, one cannot use the universal behavior of soft-gluon emission and instead has to consider the case $|I_{\text{full}}| = 1$ more explicitly. We proceed in analogy to the residue contribution, but for the special case $P_I = p_j$. The right-hand side of Fig. 3.3 then becomes the Born amplitude with the replacements $a'_i \mapsto a_i = q$ and $a_j \mapsto \bar{b}$. The left-hand side is no longer a proper amplitude but only contains three legs. Thus, its value is simply given by the corresponding splitting function of $a_j \bar{q} \leftarrow \bar{b}$ splitting. In summary, we obtain

$$|S_{\bar{q}, i}^{(0)}(\{p'_k\}, q)\rangle = \sum_{j \neq i} \mathbf{Split}_{j, n+1 \leftarrow j}^{(0)}(p_j, p'_i, p_j) \Big| M_n^{(0)}(\{p'_k\}) \Big|_{a_j \rightarrow \bar{b}}^{a'_i \rightarrow q}. \quad (3.90)$$

The *anti-soft-pole* contribution $|\bar{S}_{a_{n+1}, i}^{(0)}(\{p'_k\}, q)\rangle$ is obtained analogously, with the roles of particles i and $n+1$ interchanged. Thus, the soft-gluon expansion formula can only be used for

⁷Note that in the full amplitude, this internal momentum is never actually on-shell because x never takes the value $x_I \notin [0, 1]$.

⁸To obtain a purely subleading collinear result without any $\mathcal{O}(l_\perp)$ contributions, one should substitute $\varepsilon_{n+1}^* \mapsto \varepsilon^*(p'_i, \sigma_{n+1})$ within the operator ε_{n+1}^* in all formulae for the remainder of this section. We use ε_{n+1}^* in order to obtain concise expressions and because it still leads to a correct NLP collinear expansion.

the case $a_i = a_{n+1} = g$, and splitting functions are employed otherwise:

$$|\bar{S}_{a_{n+1},i}^{(0)}(\{p'_k\}, q)\rangle = \mathbf{E}_{i,n+1} \begin{cases} \sum_{j \neq i} \mathbf{Split}_{j,n+1 \leftarrow j}^{(0)}(p_j, p'_i, p_j) \left| M_n^{(0)}(\{p'_k\}) \right|_{a_j \rightarrow b}^{a'_i \rightarrow a_{n+1}} \rangle, & a_i \in \{q, \bar{q}\}, \\ |S_{g,i}^{(0)}(\{p'_k\}, q)\rangle, & a_i = g, \end{cases} \quad (3.91)$$

where we have used for the case $a_i = g$ that QCD amplitudes are symmetric under gluon exchange.

Symmetry under gluon exchange can also be leveraged to obtain the *linear* contribution, which vanishes unless $a_i = a_{n+1} = g$ as discussed above. To be explicit,

$$\begin{aligned} \frac{1}{x} |S\rangle + \frac{1}{1-x} |\bar{S}\rangle + \sum_I \frac{1}{x_I - x} |R_I\rangle + |C\rangle + x |L\rangle = \\ \frac{1}{1-x} |\bar{S}\rangle + \frac{1}{x} |S\rangle + \sum_I \frac{1}{x_I - (1-x)} \mathbf{E}_{i,n+1} |R_I\rangle + \mathbf{E}_{i,n+1} |C\rangle + (1-x) \mathbf{E}_{i,n+1} |L\rangle, \end{aligned} \quad (3.92)$$

where we have dropped subscripts and superscripts as well as functional dependence for brevity. After cancelling the $1-x$ poles, it is safe to set $x = 1$ to obtain an expression for $|L_{g,i}^{(0)}(\{p'_k\}, q)\rangle$ in terms of the other contributions. Furthermore, we can use

$$\mathbf{E}_{i,n+1} |R_I\rangle = -|R_{\bar{I}}\rangle, \quad \bar{I} = \{1, \dots, n\} \setminus \{i\} \setminus I, \quad x_{\bar{I}} = 1 - x_I \quad (3.93)$$

$$\implies \sum_I f(x_I) \mathbf{E}_{i,n+1} |R_I\rangle = - \sum_I f(1 - x_I) |R_I\rangle \quad (3.94)$$

to obtain⁹

$$|L_{a_{n+1},i}^{(0)}(\{p'_k\}, q)\rangle = \begin{cases} (\mathbf{E}_{i,n+1} - 1) |C_{a_{n+1},i}^{(0)}(\{p'_k\}, q)\rangle, & a_i = a_{n+1} = g, \\ 0, & \text{otherwise.} \end{cases} \quad (3.95)$$

With this, all ingredients for Eq. (3.84) are known if we can determine the *constant* contribution $|C_{a_{n+1},i}^{(0)}(\{p'_k\}, q)\rangle$. In the case $a_{n+1} = g$, we can again employ the soft limit from Eq. (3.40) in analogy to the soft-pole contribution, with the difference that now the subleading terms of the soft expansion become important. They are equal to the sum of all non-divergent contributions in Eq. (3.84) when setting $x = 0$:

$$\begin{aligned} |C_{g,i}^{(0)}(\{p'_k\}, q)\rangle + |\bar{S}_{g,i}^{(0)}(\{p'_k\}, q)\rangle + \sum_I \frac{1}{x_I} |R_{g,i,I}^{(0)}(\{p'_k\})\rangle = \\ - \sum_{j \neq i} \mathbf{T}_j \left(\frac{\boldsymbol{\epsilon}_{n+1}^* \cdot p_j}{p'_i \cdot p_j} \dim(a_i) + \frac{p'_{i,\mu} \boldsymbol{\epsilon}_{n+1,\nu}^*}{p'_i \cdot p_j} (p_j^\mu \partial_i^\nu - p_j^\nu \partial_i^\mu + i(J_j^{\mu\nu} - \mathbf{K}_j^{\mu\nu})) \right. \\ \left. - \frac{q_\mu \boldsymbol{\epsilon}_{n+1,\nu}^*}{p'_i \cdot q} i(J_i^{\mu\nu} - \mathbf{K}_i^{\mu\nu}) \right) |M_n^{(0)}(\{p'_k\})\rangle, \end{aligned} \quad (3.96)$$

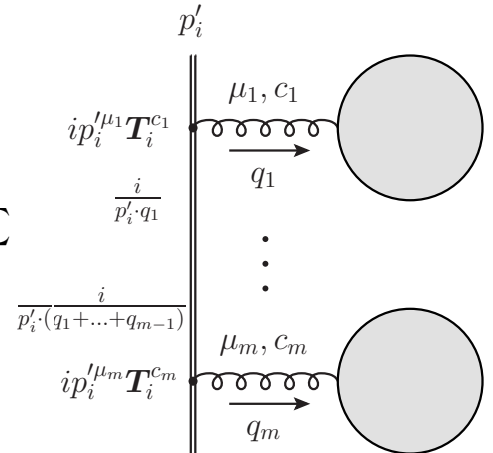
⁹The apparent difference to Eq. (4.41) of Ref. [1] is due to our definition of $|C_{a_{n+1},i}^{(0)}(\{p'_k\}, q)\rangle$ in Eq. (3.84) which differs from Ref. [1] and instead agrees with Ref. [2]. To reinstate the results from Ref. [1], one needs to substitute $|C_{g,i}^{(0)}(\{p'_k\}, q)\rangle \mapsto |C_{g,i}^{(0)}(\{p'_k\}, q)\rangle + \dim(a_i) |S_{g,i}^{(0)}(\{p'_k\}, q)\rangle - |\bar{S}_{g,i}^{(0)}(\{p'_k\}, q)\rangle - \sum_I \frac{1}{x_I} |R_{g,i,I}^{(0)}(\{p'_k\})\rangle$ and employ Eq. (3.94).

where we have used $p_j - p'_j = -xp'_i\delta_{ij}$ to obtain the term

$$-\sum_{j \neq i} \mathbf{T}_j \frac{\boldsymbol{\varepsilon}_{n+1}^* \cdot p_j}{p'_i \cdot p_j} (-p'_i \cdot \partial_i) = -\sum_{j \neq i} \mathbf{T}_j \left(\frac{p'_{i,\mu} \boldsymbol{\varepsilon}_{n+1,\nu}^*}{p'_i \cdot p_j} (-p_j^\nu \partial_i^\mu) \right), \quad (3.97)$$

which furthermore leads to the first term in Eq. (3.96), $-\sum_{j \neq i} \mathbf{T}_j (\boldsymbol{\varepsilon}_{n+1}^* \cdot \partial_i)$, by requiring the Ward identity. The dependence on $\dim(a_i)$ is necessary to correct for the derivative acting on spinors depending on p'_i instead of p_i . The last term in Eq. (3.96) corresponds to the spin-dependent x^0 contributions of Eq. (3.79). Note that we include $J_i^{\mu\nu}$ to retain the $J_i^{\mu\nu} - \mathbf{K}_i^{\mu\nu}$ structure discussed in Section 3.2. However, it vanishes upon contraction with $\boldsymbol{\varepsilon}_{n+1}^*$ and can be left out, as was done in Ref. [1].

The case $a_{n+1} = \bar{q}$ is more complicated because no general formula for the subleading behavior for the emission of a soft (anti)quark exists. While a general prescription for the determination of $|C_{\bar{q},i}^{(0)}(\{p'_k\}, q)\rangle$ was therefore not included in Ref. [1], a solution was presented in Ref. [2]. Instead of analyzing the small- x expansion, we consider the $|x| \rightarrow \infty$ limit, which isolates the constant contribution in Eq. (3.84). Note that this is only possible because the linear contribution vanishes for $a_{n+1} = \bar{q}$. Then, all other particles appear soft compared to the quark-antiquark pair. Thus, diagrams where particles i and $n+1$ are not part of the same fermion line do not contribute. Instead, we need only consider diagrams where they form a straight *eikonal* line, which is defined as a line from which only soft gluons can be radiated. The concept of eikonal lines is frequently used in the context of leading-power soft factorization [39] as mentioned in Section 3.2. The Feynman rules follow directly from the leading-power soft current, leading to

$$|C_{\bar{q},i}^{(0)}(\{p'_k\}, q)\rangle = -2\delta_{\sigma_i, -\sigma_{n+1}} \sum \frac{i}{p'_i \cdot q_1} \quad , \quad (3.98)$$


where sum runs over all possible diagrams where $m \geq 2$ gluons are attached to the eikonal line. The condition $m \geq 2$ is necessary because the case of a single gluon corresponds to the divergent diagram as displayed in Fig. 3.2. Finally, the remaining spin structure of the quark-antiquark pair yields

$$\bar{u}(p'_i, \sigma_i) \gamma^\mu v(p'_i, \sigma_{n+1}) = -2p'_i{}^\mu \delta_{\sigma_i, -\sigma_{n+1}}, \quad (3.99)$$

contributing an additional $p'_i{}^\mu$ factor, which is necessary because there is one more eikonal vertex than eikonal propagators.

In summary, we have derived the subleading collinear behavior of tree-level amplitudes to be

$$|M_{n+1}^{(0)}(\{p_k\})\rangle = \widetilde{\text{Split}}_{i,n+1 \rightarrow i}^{(0)}(p_i, p_{n+1}, p'_i) |M_n^{(0)}(\{p'_k\})\rangle + |\Delta M_{a_{n+1},i}^{(0)}(x, \{p'_k\}, q)\rangle + \mathcal{O}(\sqrt{\lambda}), \quad (3.100)$$

where the purely leading-power splitting function is defined in Eq. (3.64) with subsequent definitions in Eqs. (3.65)–(3.68) and Eqs. (3.48)–(3.51), and the subleading contribution from Eq. (3.84) contains contributions defined in Eqs. (3.86)–(3.91) and Eqs. (3.95)–(3.96).

3.4 Soft Limit of One-Loop Amplitudes

Having discussed tree-level amplitudes, the next logical step is to analyze one-loop amplitudes. For the soft expansion, performing a Taylor series in $q^\mu = \mathcal{O}(\lambda)$ is complicated by the fact that Taylor expansion and loop integration do not commute. This is obvious because momenta that do not appear in propagators cannot appear as scales in the integral. If we were to simply expand in q^μ , treating all other momenta as hard, we cannot approximate the solution of a loop integral containing q^μ correctly (the integral could e.g. render scaleless, no matter to which power in q^μ we expand). Furthermore, since we integrate over all possible values of the loop momentum l^μ , it is also possible that $|l^\mu| < |q^\mu|$, invalidating a q^μ expansion.

Still, an expansion in q^μ before having to exactly solve all integrals in which q^μ occurs is highly desirable since only this way a process-independent factorization formula seems feasible. Fortunately, the *method of regions* [147] offers a systematic procedure to perform such an expansion. While the validity of the method remains to be proven in full generality, it is well-established in the context of factorization. The first step is to write the loop momentum in light-cone coordinates:¹⁰

$$l^\mu = \frac{l_+}{2} \bar{n}^\mu + \frac{l_-}{2} n^\mu + l_\perp^\mu, \quad (3.101)$$

with reference vectors n^μ and $\bar{n}^\mu$ fulfilling

$$n^2 = \bar{n}^2 = l_\perp \cdot n = l_\perp \cdot \bar{n} = 0, \quad n \cdot \bar{n} = 2. \quad (3.102)$$

Before expanding in λ , we now have to assign a scaling behavior to the components $(l_+, l_-, l_\perp)$. This is called choosing a region of the loop momentum. For example, $(l_+, l_-, l_\perp) \sim (\lambda, \lambda, \lambda)$ is called the soft region, where $l^\mu = \mathcal{O}(\lambda)$. Now, we can first expand in λ and then solve the integral. The essence of the method of regions is that the correct series expansion of the integral is obtained by summing the contributions from all regions. While there are of course an infinite number of regions that exist in principle, it is clear that only a finite number of regions can lead to non-vanishing results. If, for example, the loop momentum is softer than any other momentum, one trivially obtains only scaleless integrals upon expansion in λ . In general, the identification of all relevant regions can be difficult, especially in the multi-loop case, and is subject to current research, e.g. using concepts from Newton polytope geometry [150]. However, for the soft expansion relevant in this section, there are only three regions contributing,

- the hard region, $(l_+, l_-, l_\perp) \sim (1, 1, 1)$,
- the soft region, $(l_+, l_-, l_\perp) \sim (\lambda, \lambda, \lambda)$,

¹⁰Note that in this thesis we use the standard definition of light-cone coordinates as used in literature on soft-collinear effective theory [148, 149], which differs from the notation of Ref. [1].

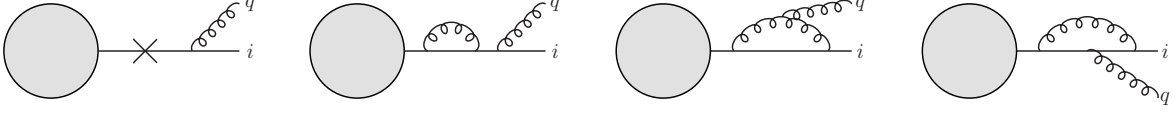


Figure 3.4: Feynman diagrams that contribute to the hard region of the expansion in the soft momentum q , additionally to the action of the tree-level soft operator. The left-most diagram contains a counterterm contribution from mass renormalization. All the diagrams are non-amputated diagrams after removal of the radiated gluon and therefore not part of the Born amplitude. In order to contribute, particle i needs to be a massive (anti-)quark. The results are truncated at $\mathcal{O}(\lambda^0)$.

- the collinear region, which is a sum of regions with $(l_+, l_-, l_\perp) \sim (\lambda, 1, \sqrt{\lambda})$, where $n^\mu = p_i^\mu / p_i^0$ defines the collinear direction and i runs over all external massless parton of the process.

In this section, we derive a process-independent soft expansion formula valid at NLP. After deriving the contribution of each region, we summarize the formula in Section 3.4.4 before confirming its validity by testing ϵ -pole cancellation and performing numerical checks. It can be applied to massive and massless one-loop QCD amplitudes and has been published in Refs. [1, 2].

3.4.1 Hard Region

Let us start by considering the hard region, $(l_+, l_-, l_\perp) \sim (1, 1, 1)$. Here, propagators which carry the loop momentum cannot become divergent and can therefore be treated as internal propagators, in equivalence to the case of soft emissions at tree level. Therefore, the term

$$\mathcal{S}_{\text{NLP}}^{(0)}(\{p_k\}, q) |M_n^{(1)}(\{p'_k\})\rangle \quad (3.103)$$

should correspond to the hard-region contribution. This is in line with LP factorization, where the soft operator and the Born amplitude can be individually expanded in α_s . At NLP, however, we observe additional contributions given by the diagrams that exist when a gluon is radiated but would not contribute to the Born amplitude with the gluon removed. As depicted in Fig. 3.4, such diagrams exist due to the condition for diagrams to be amputated. They contain either both the loop and the radiation occurring on the same external leg or radiation off a leg with a mass counterterm. Such contributions have already been pointed out for the massive-QED case in Refs. [143, 151], which was generalized to QCD in Ref. [2], whose results are used throughout this section. Because the loop momentum is considered as a hard momentum, expansion in λ removes all dependence on the soft momentum q from the propagators. When Passarino-Veltman reduction and integration-by-parts identities, explained in Sections 3.4.2 and 4.4.3, are taken into account, this leaves only the standard tadpole integral

$$A_0(m_i^2) \equiv \left(\mu^2 e^{\gamma_E}\right)^\epsilon \int \frac{d^d l}{i\pi^{d/2}} \frac{1}{l^2 - m_i^2} \quad (3.104)$$

for the contribution from Fig. 3.4. This implies that this contribution vanishes if particle i is massless because $A_0(0) = 0$ due to scalelessness. For a non-zero mass, the solution can e.g. be

found in Ref. [152] and reads

$$A_0(m^2) = -m^2 e^{\epsilon\gamma_E} \Gamma(-1 + \epsilon) \left(\frac{\mu^2}{m^2}\right)^\epsilon = m^2 \left[\frac{1}{\epsilon} + 1 + \log\left(\frac{\mu^2}{m^2}\right)\right]. \quad (3.105)$$

The value of Fig. 3.4 can then be calculated by direct calculation, analogously to the soft-region case, where the involved computation is more complicated. Therefore, more details are given when the soft region is discussed in Section 3.4.2. Still, one subtlety arises specifically in the hard region. In the calculation of $\mathcal{S}_{\text{NLP}}^{(0)}$ in Section 3.2, the Ward identity was used to obtain the contribution from internal radiation. As it turns out, Fig. 3.4 does not fulfill the Ward identity on its own. Hence, it has to be restored by hand, leading to the final expression

$$\begin{aligned} |M_{n+1}^{(1)}(\{p_k\})|_{\text{hard region}} &= \mathcal{S}_{\text{NLP}}^{(0)}(\{p_k\}, q) |M_n^{(1)}(\{p'_k\})\rangle \\ &+ \text{Fig. 3.4} - \epsilon_{n+1}^* \cdot \frac{\partial}{\partial q} [\text{Fig. 3.4}]_{\epsilon_{n+1}^* \mapsto q} + \mathcal{O}(\lambda). \end{aligned} \quad (3.106)$$

Following the discussion above, the last term should be regarded as corresponding to internal emission. The second line has the explicit value

$$\begin{aligned} \sum_i \mathbf{T}_i^c \frac{1-\epsilon}{1-2\epsilon} \left((1-2\epsilon^2)C_A + 2\epsilon(1+2\epsilon)C_F \right) \frac{A_0(m_i^2)}{m_i^2} \left(g^{\mu\nu} - \frac{2p_i^\mu p_i^\nu}{m_i^2} \right) \frac{F_{\mu\rho}}{s_{iq}} \mathbf{K}_{i\nu}{}^\rho \\ = \sum_i \mathbf{T}_i^c \left[\left(\frac{1}{\epsilon} + \ln\left(\frac{\mu^2}{m_i^2}\right) + 2 \right) C_A + 2C_F + \mathcal{O}(\epsilon) \right] \left(g^{\mu\nu} - \frac{2p_i^\mu p_i^\nu}{m_i^2} \right) \frac{F_{\mu\rho}}{s_{iq}} \mathbf{K}_{i\nu}{}^\rho. \end{aligned} \quad (3.107)$$

All λ poles contained in individual diagrams cancel and lead to a purely subleading contribution as one expects from LP factorization theorems. Therefore, no expansion of the Born amplitude with the help of derivatives is necessary. Still, one could replace $\mathbf{K}_{i\nu}{}^\rho \mapsto -(J_{i\nu}{}^\rho - \mathbf{K}_{i\nu}{}^\rho)$ to obtain the structure which is expected following the arguments presented in Section 3.2. The $J_{i\nu}{}^\rho$ dependence vanishes due to

$$\left(g^{\mu\nu} - \frac{2p_i^\mu p_i^\nu}{m_i^2} \right) \frac{F_{\mu\rho}}{s_{iq}} J_{i\nu}{}^\rho = 0. \quad (3.108)$$

When presenting the final results in Eq. (3.147), the contribution from Eq. (3.107) is added to the operator $\mathcal{S}_{\text{NLP}}^{(1)}$ together with the soft-region contribution discussed in the following chapter.

3.4.2 Soft Region

The soft region is defined by the momentum scaling $(l_+, l_-, l_\perp) \sim (\lambda, \lambda, \lambda)$. According to hard-soft-collinear factorization, this region already contributes at leading power, where the contribution had already been calculated for massless [153] and massive [154] QCD amplitudes. The scaling implies that we can perform a Taylor expansion not only in the external soft momentum q , but also in the loop momentum l . Thus, if the loop attaches to an internal line, any propagator of the form $[(P+l)^2 - m^2]^{-1}$ with $P^2 > m^2$ will always be expanded to $[P^2 - m^2]^{-1} + \mathcal{O}(l)$. For the integral not to be scaleless, we therefore need the loop to attach to external lines. This makes a fully process-independent calculation feasible since we need not consider process-dependent internal radiation. While we study the soft region by expanding standard QCD Feynman diagrams in λ , it should be noted that the flavor-diagonal part of the NLP soft-region contribution

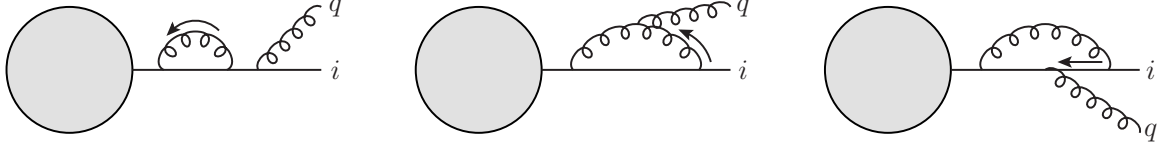


Figure 3.5: Feynman diagrams contributing to the soft region involving radiation off a single leg. The momentum routing is indicated by the arrow, which marks the line which carries the loop momentum l . The contribution is only non-vanishing if particle i is a massive (anti-)quark because in the case of massless particles, the expanded loop integral renders scaleless.

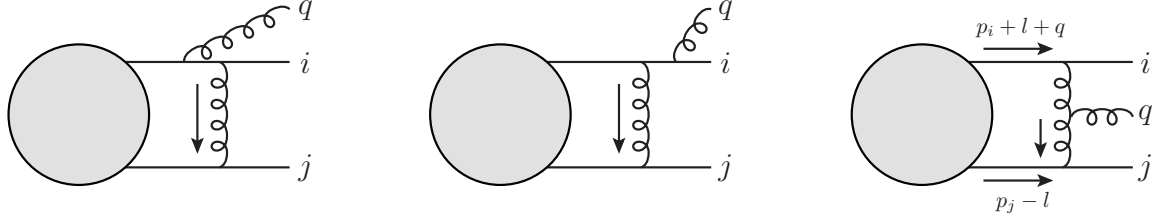


Figure 3.6: Feynman diagrams contributing to the soft region involving radiation off two legs. The momentum routing is indicated by the arrow, which marks the line which carries the loop momentum l . In the third diagram, the explicit momenta flowing out of the shaded circle are also indicated. Particles i and j can be a massive or massless (anti-)quarks as well as gluons. In the gluon case, however, there is an additional diagram where the soft gluon with momentum q attaches to both leg i and the gluon loop through a quartic vertex. Note that when performing a sum $\sum_{i \neq j}$, the third diagram requires a factor $\frac{1}{2}$ due to its symmetry under $i \leftrightarrow j$ to avoid double counting. Finally, note that only the third diagram is relevant in the case where both i and j are massless because it is the only one leading to a non-scaleless integral.

can alternatively be studied with next-to-eikonal lines [117, 118] as mentioned in the beginning of this chapter.

The contributing diagrams are identical to the leading-power case, except for the novel flavor-off-diagonal contribution discussed at the end of this section. The diagrams can involve either one or two external lines, as depicted in Figs. 3.5 and 3.6, respectively. The insertion of Feynman rules and expansion in λ can be performed analogously to the tree-level case outlined in Section 3.2. Due to the more complicated and larger number of diagrams, we perform this and the remaining steps of the calculation in the software **FORM** [155] for symbolic manipulation. Besides the increased complexity, the key conceptual difference from the tree-level case is the occurrence of loop integrals. Considering all propagators containing the loop momentum l , it is easy to see from Figs. 3.5 and 3.6 that all integrals can be brought to the form

$$\left(-\frac{\mu^2 s_{ij}}{s_{iq} s_{jq}}\right)^\epsilon I_{\alpha_1 \alpha_2 \alpha_3 \alpha_4} \equiv \left(\mu^2 e^{\gamma_E}\right)^\epsilon \int \frac{d^d l}{i\pi^{d/2}} \frac{1}{[l^2]^{\alpha_1} [(l+q)^2]^{\alpha_2} [p_i \cdot (l+q)]^{\alpha_3} [-p_j \cdot l]^{\alpha_4}}, \quad (3.109)$$

where we suppressed the $+i0^+$ contained in all propagators for brevity, and where the prefactors were included to obtain more compact results, in line with Ref. [2]. Additionally to $I_{\alpha_1 \alpha_2 \alpha_3 \alpha_4}$, the loop momentum l^μ can occur in the numerator. For example, considering the momentum routing shown in Fig. 3.6 and following the logic from Section 3.2, the momentum expansion of the shaded circle leads to terms containing $(l+q) \cdot \partial_i$. This and all other occurrences of l^μ in the numerator can be treated by performing a Passarino-Veltman reduction [156]. This reduction

method relies on the analysis of occurring scales in the integral. For example, there is

$$\int \frac{d^d l}{i\pi^{d/2}} \frac{l^\mu}{l^2(l+q)^2[p_i \cdot (l+q)][-p_j \cdot l]} = Aq^\mu + Bp_i^\mu + Cp_j^\mu \quad (3.110)$$

because q , p_i , and p_j are the only scales that exist in the integral. After contracting this equation with q_μ , $p_{i\mu}$, or $p_{j\mu}$, we can always cancel the loop momentum from the numerator using e.g.

$$\frac{l \cdot q}{l^2(l+q)^2} = \frac{1}{2} \left(\frac{1}{l^2} - \frac{1}{(l+q)^2} \right). \quad (3.111)$$

Solving the obtained system of equations for A , B , and C yields an expression of the left-hand side of Eq. (3.110) in terms of integrals without the loop momentum occurring in the numerator. Returning to the calculation of the soft-region contribution, the Taylor expansion in λ leads to integrals where some $\alpha_i > 1$. Such integrals can be reduced with integration-by-parts identities, explained in more detail in Section 4.4.3. In practice, we obtain the identities using the software *Kira* [157, 158]. The remaining master integrals are, following the naming of Ref. [2],

$$\begin{aligned} M_{1i} &\equiv (p_i \cdot q) I_{1110}, & M_{1j} &\equiv (p_j \cdot q) I_{1101}, & M_{2i} &\equiv \frac{p_i \cdot p_j}{2} I_{0111}, & M_{2j} &\equiv \frac{p_i \cdot p_j}{2} I_{1011}, \\ M_3 &\equiv (p_i \cdot q)(p_j \cdot q) I_{1111}. \end{aligned} \quad (3.112)$$

Of these integrals, only M_3 does not vanish in the massless case $m_i = m_j = 0$. Thus, the third diagram in Fig. 3.6 is the only one relevant in the massless case. The master integrals have been calculated in Ref. [154]. For convenience, we restate the results expanded to $\mathcal{O}(\epsilon^0)$ as presented in Ref. [2]. If $m_i \neq 0$ and $m_j \neq 0$, there is

$$M_{1k} = \frac{1}{2\epsilon^2} + \frac{\log(-\alpha_k)}{2\epsilon} + \frac{1}{4} \log^2(-\alpha_k) + \frac{5\pi^2}{24} + \mathcal{O}\epsilon, \quad (3.113)$$

$$M_{2k} = \frac{1}{v_{ij}} \left(-\frac{l_{x_{ij}}}{2\epsilon} + \frac{1}{2} \log(-\alpha_k) l_{x_{ij}} - \log(v_{ij}) l_{x_{ij}} - \frac{1}{4} l_{x_{ij}}^2 - \text{Li}_2(x_{ij}) + \frac{\pi^2}{6} \right) + \mathcal{O}\epsilon, \quad (3.114)$$

$$M_3 = \frac{1}{\epsilon^2} + \frac{\log(-\alpha_i) + \log(-\alpha_j)}{2\epsilon} + \frac{1}{2} \log(-\alpha_i) \log(-\alpha_j) - \frac{1}{4} l_{x_{ij}}^2 - \frac{7\pi^2}{12} + \mathcal{O}\epsilon, \quad (3.115)$$

with

$$\begin{aligned} \alpha_i &\equiv \frac{m_i^2 s_{jq}}{s_{ij} s_{iq}}, & \alpha_j &\equiv \frac{m_j^2 s_{iq}}{s_{ij} s_{jq}}, & v_{ij} &\equiv \sqrt{1 - 4\alpha_i \alpha_j} = \sqrt{1 - \frac{m_i^2 m_j^2}{(p_i \cdot p_j)^2}}, \\ x_{ij} &\equiv \frac{1 - v_{ij}}{1 + v_{ij}}, & l_{x_{ij}} &\equiv \log(x_{ij}) + 2\pi i \theta(s_{ij}). \end{aligned} \quad (3.116)$$

If $m_i \neq 0$ and $m_j = 0$, M_{1i} does not change, whereas the other integrals simplify to

$$\begin{aligned} M_{1j} &= 0, & M_{2j} &= -M_{1i}, & M_{2i} &= \frac{1}{2\epsilon^2} - \frac{\log(-\alpha_i)}{2\epsilon} + \frac{1}{4} \log(-\alpha_i)^2 + \frac{3\pi^2}{8} + \mathcal{O}(\epsilon) \\ M_3 &= \frac{3}{2\epsilon^2} + \frac{\log(-\alpha_i)}{2\epsilon} - \frac{1}{4} \log(-\alpha_i)^2 - \frac{5\pi^2}{24} + \mathcal{O}(\epsilon). \end{aligned} \quad (3.117)$$

The case $m_i = 0$, $m_j \neq 0$ can be obtained by exchanging i and j . Finally, the case $m_i = m_j = 0$ leads to the simple result

$$M_{1k} = M_{2k} = 0, \quad M_3 = \frac{2}{\epsilon^2} + \frac{\pi^2}{6} + \mathcal{O}(\epsilon). \quad (3.118)$$

With this, we have all ingredients at hand for calculating the flavor-diagonal soft-region contribution. We give the final result in Section 3.4.4, where we summarize all results. In particular, it is contained in $\mathbf{S}_{\text{NLP}}^{(1)}$, whose value can be found in Eq. (3.151) and which also contains terms from the hard region given in Eq. (3.107). Instead of also stating the final formula here, let us give some comments regarding the computation. Following the arguments laid out in Section 3.2, spin dependence is contained within the spin operator $\mathbf{K}_i^{\mu\nu}$, which only appears as a part of $J_i^{\mu\nu} - \mathbf{K}_i^{\mu\nu}$. Therefore, the simplest way to reproduce our result is

1. Insert Feynman rules for the diagrams in Figs. 3.5 and 3.6 for the case that i and j are massive quarks.
2. Expand in λ up to $\mathcal{O}(\lambda^0)$, ignoring momentum derivatives ∂_i^μ and ∂_j^μ acting on $|M_n^{(0)}\rangle$.
3. Perform color and Dirac algebra, and reduce the integrals with Passarino-Veltman and integration-by-parts reduction.
4. After simplification, the remaining occurrence of Dirac matrices should be of the form $\bar{\mathbf{u}}_k \gamma^\mu \gamma^\nu \partial_{\bar{\mathbf{u}}_{k'}} |M_n^{(0)}\rangle$ with $k = i$ or $k = j$. All terms where this occurs with both $\bar{\mathbf{u}}_i$ and $\bar{\mathbf{u}}_j$ are of $\mathcal{O}(\lambda)$ and can be neglected. Since we sum over all external legs with $\sum_{i \neq j}$, exchange $i \leftrightarrow j$ for terms with $k = j$.
5. Use $\gamma^\mu \gamma^\nu = -i\sigma^{\mu\nu} + g^{\mu\nu}$ and replace $\bar{\mathbf{u}}_i \sigma^{\mu\nu} \partial_{\bar{\mathbf{u}}_{i'}} |M_n^{(0)}\rangle \mapsto 2(J_i^{\mu\nu} - \mathbf{K}_i^{\mu\nu}) |M_n^{(0)}\rangle$. This reinstates derivatives ∂_i^μ and generalizes the result to be valid also for massless (anti-)quarks and gluons after taking the limit $m_i \rightarrow 0$, when the appropriate solutions of the master integrals are used.
6. Reinstatement momentum derivatives coming from the leading-power current being multiplied with $(1 + \sum_j (p_j - p'_j) \cdot \partial_j)$.
7. Simplify the results. In particular, bring all color structures to the form $f^{abc} \mathbf{T}_i^a \mathbf{T}_j^b$ or $\mathbf{T}_i^c \mathbf{T}_i \cdot \mathbf{T}_j$. While the single-leg diagrams from Fig. 3.5 naturally do not contain $\mathbf{T}_j$, it can be introduced by the “reversed” color conservation identity

$$\sum_i \mathbf{T}_i^a \mathbf{T}_i^b = - \sum_{i \neq j} \mathbf{T}_i^a \mathbf{T}_j^b. \quad (3.119)$$

Note that while this procedure indeed reproduces the correct result, we do not claim to have a formal proof that $J_i^{\mu\nu} - \mathbf{K}_i^{\mu\nu}$ is the only possible structure containing derivatives and spin dependence. It is therefore a valuable cross-check to perform the calculation while keeping derivatives ∂_i^μ , as well as performing separate calculations for massless quarks and gluons. Indeed, this is what we did to obtain the results of Refs. [1, 2]. In particular, the results for the massless case [1] were published before the results for the massive case [2].

In the massless case, the soft region at subleading power contains additional flavor-off-diagonal diagrams which do not contribute at leading power. They are depicted in Fig. 3.7. Their calculation is performed analogously to the flavor-diagonal case, but is more straightforward because the contribution starts only at $\mathcal{O}(\lambda^0)$, eliminating the need for further expansion in λ . As in the massless flavor-diagonal case, M_3 is the only contributing master integral. The result is a contribution to the subleading soft expansion of the form

$$\sum_{\substack{i \neq j \\ m_i=0 \\ m_j=0}} \sum_{\substack{\tilde{a}_i \neq a_i \\ \tilde{a}_j \neq a_j}} \tilde{\mathbf{S}}_{a_i a_j \leftarrow \tilde{a}_i \tilde{a}_j, ij}^{(1)}(p'_i, p'_j, q) |M_n^{(0)}(\{p'_k\})|_{a_j \rightarrow \tilde{a}_j}^{a_i \rightarrow \tilde{a}_i}, \quad (3.120)$$

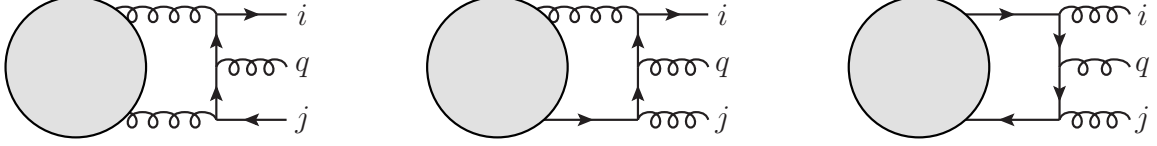


Figure 3.7: Feynman diagrams contained in the flavor-off-diagonal soft-region contribution. They only contribute in the massless case, $m_i = m_j = 0$. The center diagram also exists for antiquarks with the direction of the fermion line reversed.

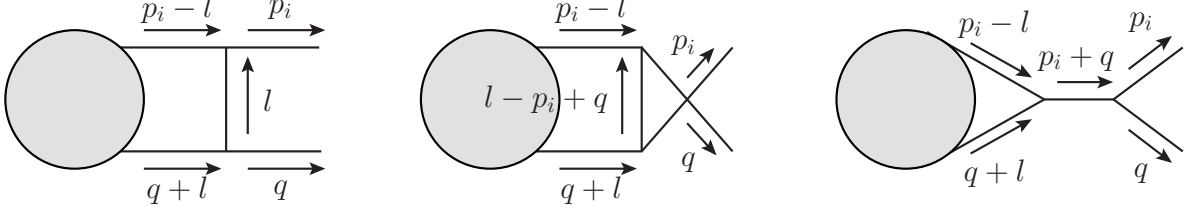


Figure 3.8: Momentum routing in diagrams contributing to the collinear region. Figure taken from Ref. [1].

where $a_i \rightarrow \tilde{a}_i$ and $a_j \rightarrow \tilde{a}_j$ denote the changed flavor of the particles according to Fig. 3.7. The expression for $\tilde{\mathcal{S}}_{a_i a_j \leftarrow \tilde{a}_i \tilde{a}_j, ij}^{(1)}(p'_i, p'_j, q)$ is shown in Eq. (3.173). It can be expressed through the splitting operators from Eq. (3.48)–(3.51), with the flavor of the splitting corresponding to the diagrams of Fig. 3.7. This constitutes another instance of a breaking of the desired

$$|M_{n+1}(\{p_k\})\rangle = \mathbf{IR} |M_n(\{p'_k\})\rangle + \text{higher-power terms}, \quad (3.121)$$

form of factorization theorems, as $\mathbf{IR}$ is now also an operator in flavor space, leading to a different underlying Born amplitude. As observed already in the collinear case at tree-level, such effects are unavoidable when going to subleading power also in the soft expansion. They will become even more pronounced in the collinear region discussed in the following section.

3.4.3 Collinear Region

In this section, we derive the contribution of the collinear region $(l_+, l_-, l_\perp) \sim (\lambda, 1, \sqrt{\lambda})$ with $n^\mu = p_i^\mu / p_i^0$, where l^μ is collinear to the momentum p_i^μ of the massless external particle i . Due to this scaling, the occurring loop integration needs to be separated into two one-dimensional integrals over l_+ and l_- and the $l_\perp$ integral in $d - 2 = 2 - 2\epsilon$ dimensions. The integration measure becomes

$$d^d l = \frac{1}{2} dl_+ dl_- d^{d-2} l_\perp. \quad (3.122)$$

The relevant diagrams in this region are of the form shown in Fig. 3.8, where the routing of the loop momentum is displayed. Diagrams without propagators of this form vanish due to scaleless integrals because the dependence on l_+ and l_- disappears from the denominator after expansion in λ . In contrast, the relevant propagators read in light-cone coordinates:

$$l^2 + i0^+ = l_+ l_- + l_\perp^2 + i0^+, \quad (3.123)$$

$$(l - p_i)^2 + i0^+ = l_+(l_- - p_{i-}) + l_\perp^2 + i0^+, \quad (3.124)$$

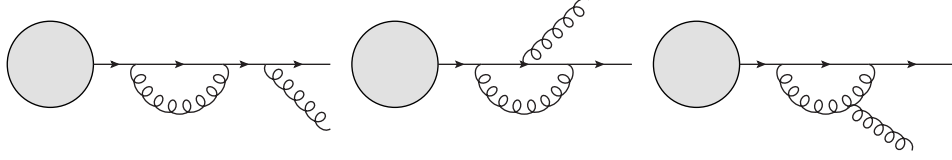


Figure 3.9: Feynman diagrams contributing to the collinear region where the two legs flowing into the shaded circle in Fig. 3.8 are connected immediately, where we consider the case that particle i is a quark. The helicity and color indices of particle i and the radiated gluon are denoted as σ_i, c_i and σ, c , respectively. The results are truncated at $\mathcal{O}(\lambda^0)$. Figure taken from Ref. [1].

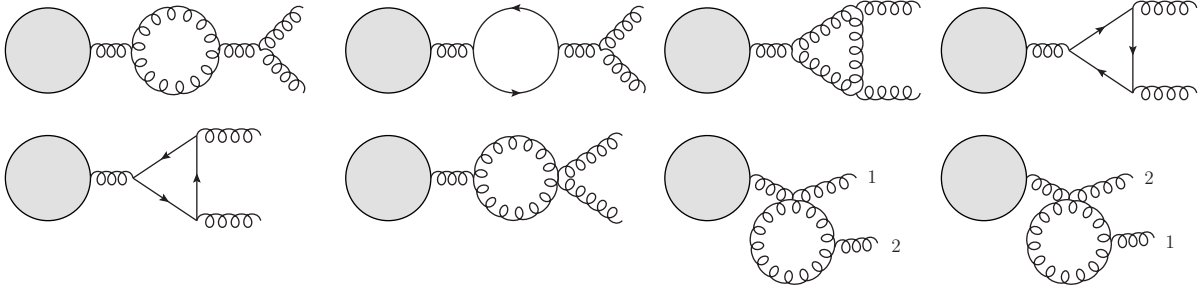


Figure 3.10: Description as for Fig. 3.9 but for the case that particle i is a gluon. In the last two diagrams, the soft gluon is labeled as “1” and particle i is labeled as “2”. However, these two diagrams do not contribute because the resulting loop integrals are scaleless.

$$\begin{aligned} (l+q)^2 + i0^+ &= (l_+ + q_+)l_- + l_\perp^2 + 2l_\perp \cdot q_\perp + l_+q_- + i0^+ \\ &= (l_+ + q_+)l_- + l_\perp^2 + i0^+ + \mathcal{O}(\lambda^{3/2}), \end{aligned} \quad (3.125)$$

$$\begin{aligned} (l-p_i+q)^2 + i0^+ &= (l_+ + q_+)(l_- - p_{i-}) + l_\perp^2 + 2l_\perp \cdot q_\perp + l_+q_- + i0^+ \\ &= (l_+ + q_+)(l_- - p_{i-}) + l_\perp^2 + i0^+ + \mathcal{O}(\lambda^{3/2}), \end{aligned} \quad (3.126)$$

where only the leading terms remain in the denominator after expansion in λ .

The main obstacle in order to obtain a process-independent expression for the collinear region is that the l_- dependence of internal propagators depends on the specific process and cannot be accessed through Taylor expansion because $l_- = \mathcal{O}(\lambda^0)$ is not a small quantity. To tackle this problem step by step, we follow the approach from Ref. [122], where the QED case was discussed. We separately treat the case where the loop attaches again to the external leg i and the case where the loop momentum flows into internal lines. In the former case, all propagator with l_- dependence are known, and the integration can be performed without problem. The diagrams corresponding to this case are displayed in Fig. 3.9 for the case $a_i = q$ and in Fig. 3.10 for $a_i = g$. To calculate their contribution—as for the soft-region calculation, it is convenient to use **FORM** for the necessary symbolic manipulations—we first insert Feynman rules in the light-cone gauge with $\bar{n}$ as the reference vector. The advantage of using a light-cone gauge is discussed below, and all final results will be expressed through gauge invariant quantities and the dependence on $\bar{n}$ will therefore disappear. The next step is to perform color and Dirac algebra and solve the loop integrals as follows. After introducing dimensionless integration variables

$$\hat{l}_+ \equiv \frac{l_+}{q_+}, \quad \hat{l}_\perp^2 \equiv \frac{l_\perp^2}{p_{i-}q_+}, \quad x \equiv \frac{l_-}{p_{i-}}, \quad (3.127)$$

the dependence on p_{i-} and q_+ is factored out from the integrands, and the propagator denominators from Eqs. (3.123)–(3.126) become

$$p_{i-}q_+[f_i + \hat{l}_\perp^2] + i0^+, \text{ with } f_i \in \{\hat{l}_+x, \hat{l}_+(x-1), (\hat{l}_++1)x, (\hat{l}_++1)(x-1)\}. \quad (3.128)$$

Furthermore, expanded integrals are proportional to $(p_{i-}q_+)^{-\epsilon} = (2p_i \cdot q)^{-\epsilon}$. Then, we can perform the $\hat{l}_+$ integration using the residue theorem. The integrand can have poles in $\hat{l}_+$ at

$$\frac{\hat{l}_\perp^2 + i0^{\text{sgn}(p_{i-}q_+)}}{-x}, \quad \frac{\hat{l}_\perp^2 + i0^{\text{sgn}(p_{i-}q_+)}}{1-x}, \quad -1 + \frac{\hat{l}_\perp^2 + i0^{\text{sgn}(p_{i-}q_+)}}{-x}, \quad -1 + \frac{\hat{l}_\perp^2 + i0^{\text{sgn}(p_{i-}q_+)}}{1-x}, \quad (3.129)$$

where $i0^{\text{sgn}(p_{i-}q_+)} \equiv i \text{sgn}(p_{i-}q_+)0^+$, depending on the occurring propagators. One can directly notice that unless

$$x \in [0, 1], \quad (3.130)$$

the integral vanishes because all imaginary parts have the same sign, one can therefore close the integration contour in the half plane without any poles, and the integral is zero due to the Cauchy integral theorem. Using the same argument, an integral needs at least one propagator with $-x < 0$ and one with $1-x > 0$ in the denominator. Then, by closing the integration contour on the corresponding side, we can choose at which of the residues we evaluate the integrand in order to perform the $\hat{l}_+$ integral. Afterwards, the $\hat{l}_\perp$ integral is performed in $2-2\epsilon$ dimensions. Because $\hat{l}_\perp$ appears only as $\hat{l}_\perp^2$ in the denominator, we can use

$$\int d^{2-2\epsilon}l_\perp f(l_\perp^2) = \frac{2\pi^{1-\epsilon}}{\Gamma(1-\epsilon)} \int_0^\infty dr r^{1-2\epsilon} f(-r^2), \quad (3.131)$$

$$\int d^{2-2\epsilon}l_\perp l_\perp^{\mu_1} \dots l_\perp^{\mu_{2n-1}} f(l_\perp^2) = 0, \quad (3.132)$$

$$\int d^{2-2\epsilon}l_\perp l_\perp^{\mu_1} \dots l_\perp^{\mu_{2n}} f(l_\perp^2) = (-1)^n g_\perp^{\{\mu_1\mu_2} \dots g_\perp^{\mu_{2n-1}\mu_{2n}}\} \frac{2\pi^{1-\epsilon}}{2^n \Gamma(n+1-\epsilon)} \int_0^\infty dr r^{2n+1-2\epsilon} f(-r^2), \quad (3.133)$$

where $g_\perp^{\mu\nu} = g^{\mu\nu} - \frac{1}{2}n^\mu \bar{n}^\nu - \frac{1}{2}n^\nu \bar{n}^\mu$ and the braces denote symmetrization. Finally, the remaining x integral, which is now a standard integral from 0 to 1, is performed to obtain

$$\begin{aligned} \text{Fig. 3.9} = r_\Gamma \left(-\frac{\mu^2}{s_{iq}} \right)^\epsilon \mathbf{T}_i^c \epsilon_\mu^*(q, p_i, \sigma) \bar{u}(p_i, \sigma_i) & \left[\frac{C_F - C_A}{1-2\epsilon} \frac{\gamma^\mu \not{q}}{2p_i \cdot q} \right. \\ & \left. - \frac{1}{1-\epsilon} \left(\frac{2C_F}{1-2\epsilon} + \frac{C_A}{\epsilon} \right) \frac{\gamma^\mu \not{\bar{n}}}{2p_i \cdot \bar{n}} - \frac{2}{1-\epsilon} \left(\frac{C_F}{\epsilon} - \frac{C_A}{1+\epsilon} \right) \frac{\bar{n}^\mu}{p_i \cdot \bar{n}} \right] \boldsymbol{\partial}_{\bar{u}_i} |M_n^{(0)}\rangle, \end{aligned} \quad (3.134)$$

$$\begin{aligned} \text{Fig. 3.10} = r_\Gamma \left(-\frac{\mu^2}{s_{iq}} \right)^\epsilon \mathbf{T}_i^c \epsilon_\mu^*(q, p_i, \sigma) \epsilon_\beta^*(p_i, \sigma_i) \\ \times \left\{ -C_A \left[\frac{1}{1-2\epsilon} \left(\frac{1}{3-2\epsilon} \frac{g^{\mu\beta} q^\alpha}{p_i \cdot q} + \frac{1}{(1-\epsilon)\epsilon} \frac{g^{\mu\beta} \bar{n}^\alpha}{p_i \cdot \bar{n}} \right) + \frac{2}{(1-\epsilon)(1+\epsilon)\epsilon} \frac{\bar{n}^\mu g^{\beta\alpha}}{p_i \cdot \bar{n}} \right] \right. \\ \left. + T_F n_l \frac{2}{(1-\epsilon)(1-2\epsilon)(3-2\epsilon)} \frac{g^{\mu\beta} q^\alpha}{p_i \cdot q} \right\} \boldsymbol{\partial}_{\epsilon_i^*, \alpha} |M_n^{(0)}\rangle, \end{aligned} \quad (3.135)$$

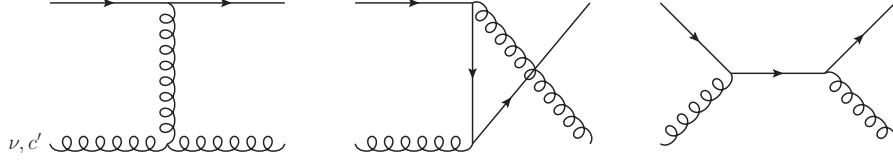


Figure 3.11: Subdiagrams of the collinear-region diagrams from Fig. 3.8 in case that particle i is a quark. Since the lines on the left-hand side attach to the shaded circle, they are not amputated and lead to propagators according to Feynman rules. We use the momentum routing shown in Fig. 3.8 but include integration over the “small” components l_+ and $l_\perp$. The results are truncated at $\mathcal{O}(\lambda^0)$. Figure taken from Ref. [1].

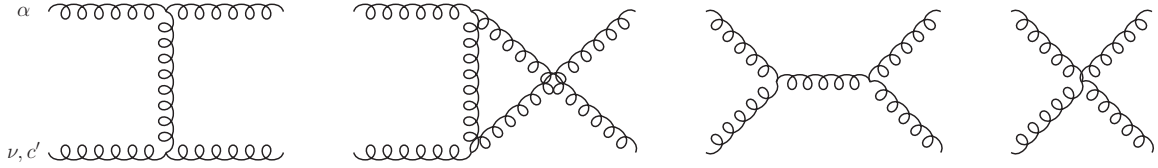


Figure 3.12: Description as in Fig. 3.11, but for the flavor-diagonal contribution in case that particle i is a gluon. Additionally, a factor $\frac{1}{2}$ needs to be included due to the symmetry of the shaded circle in Fig. 3.8 under gluon exchange.

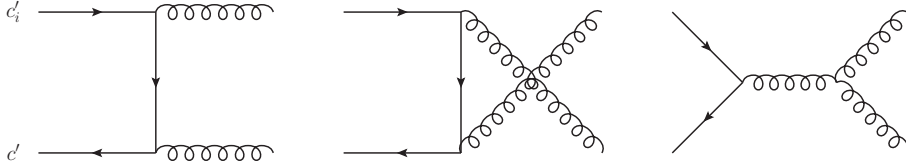


Figure 3.13: Description as in Fig. 3.11, but for the flavor-off-diagonal contribution in case that particle i is a gluon.

where $\varepsilon_\mu^*(q, p_i, \sigma) \equiv \varepsilon_{q, \mu}^* - \frac{p_i \cdot \varepsilon_q^*}{p_i \cdot q} q_\mu$ and the Mandelstam variable implicitly carries an imaginary part, $s_{iq} \equiv 2p_i \cdot q + i0^+$.

Let us now consider the case where the loop momentum actually runs on internal lines within the shaded circle of Fig. 3.8. The specific subdiagrams that attach to the circle for different flavor configurations are shown in Figs. 3.11–3.13. As discussed above, the difficulty is that now, process-dependent internal propagators contain the loop momentum with the component $l_- = xp_{i-} = \mathcal{O}(1)$. On the other hand, the dependence on $l_+ = \mathcal{O}(\lambda)$ and $l_\perp = \mathcal{O}(\sqrt{\lambda})$ can be tackled through expansion in λ . Indeed, the result presented in Ref. [122] contains terms with $l_\perp \cdot \partial / \partial l_\perp$ acting on process-dependent amplitudes. However, we find that by performing the calculation in a light-cone gauge, all such contributions vanish and neither $\partial / \partial l_\perp^\mu$ nor $\partial / \partial l_+$ is needed. This justifies the choice of light-cone gauge taken above. We reiterate that due to this choice we are able to obtain a final result that consists only on gauge-invariant quantities, which are therefore not required to be provided in a specific gauge. In analogy to above, we insert Feynman rules, perform the $\bar{l}_+$ and $\bar{l}_\perp$ integrals, and simplify the results to obtain the following

jet operators:

$$\begin{aligned} \text{Fig. 3.11} \equiv \mathbf{J}_q^{\nu, c'} &= \frac{\Gamma(1+\epsilon)}{1-\epsilon} \left(-\frac{\mu^2}{s_{iq}} \right)^\epsilon (x(1-x))^{-\epsilon} \mathbf{P}_i(\sigma_i, c_i) \left(\mathbf{T}_i^c \mathbf{T}_i^{c'} + \frac{1}{x} i f^{cdc'} \mathbf{T}_i^d \right) \\ &\quad \times \epsilon_\mu^*(q, p_i, \sigma) \bar{u}(p_i, \sigma_i) (2g^{\mu\beta} - x \gamma^\mu \gamma^\beta) g_{\perp\beta}^\nu, \end{aligned} \quad (3.136)$$

$$\begin{aligned} \text{Fig. 3.12} \equiv \mathbf{J}_g^{\alpha\nu, c'} &= \frac{\Gamma(1+\epsilon)}{1-\epsilon} \left(-\frac{\mu^2}{s_{iq}} \right)^\epsilon (x(1-x))^{-\epsilon} \mathbf{P}_i(\sigma_i, c_i) \left(\mathbf{T}_i^c \mathbf{T}_i^{c'} + \frac{1}{x} i f^{cdc'} \mathbf{T}_i^d \right) \\ &\quad \times \epsilon_\mu^*(q, p_i, \sigma) \varepsilon_\beta^*(p_i, \sigma_i) \left(g_\perp^{\mu\nu} g_\perp^{\beta\alpha} - x g^{\mu\beta} g_\perp^{\nu\alpha} + \frac{x}{1-x} g_\perp^{\mu\alpha} g_\perp^{\beta\nu} \right), \end{aligned} \quad (3.137)$$

$$\begin{aligned} \text{Fig. 3.13} \equiv \tilde{\mathbf{J}}_{c'c'_i} &= \frac{\Gamma(1+\epsilon)}{1-\epsilon} \left(-\frac{\mu^2}{s_{iq}} \right)^\epsilon (x(1-x))^{-\epsilon} \left(T^c T^{c_i} + i x f^{cdc_i} T^d \right)_{c'c'_i} \\ &\quad \times \varepsilon_\mu^*(q, p_i, \sigma) \varepsilon_\beta^*(p_i, \sigma_i) \not{p}_i (2x g^{\mu\beta} - \gamma^\mu \gamma^\beta), \end{aligned} \quad (3.138)$$

where the x integration from 0 to 1 remains to be performed. Note that from power-counting arguments, one might expect all diagrams shown in this section to diverge as $\lambda \rightarrow 0$. However, the results presented do not contain any poles in λ because they conspire to cancel. This is in line with the expectation from hard-soft-collinear factorization at leading power, where the collinear region does not contribute to the soft expansion.

The division of the calculation into the diagrams of Fig. 3.9 and 3.10, where the collinear loop momentum is radiated off leg i , and the remaining diagrams, where it is radiated off other legs, might remind the reader of the division of subleading collinear contributions at tree level in Eqs. (3.79)–(3.80). Indeed, this similarity can be leveraged to reuse the result of Section 3.3 here. The key observation is that while the diagrams contributing to $|M_{n+1}^{(0), \text{non-singular}}\rangle$ in Eqs. (3.79)–(3.80) are exactly the diagrams with which the jet operators have to be connected before performing the x integration,¹¹ the remaining terms can be used to express Eqs. (3.134)–(3.135) as convolutions in x with jet operators:

$$\text{Fig. 3.9} = \int_0^1 dx \mathbf{J}_q^{\nu, c'} \mathbf{T}_i^{c'} \frac{1}{p_i \cdot q} \left(-\frac{1}{2} \gamma_\nu \not{q} - \frac{1}{x} q_\nu \right) \partial_{\bar{u}_i} |M_n^{(0)}\rangle, \quad (3.139)$$

$$\begin{aligned} \text{Fig. 3.10} &= \int_0^1 dx \mathbf{J}_g^{\alpha\nu, c'} \mathbf{T}_i^{c'} \frac{1}{p_i \cdot q} \left(-(1-2x) g_{\alpha\nu} q_\beta - \frac{q_\nu g_{\alpha\beta}}{x} + \frac{q_\alpha g_{\nu\beta}}{1-x} \right) \partial_{\epsilon_i^*}^\beta |M_n^{(0)}\rangle \\ &\quad + n_l \int_0^1 dx \text{Tr} \left[\tilde{\mathbf{J}}_{c'c'_i} \frac{\not{q}}{p_i \cdot q} \right] T_{c'_i c'}^{c''} \frac{q_\mu}{p_i \cdot q} \partial_{\varepsilon^*(p_i, \sigma_i'')}^\mu \mathbf{P}_i(\sigma_i'', c_i'') |M_n^{(0)}\rangle, \end{aligned} \quad (3.140)$$

where we have used Eq. (3.79) with the replacements $\varepsilon_{n+1, \mu}^* \mapsto -g_{\mu\nu}$ and $\varepsilon_{i, \mu}^* \mapsto -g_{\mu\alpha}$ and Eq. (3.80) with $2\delta_{\sigma_i, -\sigma_{n+1}} = -\bar{u}(p_i, \sigma_i) \not{q} v(p_i, \sigma_{n+1}) / (p_i \cdot q) \mapsto -\not{q} / (p_i \cdot q)$, whereas the trace with an additional minus sign accounts for the closed fermion loop. Therefore, we can express the complete collinear region as a convolution of a jet operator with the subleading-collinear amplitudes $|\Delta M_{a,i}^{(0)}(x, \{p'_k\}, q)\rangle$ with $a \in \{g, \bar{q}\}$, for which gauge-invariant expressions have been

¹¹Note that external polarization vectors and spinors including their dependence on x through factors of $\sqrt{x}$ or $\sqrt{1-x}$ need to be removed because the collinear particles are no longer external but instead connected to the jet operators.

derived in Section 3.3. The case $a = \bar{q}$ is only necessary if particle i is a gluon. As a gauge invariant amplitude, $|\Delta M_{a,i}^{(0)}(x, \{p'_k\}, q)\rangle$ fulfills the Ward identity. This can be used to further simplify the jet operators by removing terms proportional to $n^\alpha \propto p_i^\alpha$ and $n^\nu \propto p'_i{}^\nu$. Effectively, this means replacing all instances of the metric $g_\perp^{\mu\nu}$ with $g^{\mu\nu}$, thereby removing all remaining $\bar{n}$ dependence in the jet operator as anticipated above. Finally, we can use the spin operators from Section 3.2. As in the soft region, one can derive an expression for the flavor-diagonal jet operator which can be used for both quarks and gluons. To achieve this, one needs to exploit the symmetry of $|\Delta M_{g,i}^{(0)}(x, \{p'_k\}, q)\rangle$ under exchange of the collinear gluons and the identity

$$\left(T_g^c T_g^{c'} + \frac{1}{x} i f^{cd c'} T_g^d\right)_{c_i c'_i} = \left(\frac{1-x}{x} T_g^c T_g^{c'} + \frac{1}{x} i f^{cd c'} T_g^d\right)_{c_i c'}, \quad (3.141)$$

which is a conveniently rewritten form of the Jacobi identity for the structure constants f^{abc} of SU(3). In summary, the contribution to the collinear region is given by¹²

$$\int_0^1 dx \left[\sum_{i, m_i=0} \mathbf{J}_i^{(1)}(x, p'_i, q) (1-x)^{-\dim(a_i)} |\Delta M_{g,i}^{(0)}(x, \{p'_k\}, q)\rangle + \sum_{i, a_i=g} \tilde{\mathbf{J}}_i^{(1)}(x, p'_i, q) (x(1-x))^{-\frac{1}{2}} |\Delta M_{\bar{q},i}^{(0)}(x, \{p'_k\}, q)\rangle \right], \quad (3.142)$$

where the x -dependent factors remove non-rational x dependence originating in external spinors, and the jet operators read

$$\begin{aligned} \mathbf{P}_{n+1} \mathbf{J}_i^{(1)}(x, p_i, q) &= \frac{\Gamma(1+\epsilon)}{1-\epsilon} \left(-\frac{\mu^2}{s_{iq}}\right)^\epsilon (x(1-x))^{-\epsilon} \sum_{\sigma' c'} \varepsilon_\mu^*(q, p_i, \sigma_{n+1}) \varepsilon_\nu(p_i, \sigma') \mathbf{P}_{n+1}(\sigma', c') \\ &\quad \times \left[\left(T_i^{c_{n+1}} T_i^{c'} + \frac{1}{x} i f^{c_{n+1} d c'} T_i^d \right) ((x-2) g^{\mu\nu} + (1+2\dim(a_i)) x i K_i^{\mu\nu}) \right] \\ &= \frac{\Gamma(1+\epsilon)}{1-\epsilon} \left(-\frac{\mu^2}{s_{iq}}\right)^\epsilon (x(1-x))^{-\epsilon} \varepsilon_\mu^*(q, p_i, \sigma_{n+1}) \cdot \varepsilon(p_i, -\sigma_{n+1}) \sum_{c'} \\ &\quad \times \mathbf{P}_g(-\sigma_{n+1}, c') \left[\left(T_i^{c_{n+1}} T_i^{c'} + \frac{1}{x} i f^{c_{n+1} d c'} T_i^d \right) (-2 + x(1 + \Sigma_{g,i})) \right], \end{aligned} \quad (3.143)$$

and

$$\begin{aligned} \tilde{\mathbf{J}}_i^{(1)}(x, p_i, q) |\dots, c'_i, \dots, c'; \dots, \sigma'_i, \dots, \sigma'\rangle &= \\ \frac{\Gamma(1+\epsilon)}{1-\epsilon} \left(-\frac{\mu^2}{s_{iq}}\right)^\epsilon (x(1-x))^{-\epsilon} \sum_{cc_i} \left(T_q^c T_q^{c_i} + x i f^{cd c_i} T_q^d \right) \sum_{c' c'_i \sigma \sigma_i} \varepsilon_\mu^*(q, p_i, \sigma) \varepsilon_\nu^*(p_i, \sigma_i) \\ &\quad \times ((1-2x) g^{\mu\nu} \mathbb{1} + 2 i K_q^{\mu\nu}(p_i))_{-\sigma' \sigma'_i} |\dots, c_i, \dots, c; \dots, \sigma_i, \dots, \sigma\rangle \end{aligned}$$

¹²Because the collinear region does not contribute at leading power, it is irrelevant whether p_i or p'_i is inserted into the jet operator because their difference is of order $\mathcal{O}(\lambda)$ for soft kinematics (not to be confused with the difference between p_i or p'_i for collinear kinematics). So far, we have refrained from using p'_i within the discussion of the collinear region for simplicity. However, for consistency with the other momentum regions, we use the primed momenta whenever possible for the final result.

$$\begin{aligned}
&= \frac{\Gamma(1+\epsilon)}{1-\epsilon} \left(-\frac{\mu^2}{s_{iq}} \right)^\epsilon (x(1-x))^{-\epsilon} \sum_{cc_i} \left(T_q^c T_q^{c_i} + x i f^{cd c_i} T_q^d \right)_{c'c'_i} \delta_{-\sigma'\sigma'_i} \sum_{\sigma\sigma_i} \delta_{\sigma\sigma_i} \varepsilon^*(q, p_i, \sigma) \cdot \varepsilon^*(p_i, \sigma_i) \\
&\quad \times (-2x + 1 + \text{sgn}(\sigma_i \sigma'_i)) |\dots, c_i, \dots, c; \dots, \sigma_i, \dots, \sigma\rangle,
\end{aligned} \tag{3.144}$$

where the equalities can be derived with

$$\varepsilon_\mu^*(q, p_i, \sigma) \varepsilon_\nu(p_i, \sigma') i K_{a_i, \sigma_i \sigma'_i}^{\mu\nu}(p_i) = -\sigma \delta_{-\sigma\sigma'} \sigma_i \delta_{\sigma_i \sigma'_i} \varepsilon^*(q, p_i, \sigma) \cdot \varepsilon(p_i, -\sigma) \tag{3.145}$$

and the operator

$$\Sigma_{g,i} |\dots, \sigma_i, \dots, \sigma\rangle \equiv \text{sgn}(\sigma \sigma_i) |\dots, \sigma_i, \dots, \sigma\rangle \tag{3.146}$$

has been introduced. The collinear amplitudes $(1-x)^{-\dim(a_i)} |\Delta M_{g,i}^{(0)}(x, \{p'_k\}, q)\rangle$ and $(x(1-x))^{-\frac{1}{2}} |\Delta M_{\bar{q},i}^{(0)}(x, \{p'_k\}, q)\rangle$ are rational functions in x which depends on gauge-invariant ingredients as shown in Eq. (3.84), below which formulae for all ingredients are derived. Due to this, the x integral can be performed explicitly. The resulting expressions are given in Eqs. (3.174) and (3.175).

3.4.4 Summary of the Subleading Soft Expansion

Summarizing the results of all regions discussed in this chapter, the expansion of one-loop QCD amplitudes in the soft limit, already presented in Refs. [1, 2], reads

$$\begin{aligned}
|M_{n+1}^{(1)}(\{p_k\})\rangle &= \mathcal{S}_{\text{NLP}}^{(0)}(\{p_k\}, \{p'_k\}, q) |M_n^{(1)}(\{p'_k\})\rangle + \mathcal{S}_{\text{NLP}}^{(1)}(\{p_k\}, \{p'_k\}, q) |M_n^{(0)}(\{p'_k\})\rangle \\
&+ \int_0^1 dx \left[\sum_{i, m_i=0} \mathcal{J}_i^{(1)}(x, p'_i, q) (1-x)^{-\dim(a_i)} |\Delta M_{g,i}^{(0)}(x, \{p'_k\}, q)\rangle \right. \\
&\quad \left. + \sum_{i, a_i=g} \tilde{\mathcal{J}}_i^{(1)}(x, p'_i, q) (x(1-x))^{-\frac{1}{2}} |\Delta M_{\bar{q},i}^{(0)}(x, \{p'_k\}, q)\rangle \right] \\
&+ \sum_{\substack{i \neq j \\ m_i=0 \\ m_j=0}} \sum_{\substack{\tilde{a}_i \neq a_i \\ \tilde{a}_j \neq a_j}} \tilde{\mathcal{S}}_{a_i a_j \leftarrow \tilde{a}_i \tilde{a}_j, ij}^{(1)}(p'_i, p'_j, q) |M_n^{(0)}(\{p'_k\})\rangle |_{a_j \rightarrow \tilde{a}_j}^{a_i \rightarrow \tilde{a}_i} + \mathcal{O}(\lambda),
\end{aligned} \tag{3.147}$$

with

$$\begin{aligned}
P_{n+1} \mathcal{S}_{\text{NLP}}^{(0)}(\{p_k\}, \{p'_k\}, q) &= - \sum_i T_i^{c_{n+1}} \mathcal{S}_i^{(0)}(\{p_k\}, \{p'_k\}, q) \equiv \\
&- \sum_i T_i^{c_{n+1}} \left[\frac{p_i \cdot \varepsilon_{n+1}^*}{p_i \cdot q} \left(1 + \sum_j (p_j - p'_j) \cdot \partial_j \right) + \frac{1}{2 p_i \cdot q} F_{\mu\nu} \left(J_i^{\mu\nu} - K_i^{\mu\nu} \right) \right],
\end{aligned} \tag{3.148}$$

taken from Eq. (3.41). For convenience, we print once more the definitions of the abelian field-strength tensor

$$F_{\mu\nu} \equiv i(q_\mu \varepsilon_{n+1, \nu}^* - q_\nu \varepsilon_{n+1, \mu}^*), \tag{3.149}$$

and the four-dimensional angular-momentum tensor operator

$$J_i^{\mu\nu} \equiv i(p_i^\mu \partial_i^\nu - p_i^\nu \partial_i^\mu). \tag{3.150}$$

The flavor-dependent spin-space operators $\mathbf{K}_i^{\mu\nu}$ are discussed in detail in Section 3.2. The one-loop operator $\mathbf{S}_{\text{NLP}}^{(1)}(\{p_k\}, \{p'_k\}, q)$, neglecting the function arguments for readability, reads

$$\begin{aligned} \mathbf{P}_{n+1} \mathbf{S}_{\text{NLP}}^{(1)} &= \sum_{i \neq j} \left(-\frac{\mu^2 s_{ij}}{s_{iq} s_{jq}} \right)^\epsilon \left[2i f^{abc_{n+1}} \mathbf{T}_i^a \mathbf{T}_j^b \mathbf{S}_{ij}^{(\text{NA})} + \mathbf{T}_i^{c_{n+1}} \mathbf{T}_j^c \mathbf{S}_{ij}^{(\text{A})} \right] \\ &+ C_F \sum_i \mathbf{T}_i^{c_{n+1}} \frac{2\epsilon(1-\epsilon)(1+2\epsilon)}{1-2\epsilon} \frac{A_0(m_i^2)}{m_i^2} \left(g^{\mu\nu} - \frac{2p_i^\mu p_i^\nu}{m_i^2} \right) \frac{F_{\mu\rho}}{s_{iq}} \mathbf{K}_{i\nu}{}^\rho, \end{aligned} \quad (3.151)$$

with the following definitions:

$$\begin{aligned} \mathbf{S}_{ij}^{(\text{NA})} &= -g_{ij}^{(1)} \mathbf{S}_i^{(0)} + \epsilon \mathbf{S}_{ij}^{(\text{A})} + a_i \left(g^{\mu\nu} - \frac{2p_i^\mu p_i^\nu}{m_i^2} \right) \frac{F_{\mu\rho}}{s_{iq}} \mathbf{K}_{i\nu}{}^\rho \\ &+ \left(b_{ij} \alpha_j g^{\mu\nu} + c_{ij} \alpha_j \frac{2p_j^\mu p_j^\nu}{m_j^2} + b_{ji} \frac{2p_j^\mu p_i^\nu}{s_{ij}} + c_{ji} \frac{2p_i^\mu p_j^\nu}{s_{ij}} \right) \frac{F_{\mu\rho}}{s_{iq}} (J_{i\nu}{}^\rho - \mathbf{K}_{i\nu}{}^\rho) \\ &+ \frac{b_{ji} + c_{ji} + 2\alpha_j (b_{ij} + c_{ij})}{v_{ij}^2} \frac{2p_i^\mu p_j^\nu F_{\mu\nu}}{s_{ij} s_{iq}} \frac{2p_i^\rho p_j^\sigma}{s_{ij}} (J_{i\rho\sigma} - \mathbf{K}_{i\rho\sigma}), \end{aligned} \quad (3.152)$$

$$-g_{ij}^{(1)} = \frac{M_{1i} + M_{1j} + (1-2\alpha_j) M_{2i} + (1-2\alpha_i) M_{2j} + (1-2\alpha_i - 2\alpha_j) M_3}{2g_{ijq}}, \quad (3.153)$$

$$S_{ij}^{(\text{A})} = -\frac{8}{v_{ij}^2} \left(\frac{2\epsilon}{1-2\epsilon} M_{1i} + (v_{ij}^2 - 1) M_{2j} \right) \frac{p_i^\mu p_j^\nu i F_{\mu\nu}}{s_{ij} s_{iq}}, \quad (3.154)$$

$$a_i = \frac{(1-\epsilon)(1-2\epsilon^2) M_{0i} - 2\epsilon M_{1i}}{1-2\epsilon}, \quad (3.155)$$

$$b_{ij} = \frac{-M_{1i} - M_{1j} + (1-2\alpha_i)(M_{2i} - M_{2j}) + M_3}{g_{ijq}}, \quad (3.156)$$

$$c_{ij} = \left[(1-2\alpha_j - (1-2\epsilon)(1-2\alpha_i)) M_{1i} \right. \quad (3.157)$$

$$\begin{aligned} &- \left((1-2\alpha_i + 2g_{ijq} - (1-2\epsilon)(1-2\alpha_j + 2g_{ijq})) M_{1j} \right. \\ &+ \left(2(1-2\epsilon)(v_{ij}^2 - g_{ijq}) + 2\epsilon(1-2\alpha_i)^2 \right) M_{2i} + \left(2g_{ijq} - 2(1-\epsilon)v_{ij}^2 \right) M_{2j} \\ &\left. + (1-2\alpha_i - (1-2\epsilon)(1-2\alpha_j)) M_3 \right] \frac{1}{2(1-2\epsilon) g_{ijq}^2}, \end{aligned} \quad (3.158)$$

$$g_{ijq} = 1 - \alpha_i - \alpha_j, \quad (3.159)$$

with the integrals M_{1k} , M_{2k} , and M_3 as shown in Section 3.4.2 for different cases depending on whether the particles i and j are massive. Their solution also contains the variables

$$\alpha_i \equiv \frac{m_i^2 s_{jq}}{s_{ij} s_{iq}}, \quad \alpha_j \equiv \frac{m_j^2 s_{iq}}{s_{ij} s_{jq}}, \quad v_{ij} \equiv \sqrt{1 - 4\alpha_i \alpha_j}. \quad (3.160)$$

The integral $A_0(m^2)$ from Eq. (3.105) also appears through the convenient definition

$$\left(-\frac{\mu^2 s_{ij}}{s_{iq}s_{jq}}\right)^\epsilon M_{0i} \equiv \frac{A_0(m_i^2)}{m_i^2}. \quad (3.161)$$

All Mandelstam variables are to be understood as containing a small imaginary part:

$$s_{ij} \equiv 2p_i \cdot p_j + i0^+, \quad s_{iq} \equiv 2p_i \cdot q + i0^+, \quad s_{jq} \equiv 2p_j \cdot q + i0^+. \quad (3.162)$$

After inserting integral solutions, the expressions can be written as expansions in ϵ . The poles in ϵ conspire with other terms of Eq. (3.147) to give the expected pole structure, as we show in Section 3.4.5. More relevant for practical application are the finite parts in ϵ which read, depending on the mass configuration, as follows. For $m_i \neq 0$ and $m_j \neq 0$, there is

$$\begin{aligned} -g_{ij}^{(1)} = & \frac{1}{v_{ij}} \left[\left(\frac{(1-2\alpha_j)\log(-\alpha_i) + (1-2\alpha_i)\log(-\alpha_j)}{4g_{ijq}} - \log(v_{ij}) - \frac{1}{4}l_{x_{ij}} \right) l_{x_{ij}} - \text{Li}_2(x_{ij}) + \frac{\pi^2}{6} \right] \\ & + \frac{(\log(-\alpha_i) - \log(-\alpha_j))^2 + l_{x_{ij}}^2 + 4\pi^2}{8g_{ijq}} + \frac{1}{2}\log(-\alpha_i)\log(-\alpha_j) - \frac{1}{4}l_{x_{ij}}^2 - \frac{7\pi^2}{12}, \end{aligned} \quad (3.163)$$

$$\epsilon S_{ij}^{(A)} = -\frac{8}{v_{ij}^2} \left[1 + \frac{2\alpha_i\alpha_j l_{x_{ij}}}{v_{ij}} \right] \frac{p_i^\mu p_j^\nu iF_{\mu\nu}}{s_{ij}s_{iq}}, \quad (3.164)$$

$$\begin{aligned} S_{ij}^{(A)} = & -\frac{8}{v_{ij}^2} \left[2 + \log(-\alpha_i) \right. \\ & \left. + \frac{\alpha_i\alpha_j}{v_{ij}} \left((4\log(v_{ij}) - 2\log(-\alpha_j) + l_{x_{ij}}) l_{x_{ij}} + 4\text{Li}_2(x_{ij}) - \frac{2\pi^2}{3} \right) \right] \frac{p_i^\mu p_j^\nu iF_{\mu\nu}}{s_{ij}s_{iq}}, \end{aligned} \quad (3.165)$$

$$a_i = -2\log(-\alpha_i) - 2\ln(-s_{ij}) + 2\ln(-s_{jq}), \quad (3.166)$$

$$b_{ij} = \frac{1}{4g_{ijq}} \left[\left(\log(-\alpha_j) - \log(-\alpha_i) + \frac{1-2\alpha_i}{v_{ij}} 2l_{x_{ij}} \right) (\log(-\alpha_i) - \log(-\alpha_j)) - l_{x_{ij}}^2 - 4\pi^2 \right], \quad (3.167)$$

$$\begin{aligned} c_{ij} = & \frac{1}{2g_{ijq}} \left[\frac{(\alpha_i - \alpha_j) \left((\log(-\alpha_i) - \log(-\alpha_j))^2 + l_{x_{ij}}^2 + 4\pi^2 \right) + 2v(\log(-\alpha_i) - \log(-\alpha_j)) l_{x_{ij}}}{2g_{ijq}} \right. \\ & \left. + (\log(-\alpha_j) - \log(-\alpha_i) - 2(1-2\alpha_i)) \frac{l_{x_{ij}}}{v_{ij}} + 2(\log(-\alpha_i) - \log(-\alpha_j)) \right], \end{aligned} \quad (3.168)$$

where we have again used

$$x_{ij} \equiv \frac{1-v_{ij}}{1+v_{ij}}, \quad l_{x_{ij}} \equiv \log(x_{ij}) + 2\pi i \theta(s_{ij}), \quad (3.169)$$

appearing in the integral solutions. For $m_i \neq 0$ and $m_j = 0$,

$$\begin{aligned}
-g_{ij}^{(1)} &= \frac{\alpha_i \log(-\alpha_i)^2 + (1 + 5\alpha_i) \frac{\pi^2}{6}}{2(1 - \alpha_i)}, \\
\epsilon S_{ij}^{(A)} &= -8 \frac{p_i^\mu p_j^\nu i F_{\mu\nu}}{s_{ij} s_{iq}}, \quad S_{ij}^{(A)} = (-16 - 8 \log(-\alpha_i)) \frac{p_i^\mu p_j^\nu i F_{\mu\nu}}{s_{ij} s_{iq}}, \\
a_i &= -2 \log(-\alpha_i) - 2 \ln(-s_{ij}) + 2 \ln(-s_{jq}), \quad b_{ij} = \frac{-\alpha_i \log(-\alpha_i)^2 + (1 - 7\alpha_i) \frac{\pi^2}{6}}{1 - \alpha_i}, \\
c_{ij} &= 4 + \frac{2\alpha_i \log(-\alpha_i)}{1 - \alpha_i} + \frac{\alpha_i (\log(-\alpha_i)^2 + \pi^2)}{(1 - \alpha_i)^2},
\end{aligned} \tag{3.170}$$

and for $m_i = 0$ and $m_j \neq 0$,

$$\begin{aligned}
-g_{ij}^{(1)} &= \frac{\alpha_j \log(-\alpha_j)^2 + (1 + 5\alpha_j) \frac{\pi^2}{6}}{2(1 - \alpha_j)}, \quad \epsilon S_{ij}^{(A)} = 0, \quad S_{ij}^{(A)} = 0, \quad a_i = 0, \\
b_{ij} &= -\frac{\log(-\alpha_j)^2 + \pi^2}{1 - \alpha_j}, \quad c_{ij} = -\frac{2 \log(-\alpha_j)}{1 - \alpha_j} - \frac{\alpha_j (\log(-\alpha_j)^2 + \pi^2)}{(1 - \alpha_j)^2}.
\end{aligned} \tag{3.171}$$

Finally, in the case $m_i = 0$ and $m_j = 0$, the coefficients take the simple form

$$-g_{ij}^{(1)} = \frac{\pi^2}{12}, \quad \epsilon S_{ij}^{(A)} = 0, \quad S_{ij}^{(A)} = 0, \quad a_i = 0, \quad b_{ij} = \frac{\pi^2}{6}, \quad c_{ij} = 4. \tag{3.172}$$

The flavor-off-diagonal soft operator reads

$$\begin{aligned}
&\tilde{S}_{a_i a_j \leftarrow \tilde{a}_i \tilde{a}_j, ij}^{(1)}(p_i, p_j, q) \mid \dots, c'_i, \dots, c'_j, \dots; \dots, \sigma'_i, \dots, \sigma'_j, \dots \rangle \\
&= -r_\Gamma \frac{\Gamma(1 - \epsilon) \Gamma(1 + \epsilon)}{\epsilon(1 - 2\epsilon)} \left(-\frac{\mu^2 s_{ij}}{s_{iq} s_{jq}} \right)^\epsilon \sum_{\sigma c} \sum_{\sigma_i c_i} \sum_{\sigma_j c_j} \sum_{\sigma'_i c'_i} \sum_{\sigma'_j c'_j} \\
&\quad \begin{cases} T_{c''_j c''_i}^c \bar{v}(p_j, \sigma''_j) \not{\epsilon}^*(q, p_i, \sigma) u(p_i, \sigma''_i) & \text{for } a_i = q \text{ or } \tilde{a}_i = \bar{q} \\ T_{c''_i c''_j}^c \bar{v}(p_i, \sigma''_i) \not{\epsilon}^*(q, p_i, \sigma) u(p_j, \sigma''_j) & \text{for } a_i = \bar{q} \text{ or } \tilde{a}_i = q \end{cases} \\
&\quad \times \langle c_i, c''_j; \sigma_i, \sigma''_j \mid \mathbf{Split}_{a_i \tilde{a}_j \leftarrow \tilde{a}_i}^{(0)}(p_i, p_j, p_i) \mid c'_i; \sigma'_i \rangle \mid c_j, c''_i; \sigma_j, \sigma''_i \mid \mathbf{Split}_{a_j \tilde{a}_i \leftarrow \tilde{a}_j}^{(0)}(p_j, p_i, p_j) \mid c'_j; \sigma'_j \rangle \\
&\quad \times \mid \dots, c_i, \dots, c_j, \dots, c; \dots, \sigma_i, \dots, \sigma_j, \dots, \sigma \rangle,
\end{aligned} \tag{3.173}$$

where the splitting function are given in Section 3.3 and the flavors $\tilde{a}_i$ and $\tilde{a}_j$ are determined by flavor conservation. Finally, given the jet operators from Eqs (3.143) and (3.144) and the decomposition of $\mid \Delta M_{a_i, i}^{(0)}(x, \{p_k\}, q) \rangle$ from Section 3.3, the x integrals in Eq. (3.147) can be performed explicitly to yield¹³

$$P_{n+1} \int_0^1 dx J_i^{(1)}(x, p'_i, q) (1 - x)^{-\dim(a_i)} \mid \Delta M_{g, i}^{(0)}(x, \{p'_k\}, q) \rangle =$$

¹³Analogously to Section 3.3, the expressions in Ref. [1] contain a different definition of $\mid C_{a_{n+1}, i}^{(0)} \rangle$ and can be recovered with $\mid C_{a_{n+1}, i}^{(0)} \rangle \mapsto \mid C_{a_{n+1}, i}^{(0)} \rangle + (\dim(a_i) - \dim(a_{n+1})) \mid S_{a_{n+1}, i}^{(0)} \rangle - \mid \bar{S}_{a_{n+1}, i}^{(0)} \rangle - \sum_I \frac{1}{x_I} \mid R_{a_{n+1}, i, I}^{(0)} \rangle$.

$$\begin{aligned}
& \frac{r_\Gamma}{\epsilon(1-\epsilon)(1-2\epsilon)} \left(-\frac{\mu^2}{s_{iq}} \right)^\epsilon \varepsilon^*(q, p_i, \sigma_{n+1}) \cdot \varepsilon(p_i, -\sigma_{n+1}) \sum_{c'} \mathbf{P}_{n+1}(-\sigma_{n+1}, c') \\
& \times \left\{ \mathbf{T}_i^{c'} \mathbf{T}_i^{c_{n+1}} \left[-\frac{1-2\epsilon}{1+\epsilon} (1-3\epsilon + (1+\epsilon)\Sigma_{g,i}) |S_{g,i}^{(0)}\rangle + (1-2\epsilon)(3-\Sigma_{g,i}) |\bar{S}_{g,i}^{(0)}\rangle \right. \right. \\
& \quad + (2-3\epsilon + \epsilon\Sigma_{g,i}) |C_{g,i}^{(0)}\rangle - \frac{\epsilon}{2} (3-\Sigma_{g,i}) |L_{g,i}^{(0)}\rangle \\
& \quad + \sum_I \left(\frac{2}{x_I} - \epsilon \frac{(2-3x_I + x_I \Sigma_{g,i})}{x_I(1-x_I)} - \epsilon \frac{(2-x_I - x_I \Sigma_{g,i})}{2x_I^2(1-x_I)} {}_2F_1(1, 1-\epsilon, 3-2\epsilon, 1/x_I) \right) |R_{g,i,I}^{(0)}\rangle \Big] \\
& \quad + \mathbf{T}_i^{c_{n+1}} \mathbf{T}_i^{c'} \left[\frac{1-\epsilon}{1+\epsilon} (3-3\epsilon + (1+\epsilon)\Sigma_{g,i}) |S_{g,i}^{(0)}\rangle - (2-\epsilon(3-\Sigma_{g,i})) |\bar{S}_{g,i}^{(0)}\rangle \right. \\
& \quad - \frac{1}{2} (4-3\epsilon + \epsilon\Sigma_{g,i}) |C_{g,i}^{(0)}\rangle + \frac{\epsilon}{2(3-2\epsilon)} (5-3\epsilon - (1-\epsilon)\Sigma_{g,i}) |L_{g,i}^{(0)}\rangle \\
& \quad \left. \left. + \sum_I \left(-2 \frac{1-\epsilon}{x_I} + \epsilon \frac{2-x_I - x_I \Sigma_{g,i}}{2x_I^2} {}_2F_1(1, 1-\epsilon, 3-2\epsilon, 1/x_I) \right) |R_{g,i,I}^{(0)}\rangle \right] \right\} \quad (3.174)
\end{aligned}$$

and

$$\begin{aligned}
& \mathbf{P}_i \mathbf{P}_{n+1} \int_0^1 dx \tilde{\mathbf{J}}_i^{(1)}(x, p'_i, q) (x(1-x))^{-\frac{1}{2}} |\Delta M_{\bar{q},i}^{(0)}(x, \{p'_k\}, q)\rangle \\
& = \frac{r_\Gamma}{(1-\epsilon)(1-2\epsilon)} \left(-\frac{\mu^2}{s_{iq}} \right)^\epsilon \varepsilon^*(q, p_i, \sigma_{n+1}) \cdot \varepsilon^*(p_i, \sigma_i) \sum_{\sigma' c'} \sum_{c'_i} \mathbf{P}_i(-\sigma', c'_i) \mathbf{P}_{n+1}(\sigma', c') \\
& \left\{ (T^{c_i} T^{c_{n+1}})_{c' c'_i} \left[2\sigma_i \sigma' |S_{\bar{q},i}^{(0)}\rangle + \frac{1-2(1-\epsilon)\sigma_i \sigma'}{\epsilon} |\bar{S}_{\bar{q},i}^{(0)}\rangle + \left(\sigma_i \sigma' - \frac{1}{2(3-2\epsilon)} \right) |C_{\bar{q},i}^{(0)}\rangle \right. \right. \\
& \quad \left. + \sum_I (2x_I - 2\sigma_i \sigma' + (1-2x_I + 2\sigma_i \sigma') {}_2F_1(1, 1-\epsilon, 2-2\epsilon, 1/x_I)) |R_{\bar{q},i,I}^{(0)}\rangle \right] \\
& \quad + (T^{c_{n+1}} T^{c_i})_{c' c'_i} \left[\frac{-1-2(1-\epsilon)\sigma_i \sigma'}{\epsilon} |S_{\bar{q},i}^{(0)}\rangle + 2\sigma_i \sigma' |\bar{S}_{\bar{q},i}^{(0)}\rangle + \left(\sigma_i \sigma' + \frac{1}{2(3-2\epsilon)} \right) |C_{\bar{q},i}^{(0)}\rangle \right. \\
& \quad \left. \left. + \sum_I \left(2(1-x_I) + 2\sigma_i \sigma' + \frac{1-x_I}{x_I} (1-2x_I + 2\sigma_i \sigma') {}_2F_1(1, 1-\epsilon, 2-2\epsilon, 1/x_I) \right) |R_{\bar{q},i,I}^{(0)}\rangle \right] \right\}. \quad (3.175)
\end{aligned}$$

3.4.5 Spurious-Pole Cancellation

In this section, we confirm analytically that our result is correct when expanded up to $\mathcal{O}(\epsilon^{-1})$. As always in this chapter, we closely follow and use equations of Refs. [1, 2]. The ϵ poles of one-loop amplitudes can be obtained from the action of a general operator on tree-level amplitudes, the $\mathbf{I}_n^{(1)}$ operator:

$$|M_{n+1}^{(1)}(\{p_k\})\rangle = \mathbf{I}_{n+1}^{(1)}(\{p_k\}) |M_{n+1}^{(0)}(\{p_k\})\rangle + \mathcal{O}(\epsilon^0). \quad (3.176)$$

It was calculated for general massless or massive one-loop amplitudes in Ref. [159] and reads

$$\begin{aligned}
\mathbf{I}_n^{(1)}(\{p_k\}) &= \frac{n-2}{2} \frac{\beta_0}{\epsilon} + \frac{1}{2\epsilon} \sum_i \Gamma_{a_i}(m_i) + \sum_{\substack{i \neq j \\ m_i=0 \\ m_j=0}} \mathbf{T}_i^c \mathbf{T}_j^c \left(\frac{1}{\epsilon^2} + \frac{1}{\epsilon} \log \left(-\frac{\mu^2}{s_{ij}} \right) \right) \\
&+ \sum_{\substack{i \neq j \\ m_i \neq 0 \\ m_j=0}} \mathbf{T}_i^c \mathbf{T}_j^c \left(\frac{1}{\epsilon^2} + \frac{1}{\epsilon} \left[\log \left(-\frac{\mu^2}{s_{ij}} \right) + \log \left(-\frac{m_i^2}{s_{ij}} \right) \right] \right) + \sum_{\substack{i \neq j \\ m_i \neq 0 \\ m_j \neq 0}} \mathbf{T}_i^c \mathbf{T}_j^c \frac{1}{2\epsilon} \frac{l_{x_{ij}}}{v_{ij}}, \quad (3.177)
\end{aligned}$$

where

$$\beta_0 \equiv \frac{11}{3}C_A - \frac{4}{3}T_f n_f \quad (3.178)$$

is the first coefficient of the beta function expansion (2.11), and

$$\Gamma_{\alpha_i}(0) \equiv \gamma_0^{\alpha_i}, \quad \Gamma_{\alpha_i}(m_i > 0) \equiv -2C_F \quad (3.179)$$

with the anomalous dimensions

$$\gamma_0^q \equiv -3C_F, \quad \gamma_0^g \equiv -\beta_0. \quad (3.180)$$

Hence, the ϵ poles of the soft expansion should read

$$|M_{n+1}^{(1)}(\{p_k\})\rangle = \mathbf{I}_{n+1}^{(1)}(\{p_k\}) \mathbf{S}_{\text{NLP}}^{(0)}(\{p_k\}, \{p'_k\}, q) |M_n^{(0)}(\{p'_k\})\rangle + \mathcal{O}(\lambda) + \mathcal{O}(\epsilon^0). \quad (3.181)$$

Commutation of the two operators, taking into account the difference between $\mathbf{I}_{n+1}^{(1)}$ and $\mathbf{I}_n^{(1)}$, and further manipulation leads to the general formula

$$\begin{aligned} \mathbf{P}_{n+1} |M_{n+1}^{(1)}\rangle &= \mathbf{P}_{n+1} \mathbf{S}^{(0)} |M_n^{(1)}\rangle \\ &+ \sum_{i \neq j} 2i f^{abc_{n+1}} \mathbf{T}_i^a \mathbf{T}_j^b \left(-\frac{\mu^2 s_{ij}}{s_{iq} s_{jq}} \right) \frac{1}{\epsilon} \left[\frac{1}{\epsilon} + \frac{1}{2} \left(\log(-\alpha_i) + \log(-\alpha_j) - \frac{l_{x_{ij}}}{v_{ij}} \right) \right] \mathbf{S}_i^{(0)} |M_n^{(0)}\rangle \\ &+ \sum_{i \neq j} \mathbf{T}_i^{c_{n+1}} \mathbf{T}_i^c \mathbf{T}_j^c \frac{1}{\epsilon} \left[-\frac{8}{v_{ij}^2} \left(1 + \frac{2\alpha_i \alpha_j l_{x_{ij}}}{v_{ij}} \right) \frac{p_i^\mu p_j^\nu}{s_{ij} s_{iq}} iF_{\mu\nu} \right] |M_n^{(0)}\rangle + \mathcal{O}(\lambda) + \mathcal{O}(\epsilon^0), \end{aligned} \quad (3.182)$$

with a smooth limit if either m_i or m_j is massless, which reads

$$\begin{aligned} \mathbf{P}_{n+1} |M_{n+1}^{(1)}\rangle &= \mathbf{P}_{n+1} \mathbf{S}^{(0)} |M_n^{(1)}\rangle + \sum_{i \neq j} 2i f^{abc_{n+1}} \mathbf{T}_i^a \mathbf{T}_j^b \left(-\frac{\mu^2 s_{ij}}{s_{iq} s_{jq}} \right) \frac{1}{\epsilon^2} \mathbf{S}_i^{(0)} |M_n^{(0)}\rangle \\ &+ \sum_{i \neq j} \mathbf{T}_i^{c_{n+1}} \mathbf{T}_i^c \mathbf{T}_j^c \frac{1}{\epsilon} \left[-\frac{8}{v_{ij}^2} \frac{p_i^\mu p_j^\nu}{s_{ij} s_{iq}} iF_{\mu\nu} \right] |M_n^{(0)}\rangle + \mathcal{O}(\lambda) + \mathcal{O}(\epsilon^0). \end{aligned} \quad (3.183)$$

Now, we can test whether our soft expansion (3.147) in fact takes this form when expanded through $\mathcal{O}(\epsilon^{-1})$. To this end, let us first consider the ϵ expansion of $\mathbf{S}_{\text{NLP}}^{(1)}$,

$$\mathbf{P}_{n+1} \mathbf{S}_{\text{NLP}}^{(1)} = \sum_{i \neq j} \left(-\frac{\mu^2 s_{ij}}{s_{iq} s_{jq}} \right) \epsilon \left[2i f^{abc_{n+1}} \mathbf{T}_i^a \mathbf{T}_j^b \mathbf{S}_{ij}^{(\text{NA})} \Big|_{\epsilon\text{-poles}} + \mathbf{T}_i^{c_{n+1}} \mathbf{T}_i^c \mathbf{T}_j^c \mathbf{S}_{ij}^{(\text{A})} \Big|_{\epsilon\text{-poles}} \right] + \mathcal{O}(\epsilon^0), \quad (3.184)$$

where the poles of $\mathbf{S}_{ij}^{(\text{NA})}$ and $\mathbf{S}_{ij}^{(\text{A})}$ depend on the mass configuration. If $m_i \neq 0$ and $m_j \neq 0$, there is

$$\begin{aligned} \mathbf{S}_{ij}^{(\text{NA})} \Big|_{\epsilon\text{-poles}} &= \frac{1}{\epsilon} \left[\frac{1}{\epsilon} + \frac{1}{2} \left(\log(-\alpha_i) + \log(-\alpha_j) - \frac{l_{x_{ij}}}{v_{ij}} \right) \right] \mathbf{S}_i^{(0)}, \\ \mathbf{S}_{ij}^{(\text{A})} \Big|_{\epsilon\text{-poles}} &= \frac{1}{\epsilon} \left[-\frac{8}{v_{ij}^2} \left(1 + \frac{2\alpha_i \alpha_j l_{x_{ij}}}{v_{ij}} \right) \frac{p_i^\mu p_j^\nu}{s_{ij} s_{iq}} iF_{\mu\nu} \right]. \end{aligned} \quad (3.185)$$

For $m_i \neq 0$ and $m_j = 0$,

$$\begin{aligned} \mathbf{S}_{ij}^{(\text{NA})} \Big|_{\epsilon\text{-poles}} &= \frac{1}{\epsilon} \left[\frac{1}{\epsilon} \mathbf{S}_i^{(0)} + 4 \frac{p_j^\mu p_j^\nu}{s_{ij} s_{jq}} F_{\mu\rho} (J_{i\nu}{}^\rho - \mathbf{K}_{i\nu}{}^\rho) \right], \\ S_{ij}^{(\text{A})} \Big|_{\epsilon\text{-poles}} &= \frac{1}{\epsilon} \left[-8 \frac{p_i^\mu p_j^\nu}{s_{ij} s_{iq}} i F_{\mu\nu} \right], \end{aligned} \quad (3.186)$$

for $m_i = 0$ and $m_j \neq 0$,

$$\begin{aligned} \mathbf{S}_{ij}^{(\text{NA})} \Big|_{\epsilon\text{-poles}} &= \frac{1}{\epsilon} \left[\frac{1}{\epsilon} \mathbf{S}_i^{(0)} + 4 \frac{p_i^\mu p_j^\nu - p_j^\mu p_i^\nu}{s_{ij} s_{iq}} F_{\mu\rho} (J_{i\nu}{}^\rho - \mathbf{K}_{i\nu}{}^\rho) \right], \\ S_{ij}^{(\text{A})} \Big|_{\epsilon\text{-poles}} &= 0, \end{aligned} \quad (3.187)$$

and finally for $m_i = m_j = 0$,

$$\begin{aligned} \mathbf{S}_{ij}^{(\text{NA})} \Big|_{\epsilon\text{-poles}} &= \frac{1}{\epsilon} \left[\frac{1}{\epsilon} \mathbf{S}_i^{(0)} + 4 \left(\frac{p_i^\mu p_j^\nu - p_j^\mu p_i^\nu}{s_{ij} s_{iq}} + \frac{p_j^\mu p_j^\nu}{s_{ij} s_{jq}} \right) F_{\mu\rho} (J_{i\nu}{}^\rho - \mathbf{K}_{i\nu}{}^\rho) \right], \\ S_{ij}^{(\text{A})} \Big|_{\epsilon\text{-poles}} &= 0. \end{aligned} \quad (3.188)$$

It is easy to see that Eq. (3.185) leads to the same pole structure as Eq. (3.182). This is expected because if both i and j are massive particles, there is neither a contribution from the jet operators nor from the flavor-off-diagonal soft operator to the soft expansion (3.147). The other cases are slightly more involved because Eq. (3.182) contains only flavor-diagonal color and spin operators acting on $|M_n^{(0)}\rangle$, at difference to the contributions from jet and flavor-off-diagonal soft operators. The key observation is that all ϵ poles in Eqs. (3.174) and (3.175) are either proportional to

$$|S_{g,i}^{(0)}\rangle \quad \text{or} \quad |C_{g,i}^{(0)}\rangle + |\bar{S}_{g,i}^{(0)}\rangle + \sum_I \frac{1}{x_I} |R_{g,i,I}^{(0)}\rangle \quad (3.189)$$

or to

$$|\bar{S}_{g,i}^{(0)}\rangle, \quad |S_{\bar{q},i}^{(0)}\rangle, \quad \text{or} \quad |\bar{S}_{\bar{q},i}^{(0)}\rangle. \quad (3.190)$$

Following Section 3.3, the former can be written as flavor-diagonal operators acting on $|M_n^{(0)}\rangle$, whereas the latter correspond to splitting functions acting on $|M_n^{(0)}(\{p'_k\})|_{a_j \rightarrow \bar{a}_j}^{a_i \rightarrow \bar{a}_i}$, in similarity to the flavor-off-diagonal soft contribution. Note that $|\bar{S}_{g,i}^{(0)}\rangle$ can belong both to the former and to the latter group, depending on whether particle i is a gluon or an (anti-)quark. Let us start with the flavor-diagonal case. Inserting Eqs. (3.89), Eqs. (3.96), and the $a_i = g$ case of Eq. (3.91), there is

$$\begin{aligned} \sum_{\substack{j \\ m_j \neq 0}} \mathbf{P}_{n+1} \int_0^1 dx \mathbf{J}_j^{(1)} (1-x)^{-\dim(a_j)} |\Delta M_{g,j}^{(0)}\rangle \\ = \sum_{\substack{i \neq j \\ m_j \neq 0}} 2i f^{abc_{n+1}} \mathbf{T}_i^a \mathbf{T}_j^b \frac{1}{\epsilon} \left[-4 \frac{p_j^\mu p_j^\nu}{s_{ij} s_{jq}} F_{\mu\rho} (J_{i\nu}{}^\rho - \mathbf{K}_{i\nu}{}^\rho) \right] |M_n^{(0)}\rangle \end{aligned}$$

$$\begin{aligned}
& + \sum_{\substack{i \neq j \\ m_j \neq 0}} 2i f^{abc_{n+1}} \mathbf{T}_i^a \mathbf{T}_j^b \frac{1}{\epsilon} \left[-4 \frac{p_i^\mu p_j^\nu - p_j^\mu p_i^\nu}{s_{ij} s_{jq}} F_{\mu\rho} (J_{j\nu}{}^\rho - \mathbf{K}_{j\nu}{}^\rho) \right] |M_n^{(0)}\rangle \\
& + \sum_{\substack{i \neq j \\ m_j \neq 0}} \mathbf{T}_j^{c_{n+1}} \mathbf{T}_j^c \mathbf{T}_i^c \frac{1}{\epsilon} \left[-8 \frac{p_j^\mu p_j^\nu}{s_{ij} s_{jq}} i F_{\mu\nu} \right] |M_n^{(0)}\rangle + \mathcal{O}(\epsilon^0) \\
& + \text{flavor-off-diagonal contributions from } |\bar{S}_{g,j}^{(0)}\rangle \text{ if } j \text{ is an (anti-)quark,} \quad (3.191)
\end{aligned}$$

which, taken together with the contributions from Eqs. (3.186), (3.187), and (3.185) reproduces the expected pole structure of Eq. (3.183). Thus, in order for spurious-pole cancellation to be fulfilled, all flavor-off-diagonal contributions must cancel. Indeed, let us consider the three convolutions related to the coefficients listed in Eq. (3.190). If particle i is an (anti-)quark,

$$\begin{aligned}
& \int_0^1 \frac{dx}{1-x} \langle \dots, c_i, \dots, c; \dots, \sigma_i, \dots, \sigma | \mathbf{J}_i^{(1)} | \bar{S}_{g,i}^{(0)} \rangle = \frac{1}{\epsilon} \epsilon_\mu^*(q, p_i, \sigma) \sum_{j \neq i} \sum_{\sigma'_i c'_i} \sum_{\sigma'_j c'_j} \sum_{\sigma' c'} \\
& \epsilon_\nu(p_i, \sigma'_i) (T_{a_i}^{c'_i} T_{a_i}^c)_{c_i c'} (g^{\mu\nu} \mathbb{1} - 2i K_{a_i}^{\mu\nu}(p_i))_{\sigma_i \sigma'} \langle c_j, c'; \sigma_j, \sigma' | \mathbf{Split}_{a_j a_i \leftarrow \bar{a}_j}^{(0)}(p_j, p_i, p_j) | c'_j; \sigma'_j \rangle \\
& \times \langle \dots, c'_i, \dots, c'_j, \dots; \dots, \sigma'_i, \dots, \sigma'_j, \dots | M^{(0)}(\{p_i\}) \Big|_{a_j \rightarrow \bar{a}_j}^{a_i \rightarrow g} \rangle + \mathcal{O}(\epsilon^0) \\
& \equiv \frac{1}{\epsilon} \sum_{j \neq i} \sum_{\sigma'_i c'_i} \sum_{\sigma'_j c'_j} J_{a_i a_j \leftarrow g \bar{a}_j}^{(1,-1)} \langle \dots, c'_i, \dots, c'_j, \dots; \dots, \sigma'_i, \dots, \sigma'_j, \dots | M^{(0)}(\{p_i\}) \Big|_{a_j \rightarrow \bar{a}_j}^{a_i \rightarrow g} \rangle + \mathcal{O}(\epsilon^0). \quad (3.192)
\end{aligned}$$

If particle i is a gluon, we instead have the following contribution from the flavor-off-diagonal jet operator:

$$\begin{aligned}
& \int_0^1 \frac{dx}{x} \langle \dots, c_i, \dots, c; \dots, \sigma_i, \dots, \sigma | \tilde{\mathbf{J}}_i^{(1)} | S_{\bar{q},i}^{(0)} \rangle = \frac{1}{\epsilon} \epsilon_\mu^*(q, p_i, \sigma) \epsilon_\nu^*(p_i, \sigma_i) \sum_{j \neq i} \sum_{\sigma'_i c'_i} \sum_{\sigma'_j c'_j} \sum_{\sigma' c'} \\
& (T^c T^{c_i})_{c' c'_i} (-g^{\mu\nu} \mathbb{1} - 2i K_q^{\mu\nu}(p_i))_{-\sigma' \sigma'_i} \langle c_j, c'; \sigma_j, \sigma' | \mathbf{Split}_{a_j \bar{q} \leftarrow \bar{a}_j}^{(0)}(p_j, p_i, p_j) | c'_j; \sigma'_j \rangle \\
& \times \langle \dots, c'_i, \dots, c'_j, \dots; \dots, \sigma'_i, \dots, \sigma'_j, \dots | M^{(0)}(\{p_i\}) \Big|_{a_j \rightarrow \bar{a}_j}^{a_i \rightarrow q} \rangle + \mathcal{O}(\epsilon^0) \\
& \equiv \frac{1}{\epsilon} \sum_{j \neq i} \sum_{\sigma'_i c'_i} \sum_{\sigma'_j c'_j} \tilde{J}_{a_i a_j \leftarrow q \bar{a}_j}^{(1,-1)} \langle \dots, c'_i, \dots, c'_j, \dots; \dots, \sigma'_i, \dots, \sigma'_j, \dots | M^{(0)}(\{p_i\}) \Big|_{a_j \rightarrow \bar{a}_j}^{a_i \rightarrow q} \rangle + \mathcal{O}(\epsilon^0), \quad (3.193)
\end{aligned}$$

$$\begin{aligned}
& \int_0^1 \frac{dx}{1-x} \langle \dots, c_i, \dots, c; \dots, \sigma_i, \dots, \sigma | \tilde{\mathbf{J}}_i^{(1)} | \bar{S}_{\bar{q},i}^{(0)} \rangle = \frac{1}{\epsilon} \epsilon_\mu^*(q, p_i, \sigma) \epsilon_\nu^*(p_i, \sigma_i) \sum_{j \neq i} \sum_{\sigma'_i c'_i} \sum_{\sigma'_j c'_j} \sum_{\sigma' c'} \\
& (T^{c_i} T^c)_{c'_i c'} (g^{\mu\nu} \mathbb{1} - 2i K_q^{\mu\nu}(p_i))_{-\sigma'_i \sigma'} \langle c_j, c'; \sigma_j, \sigma' | \mathbf{Split}_{a_j q \leftarrow \bar{a}_j}^{(0)}(p_j, p_i, p_j) | c'_j; \sigma'_j \rangle \\
& \times \langle \dots, c'_i, \dots, c'_j, \dots; \dots, \sigma'_i, \dots, \sigma'_j, \dots | M^{(0)}(\{p_i\}) \Big|_{a_j \rightarrow \bar{a}_j}^{a_i \rightarrow \bar{q}} \rangle + \mathcal{O}(\epsilon^0)
\end{aligned}$$

$$\equiv \frac{1}{\epsilon} \sum_{j \neq i} \sum_{\sigma'_i c'_i} \sum_{\sigma'_j c'_j} \tilde{J}_{a_i a_j \leftarrow \bar{q} \bar{a}_j}^{(1,-1)} \langle \dots, c'_i, \dots, c'_j, \dots; \dots, \sigma'_i, \dots, \sigma'_j, \dots | M^{(0)}(\{p_i\}) \Big|_{a_j \rightarrow \bar{a}_j}^{a_i \rightarrow \bar{q}} \rangle + \mathcal{O}(\epsilon^0). \quad (3.194)$$

After inserting the splitting operators from Eqs. (3.48)–(3.51), the defined functions read

$$\begin{aligned} J_{q\bar{q} \leftarrow g\bar{g}}^{(1,-1)} &= -\frac{1}{2 p_i \cdot p_j} (T^{c'_i} T^c T^{c'_j})_{c_i c_j} \bar{u}(p_i, \sigma_i) \not{\epsilon}(p_i, \sigma'_i) \not{\epsilon}^*(q, p_i, \sigma) \not{\epsilon}(p_j, \sigma'_j) v(p_j, \sigma_j), \\ J_{q\bar{g} \leftarrow g\bar{q}}^{(1,-1)} &= -\frac{1}{2 p_i \cdot p_j} (T^{c'_i} T^c T^{c_j})_{c_i c'_j} \bar{u}(p_i, \sigma_i) \not{\epsilon}(p_i, \sigma'_i) \not{\epsilon}^*(q, p_i, \sigma) \not{\epsilon}^*(p_j, \sigma_j) u(p_j, \sigma'_j), \\ J_{\bar{q}\bar{q} \leftarrow g\bar{q}}^{(1,-1)} &= +\frac{1}{2 p_i \cdot p_j} (T^{c_j} T^c T^{c'_i})_{c'_j c_i} \bar{v}(p_j, \sigma'_j) \not{\epsilon}^*(p_j, \sigma_j) \not{\epsilon}^*(q, p_i, \sigma) \not{\epsilon}(p_i, \sigma'_i) v(p_i, \sigma_i), \\ \tilde{J}_{g\bar{q} \leftarrow q\bar{g}}^{(1,-1)} &= +\frac{1}{2 p_i \cdot p_j} (T^{c'_j} T^c T^{c_i})_{c'_j c_i} \bar{u}(p_j, \sigma_j) \not{\epsilon}(p_j, \sigma'_j) \not{\epsilon}^*(q, p_i, \sigma) \not{\epsilon}^*(p_i, \sigma_i) v(p_i, -\sigma'_i), \\ \tilde{J}_{g\bar{g} \leftarrow q\bar{q}}^{(1,-1)} &= -\frac{1}{2 p_i \cdot p_j} (T^{c_j} T^c T^{c_i})_{c'_j c_i} \bar{v}(p_j, \sigma'_j) \not{\epsilon}^*(p_j, \sigma_j) \not{\epsilon}^*(q, p_i, \sigma) \not{\epsilon}^*(p_i, \sigma_i) v(p_i, -\sigma'_i), \\ \tilde{J}_{g\bar{g} \leftarrow \bar{q}\bar{q}}^{(1,-1)} &= -\frac{1}{2 p_i \cdot p_j} (T^{c_i} T^c T^{c_j})_{c'_i c'_j} \bar{u}(p_i, -\sigma'_i) \not{\epsilon}^*(p_i, \sigma_i) \not{\epsilon}^*(q, p_i, \sigma) \not{\epsilon}^*(p_j, \sigma_j) u(p_j, \sigma'_j), \\ \tilde{J}_{g\bar{q} \leftarrow \bar{q}\bar{g}}^{(1,-1)} &= -\frac{1}{2 p_i \cdot p_j} (T^{c_i} T^c T^{c'_j})_{c'_i c_j} \bar{u}(p_i, -\sigma'_i) \not{\epsilon}^*(p_i, \sigma_i) \not{\epsilon}^*(q, p_i, \sigma) \not{\epsilon}(p_j, \sigma'_j) v(p_j, \sigma_j). \end{aligned} \quad (3.195)$$

After inserting $\not{p}_i$ or $\not{p}_j$ into the spinor chains with equalities like

$$\begin{aligned} \bar{u}(p_i, \sigma_i) \not{\epsilon}(p_i, \sigma'_i) \not{\epsilon}^*(q, p_i, \sigma) \not{\epsilon}(p_j, \sigma'_j) v(p_j, \sigma_j) = \\ -\frac{1}{2 p_i \cdot p_j} \bar{u}(p_i, \sigma_i) \not{\epsilon}(p_i, \sigma'_i) \not{p}_j \not{\epsilon}^*(q, p_i, \sigma) \not{p}_i \not{\epsilon}(p_j, \sigma'_j) v(p_j, \sigma_j) \end{aligned} \quad (3.196)$$

and transforming them to spinors with

$$\not{p} = \sum_{\sigma''} u(p, \sigma'') \bar{u}(p, \sigma'') = \sum_{\sigma''} v(p, \sigma'') \bar{v}(p, \sigma''), \quad (3.197)$$

one recovers all terms of the sum over the flavor-off-diagonal soft operator $\mathcal{S}_{a_i a_j \leftarrow \bar{a}_i \bar{a}_j, ij}^{(1)}$ shown in Eq. (3.173) with opposite sign. Thus, all ϵ poles from flavor-off-diagonal contributions cancel, and we have successfully shown that the soft expansion (3.147) is correct through $\mathcal{O}(\epsilon^{-1})$.

3.4.6 Numerical Checks

While a correct pole structure shown in the previous section is a good indicator for the correctness of our result, the behavior at $\mathcal{O}(\epsilon^0)$ is what is relevant for practical application after all. Hence, it is desirable to perform a check of its correctness. To achieve this, we make use of existing numerical implementations which can calculate arbitrary one-loop QCD amplitudes, including $|M_{n+1}^{(1)}\rangle$ and $|M_n^{(1)}\rangle$ once a specific Born process is chosen. Then, we can numerically calculate

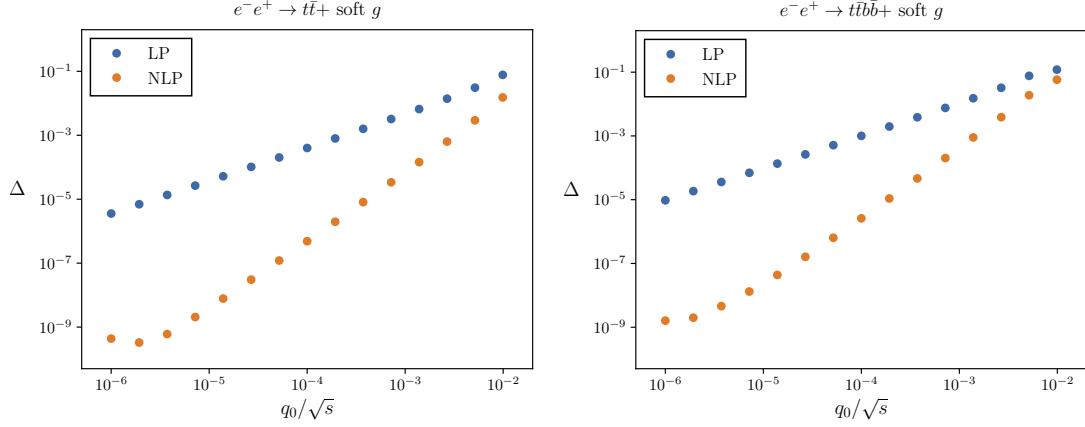


Figure 3.14: Numerical probes of $\Delta_{\text{LP/NLP}}$ defined in Eq. (3.198) for different $\lambda = q_0/\sqrt{s}$, where q_0 is the energy component of the soft gluon and $\sqrt{s}$ the center-of-mass energy of the phase-space point, for two different processes containing massive quarks. Figure taken from Ref. [2].

the quantity

$$\Delta_{\text{LP/NLP}} \equiv \frac{1}{N} \sum_{\substack{\text{singular} \\ \text{color flows } \{c_k\} \\ \text{helicities } \{\sigma_k\}}} \left| \frac{\left[\langle \{c_k\}, \{\sigma_k\} | M_{n+1}^{(1)} \rangle - \langle \{c_k\}, \{\sigma_k\} | M_{n+1}^{(1)} \rangle_{\text{LP/NLP}} \right]_{\mathcal{O}(\epsilon^0)}}{\left[\langle \{c_k\}, \{\sigma_k\} | M_{n+1}^{(1)} \rangle \right]_{\mathcal{O}(\epsilon^0)}} \right|, \quad (3.198)$$

where $|M_{n+1}^{(1)}\rangle_{\text{LP/NLP}}$ denotes the amplitude in the soft approximation from Eq. (3.147) at LP or NLP, respectively, for arbitrary phase-space points. If the momentum $q = p_{n+1}$ is soft, $\Delta_{\text{LP/NLP}}$ should be a small quantity if our approximation is correct. To ensure this for all possible color¹⁴ and helicity configurations for which a soft singularity exists, we perform a sum of absolute values over them. The number of such configurations is denoted as N .

In Refs. [1, 2], we computed $\Delta_{\text{LP/NLP}}$ in practice with the help of the software package **Recola** [161, 162], which allows the numerical calculation of non-squared one-loop amplitudes. For the necessary evaluations of $|M_n^{(0)}\rangle$, $|M_n^{(1)}\rangle$ and their derivatives, we used the standard implementation of **Recola**, which is linked to **Collier** [163–165] for the reduction and evaluation of one-loop integrals. Since we evaluate $|M_{n+1}^{(1)}\rangle$ in infrared phase-space regions, a particularly numerically stable implementation is desirable. To this end, we instead linked **Recola** to **CutTools** [166] for the reduction and **OneLoop** [167, 168] for the evaluation of integrals at quadruple precision. A similar implementation is publicly available within the **ggxy** software package [169]. For the collinear regions, the necessary building blocks of $|\Delta M_{a_i, i}^{(0)}\rangle$ were by default calculated by direct implementation of Eqs. (3.79) and (3.80) into **avhlib** [170, 171]. The x dependence was obtained by means of numerical fitting. The correctness of the explicit representations of the ingredients of $|\Delta M_{a_i, i}^{(0)}\rangle$ described in Section 3.4.3 was confirmed with separate numerical tests. Finally, due to the appearance of flavor-off-diagonal contributions, appropriate sign factors had to be included to take into account conventions of different software packages.

The resulting numerical probes of $\Delta_{\text{LP/NLP}}$ are shown in Figs. 3.14–3.16 for different Born processes, containing both massive and massless (anti-)quarks, as well as gluons and uncolored

¹⁴To be specific, we work in the color-flow basis of color configurations introduced in Ref. [160].

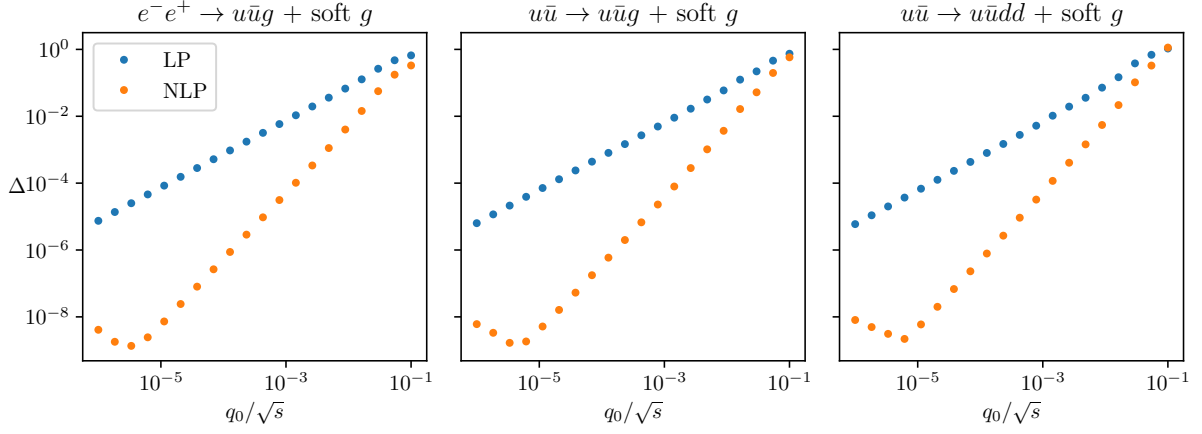


Figure 3.15: Description as in Fig. 3.14, except with massless partons. Taken instead from Ref. [1].

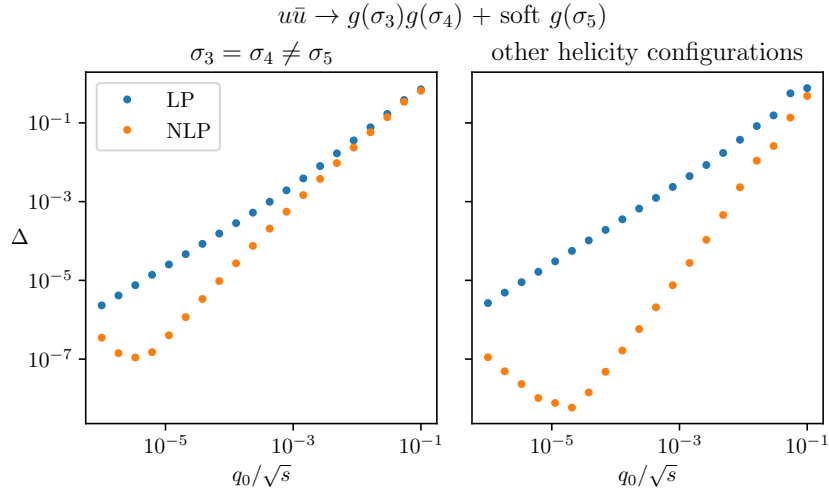


Figure 3.16: Description as in Fig. 3.15, for the case that two gluons are contained in the Born process. The helicity sum is divided into two parts as indicated in the figure titles.

particles. According to the soft expansion, one expects $\Delta_{\text{LP/NLP}}$ to behave as follows:

$$\Delta_{\text{LP}} = \left(c_0 + c_1 \log(\lambda) + c_2 \log(\lambda)^2 \right) \lambda + \mathcal{O}(\lambda^2), \quad (3.199)$$

$$\Delta_{\text{NLP}} = \left(d_0 + d_1 \log(\lambda) + d_2 \log(\lambda)^2 \right) \lambda^2 + \mathcal{O}(\lambda^3). \quad (3.200)$$

Indeed, we observe this behavior for all observed processes, indicating the correctness of our results. Additionally, we observe that there is a value of λ for which Δ_{NLP} stops getting smaller even if λ is further decreased. This can be explained by the numerical limitations when calculating $|M_{n+1}^{(1)}\rangle$ in infrared regions. For these phase-space regions, our NLP approximation exceeds the precision of our numerical implementation of the exact scattering amplitude, indicating that it could be used for numerical stabilization of cross-section calculations, as alluded to in the introduction when referring to Refs. [142, 143].

For the process

$$q(\sigma_1) + \bar{q}(\sigma_2) \rightarrow g(\sigma_3) + g(\sigma_4) + g(q, \sigma_5) \quad (3.201)$$

shown in Fig. 3.16, one sees that the improvement by going to NLP is less pronounced for a specific set of helicity configurations, even though it still agrees with the expectation from Eq. (3.200). As discussed in Ref. [1], this can be explained from the absence of soft logarithms through NLP for these helicities because the tree-level scattering amplitudes of

$$q(\sigma_1) + \bar{q}(\sigma_2) \rightarrow a_3(\sigma_3) + a_4(\sigma_4) \quad (3.202)$$

and

$$q(\sigma_1) + \bar{q}(\sigma_2) \rightarrow g(\sigma_3) + g(\sigma_4) + g(-\sigma_5) \quad (3.203)$$

vanish due to helicity conservation. Additionally, the flavor-off-diagonal jet operator vanishes for the same reason. Therefore, all contributions to Eq. (3.147) except for $\mathcal{S}_{\text{NLP}}^{(0)} |M_n^{(1)}\rangle$ are zero, and no logarithms $\log(\lambda)$ appear through NLP. Assuming that this changes starting from next-to-next-to-leading power (NNLP), one can expect such NNLP corrections to have a larger relative impact for these helicities, as observed in Fig. 3.16. In practical applications, when usually squared amplitudes summed over all helicities are relevant, this is not expected to cause a problem because the other helicity configurations dominate numerically, as one expects because they contain soft logarithms already at LP.

Chapter 4

Six-Point Amplitudes at One-Loop Order in QCD

After the theoretical study of the process-independent behavior of QCD amplitudes in the previous chapter, we discuss state-of-the-art techniques for the calculation of amplitudes for specific processes of interest. In particular, we discuss the calculation of an analytic expression for the amplitudes of the processes

$$0 \rightarrow \gamma(p_1, \sigma_1) + \gamma(p_2, \sigma_2) + g(p_3, \sigma_3, c_3) + g(p_4, \sigma_4, c_4) + q(p_5, \sigma_5, c_5) + \bar{q}(p_6, \sigma_6, c_6), \quad (4.1)$$

$$0 \rightarrow \gamma(p_1, \sigma_1) + \gamma(p_2, \sigma_2) + q'(p_3, \sigma_3, c_3) + \bar{q}'(p_4, \sigma_4, c_4) + q(p_5, \sigma_5, c_5) + \bar{q}(p_6, \sigma_6, c_6), \quad (4.2)$$

at one-loop order. The quark flavors q and q' may be equal or different. For brevity, we denote the amplitudes with the shorthand notations $M_g^{(L)} \equiv M_{0 \rightarrow \gamma\gamma gg q\bar{q}}^{(L)}$, $M_{q'}^{(L)} \equiv M_{0 \rightarrow \gamma\gamma q' \bar{q}' q\bar{q}}^{(L)}$ for $q' \neq q$, and $M_q^{(L)} \equiv M_{0 \rightarrow \gamma\gamma q \bar{q} q\bar{q}}^{(L)}$. $M_g^{(1)}$, $M_{q'}^{(1)}$, and $M_q^{(1)}$ are necessary to compute the double-real-single-virtual corrections to the cross section $\sigma_{pp \rightarrow \gamma\gamma}$, and are therefore necessary when this cross section is calculated at N³LO, the main phenomenological result of this thesis. While numerical tools for the calculation of arbitrary one-loop amplitudes are available, see e.g. the discussion in Section 3.4.6, we require an implementation with high efficiency and precision due to the usage of slicing methods, see Section 2.2 and Chapter 5. Obtaining such an implementation by using an analytic result is the main motivation of the calculation discussed in this chapter. While fully analytic results for six-point one-loop amplitudes have been published for the six-gluon case [172], no such results are available for our desired processes. In this chapter, we also review theoretical foundations for modern amplitude calculations, in particular those presented in Ref. [173]. Such state-of-the-art methods have also been applied at two-loop level, see Ref. [174] for a recent example. Still, the present discussion of a one-loop amplitude calculation is sufficient to understand the underlying concepts.

The calculation presented here has already been discussed in Ref. [3], where we have published the results of the N³LO calculation of $\sigma_{pp \rightarrow \gamma\gamma}$. However, the description in this chapter is much more detailed.¹

¹A note on the author's personal contribution to the amplitude-calculation part of Ref. [3]. While I have received supervision and had useful discussions with M. Czakon and R. Poncelet, the implementation and calculation presented here was fully performed by myself using the available literature to which we refer in this chapter when used.

4.1 Kinematics

Due to momentum conservation,

$$\sum_{i=1}^6 p_i = 0, \quad (4.3)$$

and on-shellness, $p_i^2 = 0$ for $i = 1, \dots, 6$, all scalar products $p_i \cdot p_j$ of two momenta can be written as functions of nine Mandelstam variables

$$\vec{s} = \{s_{12}, s_{23}, s_{34}, s_{45}, s_{56}, s_{61}, s_{123}, s_{234}, s_{345}\}, \quad (4.4)$$

with $s_{ij} = (p_i + p_j)^2$, $s_{ijk} = (p_i + p_j + p_k)^2$. In scattering amplitudes, there furthermore appears the parity-odd quantity

$$\text{tr}_5(1234) \equiv \text{tr}(\gamma_5 \not{p}_1 \not{p}_2 \not{p}_3 \not{p}_4) = 4i\epsilon_{\mu\nu\rho\sigma} p_1^\mu p_2^\nu p_3^\rho p_4^\sigma \equiv 4i\epsilon_{p_1 p_2 p_3 p_4}, \quad (4.5)$$

with $\gamma_5 \equiv i\gamma^0\gamma^1\gamma^2\gamma^3$. It can be expressed as a non-rational function of the Mandelstam variables via the following representation of the Levi-Civita tensor:

$$\epsilon^{\alpha\beta\gamma\delta} = \frac{-1}{\epsilon_{p_1 p_2 p_3 p_4}} \sum_{\sigma \in \Sigma_4} \text{sgn}(\sigma) p_{\sigma(1)}^\alpha p_{\sigma(2)}^\beta p_{\sigma(3)}^\gamma p_{\sigma(4)}^\delta, \quad (4.6)$$

where Σ_4 denotes all permutations of $\{1, 2, 3, 4\}$. Contraction with $p_\alpha p_\beta p_\gamma p_\delta$ leads to

$$(\text{tr}_5(1234))^2 = -16(\epsilon_{p_1 p_2 p_3 p_4})^2 = \det(\{s_{ij}\}_{i,j=1,\dots,4}) \equiv G_5(1234), \quad (4.7)$$

where $G_5(1234)$ is a *Gram determinant*. Finally, we can determine the sign of $\text{tr}_5(1234)$ by requiring that our convention, $\epsilon_{0123} = +1$ and therefore $\epsilon^{0123} = -1$, is fulfilled. Note that all other tr_5 quantities can be related to $\text{tr}_5(1234)$ via

$$\text{tr}_5(ijkl) = \frac{\text{tr}_5(ijkl) \text{tr}_5(1234)}{(\text{tr}_5(1234))^2} \text{tr}_5(1234), \quad (4.8)$$

where the prefactor is a rational function of the Mandelstam variables which can be obtained with Eq. (4.6). This, however, implies that choosing $\text{tr}_5(1234)$ as the variable to split a scattering amplitude into a parity-even and a parity-odd part, as commonly done for five-point amplitudes (see e.g. Ref. [68]), is an ad-hoc choice when working with six-point kinematics. Furthermore, the Gram determinant

$$\begin{aligned} G_6(12345) \equiv \det(\{s_{ij}\}_{i,j=1,\dots,5}) = & -2 \left[s_{12}^2 (-s_{45}) ((s_{23} - s_{234})(s_{61} - s_{234}) + s_{234}s_{45}) \right. \\ & + s_{12} (s_{123}(s_{61} - s_{234})(s_{23}(s_{345} - s_{34}) - s_{234}s_{345} + s_{34}s_{61}) - s_{123}s_{45}(s_{234}(-s_{234} + s_{34} - 2s_{345}) \\ & + s_{61}(s_{234} + s_{34})) - s_{56} (s_{45}(s_{23}(s_{234} - 2s_{34} + s_{345}) + s_{61}(-2s_{23} + s_{234} - 2s_{34}) + s_{234}s_{345}) \\ & + (s_{61} - s_{23})(s_{23}(s_{345} - s_{34}) - s_{234}s_{345} + s_{34}s_{61}) + s_{45}^2 (s_{34} - s_{234})) \\ & + s_{45} (s_{234}(-s_{23}(s_{34} + s_{345}) + s_{234}s_{345} - s_{234}s_{45} + s_{34}s_{45}) + s_{34}s_{61}(2s_{23} - s_{234}))) \\ & \left. - s_{123}^2 (-s_{234} + s_{34} - s_{345} + s_{61})(s_{34}s_{61} - s_{234}s_{345}) \right. \\ & \left. + s_{123}s_{56} (-s_{61}(s_{23}(s_{34} + s_{345}) + s_{234}(s_{345} - s_{45}) + s_{34}(s_{345} + s_{45})) \right) \end{aligned}$$

$$\begin{aligned}
& + s_{345}(s_{23}(2s_{234} - s_{34} + s_{345}) + s_{234}(s_{345} - s_{45}) + s_{34}s_{45}) + s_{34}s_{61}^2) \\
& - s_{123}(s_{34}s_{61} - s_{234}s_{345})(s_{23}(s_{345} - s_{34}) - s_{234}s_{345} + s_{234}s_{45} - s_{34}s_{45} + s_{34}s_{61}) \\
& + s_{23}\left(s_{345}\left(s_{56}(s_{23}(s_{34} - s_{345}) - s_{45}(s_{234} + s_{34}) + s_{234}s_{345}) - s_{56}^2(s_{23} + s_{345} - s_{45})\right.\right. \\
& \left.\left.+ s_{234}s_{34}s_{45}\right) - s_{61}(s_{34} - s_{56})(s_{34}s_{45} + s_{56}(s_{345} - s_{45}))\right)\Big] \tag{4.9}
\end{aligned}$$

vanishes in four dimensions, which leads to a highly non-trivial dependence between the Mandelstam variables (4.4). The ad-hoc choice of a tr_5 as well as potential hidden occurrences of G_6 imply that Mandelstam variables are no longer well-suited variables for helicity amplitudes if the number of external legs exceeds five.

A potential solution for massless kinematics is given by *momentum-twistor variables* [175], two possible explicit parameterizations for six-point kinematics can be found in Refs. [176, 177]. The eight variables (in contrast to nine Mandelstam variables) explicitly encode $G_6 = 0$ and rationalize tr_5 , eliminating the need for an additional parity-odd variable. However, since the parameterization is not unique, it is unclear whether there exists one that yields particularly compact amplitudes or how to identify it. Notably, Mandelstam variables are not polynomial but rather rational in the momentum twistors. This complicates the analysis of usually simple denominators of helicity amplitudes, as well as the potential to perform partial fractioning (see Section 4.5) to obtain more compact expressions.

Another approach is given by the *spinor-helicity formalism*. There, the basic variables, the *spinor brackets*, are not scalar products of momenta, but rather of massless Dirac bispinors:

$$\langle ij \rangle \equiv \langle i|j \rangle \equiv \bar{u}(p_i, -\tfrac{1}{2})u(p_j, +\tfrac{1}{2}), \quad [ij] \equiv [i|j] \equiv \bar{u}(p_i, +\tfrac{1}{2})u(p_j, -\tfrac{1}{2}). \tag{4.10}$$

The notation is natural when rewriting the definition in terms of the two-component Weyl spinors, defined in Section A.2, instead of Dirac bispinors:

$$\langle ij \rangle = \lambda_i^\alpha \lambda_{j\alpha}, \quad [ij] = \tilde{\lambda}_{i\dot{\alpha}} \tilde{\lambda}_j^{\dot{\alpha}}, \tag{4.11}$$

where we have used the notation $\lambda_i^\alpha \equiv \lambda^\alpha(p_i)$. Some basic properties are

$$\langle ij \rangle = -\langle ji \rangle, \quad [ij] = -[ji], \quad \langle ij \rangle^* = [ji]. \tag{4.12}$$

It is a convenient notation for fermion chains, e.g.

$$\bar{u}(p_i, -\tfrac{1}{2})\not{p}_k u(p_j, -\tfrac{1}{2}) = \langle ik \rangle [kj] \equiv \langle i|k|j]. \tag{4.13}$$

Sums appearing in fermion chains are written as

$$\langle i|k+l|j] \equiv \langle ik \rangle [kj] + \langle il \rangle [lj]. \tag{4.14}$$

Mandelstam variables can be expressed via

$$s_{ij} = \langle ij \rangle [ji], \tag{4.15}$$

which can be also applied to $s_{ijk} = s_{ij} + s_{ik} + s_{jk}$. When imagining spinor brackets as “square roots” of Mandelstam variables, it is not surprising that tr_5 becomes a simple polynomial in

spinor space:

$$\text{tr}_5(ijkl) = [ij] \langle jk \rangle [kl] \langle li \rangle - \langle ij \rangle [jk] \langle kl \rangle [li]. \quad (4.16)$$

Furthermore, with the *Schouten identity*,

$$\langle ij \rangle \langle kl \rangle + \langle ik \rangle \langle lj \rangle + \langle il \rangle \langle jk \rangle = 0, \quad (4.17)$$

and momentum conservation,

$$\sum_{k=1}^6 \langle i|k|j \rangle = 0, \quad (4.18)$$

$G_6 = 0$ holds analytically, as we show in Section 4.2. Spinor brackets therefore—like momentum twistors—solve the problems that appear when using Mandelstam variables. A downside compared to momentum twistors is that we move from eight independent variables to 30 variables which are related via Eqs. (4.17) and (4.18). On the other hand, variables correspond to the behavior of specific particles in an obvious way, in particular, their behavior in infrared limits are easy to understand. Furthermore, expressing amplitudes through spinor brackets leads to simple denominator factors and enables the partial-fractioning analysis described in Section 4.5. For the rest of this chapter, we therefore proceed to work with spinor brackets. A way to deal with the ambiguities posed by Schouten and momentum-conservation identities is described in Section 4.2.

4.2 The Polynomial Ring of Spinors

In this section, we briefly introduce the concepts of *polynomial rings*, *ideals*, *Gröbner bases*, and *quotient rings*. We follow Ref. [173], from where we also borrow the notation. For a thorough and pedagogical treatment, see also Ref. [178].

A *polynomial ring* over the field $\mathbb{F}$,

$$R \equiv \mathbb{F}[x_1, \dots, x_n], \quad (4.19)$$

is the set (together with the usual operations of addition and multiplication) of all polynomials in the variables $\{x_1, \dots, x_n\}$ with coefficients in the field $\mathbb{F}$. An example is the polynomial ring in all spinor brackets in the six-point phase-space of Section 4.1:

$$\mathcal{S}_6 \equiv \mathbb{F}[\langle 12 \rangle, \langle 13 \rangle, \dots, \langle 56 \rangle, [12], [13], \dots, [56]]. \quad (4.20)$$

For brevity, we introduce the vector containing all spinor brackets

$$\vec{b} \equiv \{\langle 12 \rangle, \langle 13 \rangle, \dots, \langle 56 \rangle, [12], [13], \dots, [56]\} \in \mathbb{F}^{30} \quad (4.21)$$

and write $\mathcal{S}_6 = \mathbb{F}[\vec{b}]$.

An *ideal* generated by $\{p_1, \dots, p_k\} \in R$ is a subset of the polynomial ring R and defined as

$$\langle p_1, \dots, p_k \rangle_R \equiv \left\{ \sum_{i=1}^k c_i p_i, \ c_i \in R \right\}. \quad (4.22)$$

Notice that any member of an ideal vanishes when all generators vanish. Examples are the subsets of $\mathcal{S}_6$ generated by momentum conservation and Schouten identities:

$$\mathcal{J}_{\Lambda_6} = \left\langle \sum_{j=1}^6 \langle ij \rangle [jk] : 1 \leq i \leq 6, 1 \leq k \leq 6 \right\rangle_{\mathcal{S}_6}, \quad (4.23)$$

$$\mathcal{K}_{\Lambda_6} = \langle \langle ij \rangle \langle kl \rangle + \langle ik \rangle \langle lj \rangle + \langle il \rangle \langle jk \rangle : 1 \leq i \leq j \leq k \leq l \leq 6 \rangle_{\mathcal{S}_6}, \quad (4.24)$$

$$\overline{\mathcal{K}}_{\Lambda_6} = \langle [ij][kl] + [ik][lj] + [il][jk] : 1 \leq i \leq j \leq k \leq l \leq 6 \rangle_{\mathcal{S}_6}. \quad (4.25)$$

There exist definitions of algebraic operations between ideals, for example the *ideal sum*,

$$\langle p_1, \dots, p_k \rangle_R + \langle q_1, \dots, q_l \rangle_R \equiv \langle p_1, \dots, p_k, q_1, \dots, q_l \rangle_R, \quad (4.26)$$

and the *ideal product*,

$$\langle p_1, \dots, p_k \rangle_R \langle q_1, \dots, q_l \rangle_R \equiv \langle p_i q_j : 1 \leq i \leq k, 1 \leq j \leq l \rangle_R. \quad (4.27)$$

Addition therefore enlarges ideals, whereas multiplication confines them:

$$J + K \supset J, K, \quad JK \subset J, K. \quad (4.28)$$

An example of an ideal sum is $\mathcal{J}_{\Lambda_6} + \mathcal{K}_{\Lambda_6} + \overline{\mathcal{K}}_{\Lambda_6}$, whose members vanish on all physical phase-space points due to relations between spinor brackets.

We now want to apply the concept of an ideal to calculations with polynomials. Any polynomial is a sum of monomials:

$$p = \sum_{\alpha \in \mathbb{Z}_{\geq 0}^n} c_{\alpha} \prod_{i=1}^n x_i^{\alpha_i} \equiv \sum_{\alpha \in \mathbb{Z}_{\geq 0}^n} c_{\alpha} \underline{x}^{\alpha} \in R = \mathbb{F}[x_1, \dots, x_n], \quad (4.29)$$

where we associate each monomial with a vector $\underline{\alpha}$ containing the powers to which the variables $\{x_1, \dots, x_n\}$ are raised. Using these vectors, one can check whether one monomial is a factor of another, which we denote by $|$ and $\nmid$, respectively:

$$\underline{x}^{\alpha} | \underline{x}^{\beta}, \quad \text{if } \alpha_i - \beta_i \geq 0 \quad \forall i, \quad \underline{x}^{\alpha} \nmid \underline{x}^{\beta}, \quad \text{otherwise.} \quad (4.30)$$

Furthermore, we can define a *monomial ordering* denoted by $\succeq$. We choose the *degree reverse lexicographic* ordering, defined as

$$\underline{x}^{\alpha} \succeq \underline{x}^{\beta} \iff |\underline{\alpha}|_1 > |\underline{\beta}|_1 \vee (|\underline{\alpha}|_1 = |\underline{\beta}|_1 \wedge \underline{\alpha} \geq^{\text{revlex}} \underline{\beta}), \quad (4.31)$$

where $|\underline{\alpha}|_1 = \sum_i \alpha_i$ denotes the 1-norm and $\underline{\alpha} \geq^{\text{revlex}} \underline{\beta}$ means that the *rightmost* non-zero element of $\underline{\alpha} - \underline{\beta}$ is *negative*. This choice usually leads to faster computations compared to other orderings. With a monomial order established, the *lead monomial* of a polynomial, $\text{LM}(p)$, is the monomial which is maximal with respect to $\succeq$. Given two polynomials p and h , we call p *reducible* by h if $\text{LM}(p) | \text{LM}(h)$, and *irreducible* otherwise.

With these definitions at hand, we can finally discuss the main computing method of this section, namely *polynomial reduction*. Reducing a polynomial p with respect to a set of polynomials $H = \{h_1, \dots, h_k\}$ means writing

$$p = q_1 h_1 + \dots + q_k h_k + \Delta_H(p), \quad (4.32)$$

where $\Delta_H(p)$ is called the *remainder* modulo H and is irreducible by any of the h_i . The importance of $\Delta_H(p)$ can be understood when thinking of H as generators of an ideal. In this case, if $\Delta_H(p) = 0$, p clearly belongs to the ideal. However, unfortunately, there are multiple sets of H all generating the same ideal, and they can all lead to different remainders. A solution is given by *Gröbner bases*. The *Gröbner basis* of an ideal J , $\mathcal{G}(J)$, can be computed from any set of generators and has the property that the remainder $\Delta_{\mathcal{G}(J)}$ is unique. In particular,

$$p \in J \iff \Delta_{\mathcal{G}(J)}(p) = 0. \quad (4.33)$$

We make no attempt to describe algorithms for polynomial reduction and Gröbner basis calculation in this work, however, they are implemented in many computer algebra systems.² One immediate application given the examples so far is to check if spinor expressions vanish due to momentum conservation and Schouten identities. Indeed, it is easy to check on a computer algebra system that the Gram determinant from Eq. (4.9) vanishes:

$$\Delta_{\mathcal{G}(\mathcal{J}_{\Lambda_6} + \mathcal{K}_{\Lambda_6} + \overline{\mathcal{K}}_{\Lambda_6})}(G_6(12345)) = 0. \quad (4.34)$$

Equipped with the ability to identify polynomials in $\mathcal{S}_6$ that belong to the ideal $\mathcal{J}_{\Lambda_6} + \mathcal{K}_{\Lambda_6} + \overline{\mathcal{K}}_{\Lambda_6}$ and therefore vanish due to Schouten or momentum-conservation identities, we can address the issue of dependent spinor brackets by defining an *equivalence class* of polynomials. We denote equivalence using $\sim$ and define for two polynomials $p, q \in \mathcal{S}_6$:

$$p \sim q \iff p - q \in \mathcal{J}_{\Lambda_6} + \mathcal{K}_{\Lambda_6} + \overline{\mathcal{K}}_{\Lambda_6}. \quad (4.35)$$

All equivalent polynomials $\{p_i\}$ share the same remainder $\Delta_{\mathcal{G}(\mathcal{J}_{\Lambda_6} + \mathcal{K}_{\Lambda_6} + \overline{\mathcal{K}}_{\Lambda_6})}(p_i)$, which we can hence choose as the *representative* of the equivalence class. The set of all independent representatives forms the *quotient ring*

$$\mathcal{R}_6 = \mathcal{S}_6 / (\mathcal{J}_{\Lambda_6} + \mathcal{K}_{\Lambda_6} + \overline{\mathcal{K}}_{\Lambda_6}). \quad (4.36)$$

The quotient ring is the basis for further calculations with ideals, that can for example be used to perform partial fractioning, as we will describe in Section 4.5.1.

4.3 Finite Fields

As we describe in Section 4.4, obtaining helicity amplitudes from Feynman diagrams requires many steps, all requiring algebraic manipulation increasing the size of the occurring expressions. It turns out that usually, the final helicity amplitude can be simplified to a form orders of magnitude smaller than the intermediate expressions. This *intermediate expression swell* makes a complete analytic calculation of the amplitude computationally prohibitive. An alternative is to perform the computation steps numerically. This can still yield an analytic result given two conditions:

²For example, given a set of variables $\mathbf{r}$ that define a polynomial ring and list of generators $\mathbf{g}$ of an ideal, **Mathematica** can calculate the Gröbner basis of said ideal with `gb = GroebnerBasis[g,r]`. The polynomial reduction of a polynomial $\mathbf{p}$ can then be performed using `PolynomialReduce[p,gb,r]`. Both functions can be given the option `MonomialOrder -> DegreeReverseLexicographic` for usually faster computation—it is however important to use a consistent monomial order for all operations.

1. There exists an ansatz for the solution, with only numerical coefficients to be fixed (e.g. it is known that the solution is a polynomial in the spinor-helicity variables with mass dimension 4).
2. The numerical computation is exact, i.e. without precision loss.

This way, the unknown numerical coefficients in the ansatz can be determined by running the numerical computation with several random values for the variables (in the case of spinor-helicity variables, for random phase-space points). If the number of numerical probes is the same as that of unknown coefficients, the latter can be inferred by solving the numerical system of equations. The first condition, getting a correct ansatz for the desired helicity amplitude, is discussed in Section 4.5. This section focuses on the second part, performing computations on a computer without precision loss. An obvious idea is the usage of rational numbers throughout, this can however also suffer from the intermediate expression swell, since their size is not bounded and more complicated expressions lead to larger integers in numerator and denominator.

An alternative is given by *finite fields*. They are standard tools in computer algebra, and a pedagogical introduction can for example be found in Ref. [179]. Here, we will quickly review the main concepts which are needed for this thesis. A finite field $\mathbb{F}_p$ characterized by the prime number p contains all non-negative integers up to $p - 1$. It is therefore bounded, and the upper bound can be chosen in any way, in particular such that the size of its elements is restricted to machine-sized integers. Like rational numbers (but unlike integers), finite fields form a field, i.e. they are closed not just under addition and multiplication, but also under subtraction and division. Of course, the four basic arithmetic operations have to be adapted to accommodate these conditions. For addition, subtraction, and multiplication, one can simply reuse the standard rules for integers, and if the result lies outside the allowed range, map back to $[0, p - 1]$ by applying the modulo operation. For example, in $\mathbb{F}_{11}$ there is

$$4 + 9 = 13 \bmod 11 = 2, \quad 3 - 5 = -2 \bmod 11 = 9, \quad 3 \times 8 = 24 \bmod 11 = 2. \quad (4.37)$$

Division can be defined as multiplication by the multiplicative inverse, where the (unique) multiplicative inverse a^{-1} of a number a is defined by $a \times a^{-1} = 1$. a^{-1} can be found either by trying out all numbers in $\mathbb{F}_p$ (brute force) or by using algorithms like the *Extended Euclidean Algorithm* (EEA), described e.g. in Ref. [179]. The EEA takes two integers a, b as input, calculates their greatest common divisor (gcd) and returns x, y such that

$$ax + by = \gcd(a, b). \quad (4.38)$$

It proceeds by iterating over integer triplets $\{x_i, y_i, r_i\}$ which all fulfill

$$ax_i + by_i = r_i \quad (4.39)$$

using the following prescription:

$$\begin{pmatrix} x_0 \\ y_0 \\ r_0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ a \end{pmatrix}, \quad \begin{pmatrix} x_1 \\ y_1 \\ r_1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ b \end{pmatrix}, \quad \begin{pmatrix} x_{i+1} \\ y_{i+1} \\ r_{i+1} \end{pmatrix} = \begin{pmatrix} x_{i-1} \\ y_{i-1} \\ r_{i-1} \end{pmatrix} - q_i \begin{pmatrix} x_i \\ y_i \\ r_i \end{pmatrix}, \quad \text{where } q_i = \left\lfloor \frac{r_{i-1}}{r_i} \right\rfloor. \quad (4.40)$$

When $r_{n+1} = 0$, there is $r_n = \gcd(a, b)$ and we have found a solution for Eq. (4.38) by setting $x = x_n$, $y = y_n$. This algorithm can be used to find the multiplicative inverse of a in $\mathbb{F}_p$ by

setting $b = p$ because $\gcd(a, p) = 1$ for any prime number p and therefore

$$ax + py = 1 \implies ax \bmod p = 1 \implies x = a^{-1} \text{ in } \mathbb{F}_p. \quad (4.41)$$

Having defined the division operation, we can generalize the modulo operator as a map from rational numbers to a finite field. That is, we write e.g. $1/3 \bmod 11 = 4$.

It is important to note that besides the basic operations just discussed, other operations like square roots, logarithms, etc. cannot be implemented as exact operation within finite fields. The numerical implementation can therefore only contain the former. The desired analytic expressions in our application, one-loop scattering amplitudes, however contain square roots and (di-)logarithms. It is thus necessary to list all non-rational functions that can appear and build a numerical workflow that returns not a single number but a vector of numbers which are the coefficients of these non-rational functions. Each element of the vector corresponds to a rational function in the input variables, which can be reconstructed with finite fields. A detailed description of the decomposition into rational and non-rational parts is given in Section 4.4.

If we implement the whole workflow using finite-field arithmetic, solving the numerical system of equations leads to an analytic solution where all numbers are elements of the finite field. For the correct solution, we need to map back from $\mathbb{F}_p$ to the rational numbers $\mathbb{Q}$. Of course, the relation between the two fields cannot be one-to-one since $\mathbb{F}_p$ is finite whereas $\mathbb{Q}$ is infinite. For example, the numbers 6, -5 , and $1/2$ all map to 6 in $\mathbb{F}_{11}$. In general, a valid reconstruction $r/s \in \mathbb{Q}$ of a finite-field number $a \in \mathbb{F}_p$ has to fulfill $r/s \bmod p = a$, or there has to exist a $y \in \mathbb{Z}$ such that $as + py = r$. This is exactly the equation that is solved by all steps in the EEA from Eq. (4.40) if we set $b = p$, $x_i = s$, $y_i = y$, $r_i = r$. Hence, all r_i/x_i for which $x_i \neq 0$ are valid reconstructions of a . Furthermore, it was noticed in Refs. [180, 181] that if for the smallest i for which $r_i < \sqrt{p/2}$ there is also $|x_i| < \sqrt{p/2}$, then r_i/x_i is the unique reconstruction of a for which both numerator and denominator are smaller than $\sqrt{p/2}$. If $|x_i| > \sqrt{p/2}$, no such reconstruction exists. In any case, we can use $r/s = r_i/x_i$ obtained in this way as a guess for the rational coefficient. The correctness of such a guess can always be checked by a numerical probe on a different prime field $\mathbb{F}_{p'}$.

We are now able to guess a rational solution given a solution on finite fields and test if this solution is correct. However, if the correct rational coefficient r/s consists of integers too large for $2r^2$ or $2s^2$ to be saved as machine-sized integers, we can never make the correct guess for r/s while retaining the computational efficiency of finite fields. Luckily, we can make use of the *Chinese Remainder Theorem*, known in number theory for a very long time and described for example in Ref. [179]. It allows, given finite-field values $a_1, a_2, \dots, a_n$ on multiple prime fields $\mathbb{F}_{p_1}, \mathbb{F}_{p_2}, \dots, \mathbb{F}_{p_n}$ corresponding to the same rational number r/s , to calculate $a = (r/s \bmod p) \in \mathbb{F}_p$, where $p = p_1 p_2 \dots p_n$. For each p_i , we define the two integers $P_i \equiv p/p_i$ and its multiplicative inverse on $\mathbb{F}_{p_i}$, $Q_i = 1/P_i \bmod p_i$, which can be calculated with the EEA from Eq. (4.40). Then, a can be calculated as

$$a = \sum_{i=1}^n a_i P_i Q_i. \quad (4.42)$$

In summary, with the two tools reviewed in this section, the Extended Euclidean Algorithm and the Chinese Remainder Theorem, it is possible to reconstruct any rational number given probes on sufficiently many prime fields $\mathbb{F}_p$. The usage of finite fields for calculations in quantum field theory was proposed in Ref. [182], and since then multiple public software tools accommodating calculations within finite fields have been published, including **FiniteFlow** [183]

and **FireFly** [184, 185]. For details on how we implement finite fields in our calculation, see Section 4.4.5.

4.4 From Feynman diagrams to Helicity Amplitudes

In this section, we describe the necessary steps to obtain an analytic expression for the one-loop amplitude of the process (4.1). In Sections 4.4.1–4.4.4, we introduce the methods that in principle enable a complete calculation of the amplitude. However, as alluded to in Section 4.3, applying all these methods analytically is computationally too expensive and some have to be implemented in a numerical framework using finite-field arithmetic. Therefore, in Section 4.4.5, we will describe which parts of the calculation are performed analytically and which numerically, and how we implement the methods into a practical software tool chain. While there exists the public software **Caravel** [186] for numerical amplitude computations with finite-field arithmetic, it does not allow for six-point kinematics necessary for our calculation.

4.4.1 Amplitude Structure

The first step in an amplitude calculation is to generate all possible diagrams and substitute the Feynman rules. The Feynman rules relevant for our processes are summarized in Appendix A.1. We do not include any massive quarks in the calculation. Furthermore, we work in dimensional regularization with all loop momenta having space-time dimension $d = 4 - 2\epsilon$. The first simplification can be made by treating the color structure with the Cvitanovic algorithm [187]. For our processes, the scattering amplitudes can be decomposed as

$$\begin{aligned} M_g^{(L)}(c_3, \dots, c_6) &= (T^{c_3} T^{c_4})_{c_5 c_6} \mathcal{A}_{g,34}^{(L)} + (T^{c_4} T^{c_3})_{c_5 c_6} \mathcal{A}_{g,43}^{(L)} + \delta^{c_3 c_4} \delta_{c_5 c_6} \mathcal{A}_{g,\delta}^{(L)}, \\ M_{q'}^{(L)}(c_3, \dots, c_6) &= \delta_{c_3 c_4} \delta_{c_5 c_6} \mathcal{A}_{q',\delta_1}^{(L)} + \delta_{c_3 c_6} \delta_{c_4 c_5} \mathcal{A}_{q',\delta_2}^{(L)}, \\ M_q^{(L)}(c_3, \dots, c_6) &= \delta_{c_3 c_4} \delta_{c_5 c_6} \mathcal{A}_{q,\delta_1}^{(L)} + \delta_{c_3 c_6} \delta_{c_4 c_5} \mathcal{A}_{q,\delta_2}^{(L)}, \end{aligned} \quad (4.43)$$

where the notation is inspired by Ref. [68] and we have suppressed the momentum and helicity dependence for brevity. Note that due to Bose symmetry, $\mathcal{A}_{g,34}^{(L)}$ and $\mathcal{A}_{g,43}^{(L)}$ are not independent:

$$\mathcal{A}_{g,43}^{(L)} = \mathcal{A}_{g,34}^{(L)} \Big|_{p_3 \leftrightarrow p_4, \sigma_3 \leftrightarrow \sigma_4}. \quad (4.44)$$

In practical applications, where the squared amplitude $|M|^2$ is expanded in α_s , the relevant quantity is the interference term $2 \operatorname{Re}([M^{(0)}]^* M^{(1)})$ summed over color and helicity. Substituting $\mathcal{A}_{g,\delta}^{(0)} = 0$, there is

$$\begin{aligned} \sum_{\text{color}} [M_g^{(0)}]^* M_g^{(1)} &= \frac{(N_c^2 - 1)^2}{4N_c} \left([\mathcal{A}_{g,34}^{(0)}]^* \mathcal{A}_{g,34}^{(1)} + [\mathcal{A}_{g,43}^{(0)}]^* \mathcal{A}_{g,43}^{(1)} \right) \\ &\quad - \frac{N_c^2 - 1}{4N_c} \left([\mathcal{A}_{g,34}^{(0)}]^* \mathcal{A}_{g,43}^{(1)} + [\mathcal{A}_{g,43}^{(0)}]^* \mathcal{A}_{g,34}^{(1)} \right) + \frac{N_c^2 - 1}{2} \left([\mathcal{A}_{g,34}^{(0)}]^* + [\mathcal{A}_{g,43}^{(0)}]^* \right) \mathcal{A}_{g,\delta}^{(1)} \end{aligned} \quad (4.45)$$

in the gluon case and

$$\begin{aligned} \sum_{\text{color}} [M_{q'}^{(0)}]^* M_{q'}^{(1)} &= N_c^2 \left([\mathcal{A}_{q',\delta_1}^{(0)}]^* \mathcal{A}_{q',\delta_1}^{(1)} + [\mathcal{A}_{q',\delta_2}^{(0)}]^* \mathcal{A}_{q',\delta_2}^{(1)} \right) \\ &\quad + N_c \left([\mathcal{A}_{q',\delta_1}^{(0)}]^* \mathcal{A}_{q',\delta_2}^{(1)} + [\mathcal{A}_{q',\delta_2}^{(0)}]^* \mathcal{A}_{q',\delta_1}^{(1)} \right) \end{aligned} \quad (4.46)$$

for the quark case, with the identical formula for $M_{q'}^{(L)} \mapsto M_q^{(L)}$. Besides color indices, the amplitudes depend on the external quark charges Q_q and $Q_{q'}$ as well as the sum over the charges Q_l of all quarks that can run in loops. Furthermore, it depends on the number of colors N_c and the number of massless fermions which can run in loops, n_f . While we can for our applications set them to the fixed values

$$Q_q = \begin{cases} \frac{2}{3}, & q \in \{u, c\}, \\ -\frac{1}{3}, & q \in \{d, s, b\}, \end{cases} \quad \sum_l Q_l = \frac{1}{3}, \quad \sum_l Q_l^2 = \frac{11}{9}, \quad N_c = 3, \quad n_f = 5, \quad (4.47)$$

they are from the theory point of view free parameters that could take any values. We can therefore decompose the amplitude by the dependence on them, where each term is a well-defined, gauge-invariant quantity. Specifically, for our processes, the decompositions read at tree level

$$\mathcal{A}_{g,34}^{(0)} = Q_q^2 A_{g,34}^{(0)}, \quad (4.48)$$

$$\mathcal{A}_{q',\delta_1}^{(0)} = \frac{1}{N_c} \left(Q_q^2 A_{q',\delta_1;qq}^{(0)} + Q_q Q_{q'} A_{q',\delta_1;qq'}^{(0)} + Q_{q'}^2 A_{q',\delta_1;q'q'}^{(0)} \right), \quad \mathcal{A}_{q',\delta_2}^{(0)} = -N_c \mathcal{A}_{q',\delta_1}^{(0)}. \quad (4.49)$$

For the one-loop amplitudes, there is

$$\mathcal{A}_{g,34}^{(1)} = Q_q^2 \left(N_c A_{g,34;qq}^{(1),N_c} + \frac{1}{N_c} A_{g,34;qq}^{(1),1/N_c} + n_f A_{g,34;qq}^{(1),n_f} \right) + Q_q \left(\sum_l Q_l \right) A_{g,34;ql}^{(1)} + \left(\sum_l Q_l^2 \right) A_{g,34;ll}^{(1)}, \quad (4.50)$$

$$\mathcal{A}_{g,\delta}^{(1)} = Q_q^2 A_{g,\delta;qq}^{(1)} + Q_q \left(\sum_l Q_l \right) \frac{1}{N_c} A_{g,\delta;ql}^{(1)}, \quad (4.51)$$

for M_g and

$$\mathcal{A}_{q',\delta_1}^{(1)} = A_{q',\delta_1}^{(1)} + \frac{1}{N_c^2} A_{q',\delta_1}^{(1),1/N_c^2} + \frac{n_f}{N_c} A_{q',\delta_1}^{(1),n_f/N_c} + \left(\sum_l Q_l^2 \right) \frac{1}{N_c} A_{q',\delta_1;ll}^{(1)}, \quad (4.52)$$

$$\mathcal{A}_{q',\delta_2}^{(1)} = N_c A_{q',\delta_2}^{(1),N_c} + \frac{1}{N_c} A_{q',\delta_2}^{(1),1/N_c} + n_f A_{q',\delta_2}^{(1),n_f} + \left(\sum_l Q_l^2 \right) A_{q',\delta_2;ll}^{(1)} \quad (4.53)$$

for $M_{q'}$, where the coefficients have the additional charge decomposition

$$A_{q',\delta_i}^{(1),c} = Q_q^2 A_{q',\delta_i;qq}^{(1),c} + Q_q Q_{q'} A_{q',\delta_i;qq'}^{(1),c} + Q_{q'}^2 A_{q',\delta_i;q'q'}^{(1),c}. \quad (4.54)$$

To all loop orders, the coefficients needed for M_q can be obtained from those in $M_{q'}$ as follows:

$$\mathcal{A}_{q,\delta_1}^{(L)} = \left(\mathcal{A}_{q',\delta_1}^{(L)} - N_c \mathcal{A}_{q',\delta_2}^{(L)} \Big|_{p_3 \leftrightarrow p_5, \sigma_3 \leftrightarrow \sigma_5} \right) \Big|_{Q_{q'} \mapsto Q_q}, \quad (4.55)$$

$$\mathcal{A}_{q,\delta_2}^{(L)} = \left(\mathcal{A}_{q',\delta_2}^{(L)} - \frac{1}{N_c} \mathcal{A}_{q',\delta_1}^{(L)} \Big|_{p_3 \leftrightarrow p_5, \sigma_3 \leftrightarrow \sigma_5} \right) \Big|_{Q_{q'} \mapsto Q_q}. \quad (4.56)$$

We call the gauge-invariant coefficients, $\mathcal{A}_{g,34}^{(0)}$ etc., *partial amplitudes*. Calculating these partial amplitudes for all helicity configurations is the objective of this chapter. In principle, one might expect that one has to perform the calculation for $2^6 = 64$ different helicities. However, the amplitude vanishes unless the fermions have opposite helicity, $\sigma_6 = -\sigma_5$ for M_g and additionally

$\sigma_4 = -\sigma_3$ for $M_{q'}$. Furthermore, we can relate helicities via symmetry under exchange of the two photons or the two gluons, via charge conjugation of the fermions, and via parity. Finally, since for practical applications we only need the interference between the one-loop and the tree-level amplitude, it is not necessary to calculate the amplitude for the case of more than four particles having equal helicity. This is due to the fact that at tree level, a *maximally helicity-violating (MHV) amplitude* needs two particles to differ in helicity. In summary, it suffices to calculate the partial amplitudes for the helicity configurations

$$+ - + - + -, \quad + - + + + -, \quad + + + - + -, \quad + + - - + -, \quad \text{for } M_g, \quad (4.57)$$

$$+ - + - + -, \quad + - - + + -, \quad + + + - + -, \quad + + - + + -, \quad \text{for } M_{q'}, \quad (4.58)$$

where we label a configuration simply by the sign of the six helicities $\sigma_1, \dots, \sigma_6$. For fixed helicity, the partial amplitudes depend on nothing but the external momenta and the dimensional regulator ϵ , and if we do not refer to a specific partial amplitude, we simply denote them as $A(\{p_i\}_{i=1,\dots,6}, \epsilon)$. As explained in Section 4.3, we divide each partial amplitude into rational functions of the spinor brackets and non-rational functions of the Mandelstam variables. For this, we write $A(\{p_i\}_{i=1,\dots,6}, \epsilon)$ as a Laurent series in ϵ and consider each order separately. In the end, the ϵ poles of the bare amplitude are subtracted and powers in ϵ larger than zero irrelevant. We are therefore only interested in the ϵ^0 part of the amplitude and write

$$A(\{p_i\}_{i=1,\dots,6}) \equiv A(\{p_i\}_{i=1,\dots,6}, \epsilon)|_{\epsilon^0} \equiv \sum_i C_i(\vec{b}) \times F_i(\vec{s}). \quad (4.59)$$

Hereafter, we will use the term partial amplitude to only refer to this ϵ^0 part of the amplitude, since only this is relevant to us. Finally, to refer to the rational coefficient belonging to a specific function, we will use the notation

$$C[F_i](\vec{b}) \equiv C_i(\vec{b}). \quad (4.60)$$

The list of occurring functions F_i is given in Section 4.4.4.

4.4.2 Projection to Helicity Amplitudes

After applying Feynman rules to all diagrams, the loop momentum l^μ appears oftentimes in a form different from standard propagators $((l + P)^2)^n$, which are however required to map all appearing integrals to a basis of *master integrals* using *integration-by-parts identities* (see Section 4.4.3). If l^μ is contracted with an ordinary momentum, it can be easily mapped to standard propagators using relations in the form of

$$l \cdot p_1 = \frac{1}{2} \left((l + p_1)^2 - l^2 \right), \quad l \cdot p_2 = \frac{1}{2} \left((l + p_1 + p_2)^2 - (l + p_1)^2 - s_{12} \right), \quad \dots \quad (4.61)$$

This, however, does not work if l^μ is contracted with a polarization vector $\varepsilon^{*\mu}(p_i)$ or a Dirac matrix γ^μ . A possibility to treat numerators of the form l^μ at one-loop order is given by *Passarino-Veltman reduction* [156], which we discuss in a different context in Section 3.4.2. This method, however, does not generalize beyond one loop, and our objective is to build a tool chain which is easily extendable to higher loop orders. Instead, we replace all external wave functions by projectors depending only on the external momenta. They should directly project onto the desired helicity amplitudes (and therefore depend on the helicities of the particles), and retain d -dimensionality in order to not lose the ϵ -dimensional part of the loop momentum. Such

a d -dimensional projection method was proposed in Ref. [188], and we describe how to apply this method specifically to our amplitude in the remainder of this section.

Starting with the polarization vectors, we deal with them by substituting them in the following way:

$$\varepsilon_{\sigma_1}^{*\mu}(p_1) \mapsto T_{1,\sigma_1}^\mu, \quad \varepsilon_{\sigma_2}^{*\mu}(p_2) \mapsto T_{1,-\sigma_2}^\mu, \quad \varepsilon_{\sigma_3}^{*\mu}(p_3) \mapsto T_{3,\sigma_3}^\mu, \quad \varepsilon_{\sigma_4}^{*\mu}(p_4) \mapsto T_{3,-\sigma_4}^\mu, \quad (4.62)$$

where

$$\begin{aligned} T_{1,\sigma_1}^\mu &\equiv s_{23} \left[1 + \frac{\sigma_1}{\text{tr}_5} (s_{12}s_{34} + s_{13}s_{24} - s_{14}s_{23}) \right] p_1^\mu + s_{13} \left[1 + \frac{\sigma_1}{\text{tr}_5} (s_{12}s_{34} - s_{13}s_{24} + s_{14}s_{23}) \right] p_2^\mu \\ &\quad - s_{12} \left[1 - \frac{\sigma_1}{\text{tr}_5} (-s_{12}s_{34} + s_{13}s_{24} + s_{14}s_{23}) \right] p_3^\mu - \left[\frac{\sigma_1}{\text{tr}_5} 2s_{12}s_{13}s_{23} \right] p_4^\mu, \end{aligned} \quad (4.63)$$

$$T_{3,\sigma_3}^\mu \equiv T_{1,\sigma_1}^\mu \Big|_{(1 \leftrightarrow 3), (2 \leftrightarrow 4)}, \quad (4.64)$$

with $\text{tr}_5 \equiv \text{tr}_5(1234)$ defined in Eq. (4.8). Of course, we only use T_{1,σ_1}^μ in the case of $M_{q'}$ because particles 3 and 4 are quarks. For any expression only depending on the four-dimensional external momenta, these projectors can be related to the four-dimensional spinor-helicity representation of polarization vectors,

$$\varepsilon_{\text{SH},+1}^{*\mu}(p, q) = \frac{[p|\gamma^\mu|q\rangle}{\sqrt{2}\langle qp\rangle}, \quad \varepsilon_{\text{SH},-1}^{*\mu}(p, q) = -\frac{\langle p|\gamma^\mu|q\rangle}{\sqrt{2}[qp]}, \quad (4.65)$$

in the following way:

$$\begin{aligned} \varepsilon_{\text{SH},\sigma_1}^{*\mu}(p_1, p_2) \varepsilon_{\text{SH},\sigma_2}^{*\mu}(p_2, p_1) \varepsilon_{\text{SH},\sigma_3}^{*\mu}(p_3, p_4) \varepsilon_{\text{SH},\sigma_4}^{*\mu}(p_4, p_3) M_{\mu\nu\rho\sigma}(\{p_i\}_{i=1,\dots,6}) \\ = \frac{\phi_{12}(\sigma_1, \sigma_2) \phi_{34}(\sigma_3, \sigma_4)}{\mathcal{N}_{12}\mathcal{N}_{34}} T_{1,\sigma_1}^\mu T_{1,-\sigma_2}^\nu T_{3,\sigma_3}^\rho T_{4,\sigma_4}^\sigma M_{\mu\nu\rho\sigma}(\{p_i\}_{i=1,\dots,6}), \end{aligned} \quad (4.66)$$

with the normalization factors

$$\mathcal{N}_{12} = 2s_{12}s_{13}s_{23}, \quad \mathcal{N}_{34} = 2s_{13}s_{14}s_{34} \quad (4.67)$$

and the phase factors

$$\phi_{12}(+1, +1) = \frac{[12]}{\langle 12 \rangle}, \quad \phi_{12}(+1, -1) = -\frac{[1|3|2]}{\langle 1|3|2 \rangle}, \quad \phi_{34}(\sigma_3, \sigma_4) = \phi_{12}(\sigma_1, \sigma_2) \Big|_{(1 \leftrightarrow 3), (2 \leftrightarrow 4)}, \quad (4.68)$$

with the phase factors for other helicity configurations related by parity transformation. This normalization difference can simply be accounted for by appropriate multiplication at the end of our tool chain. As long as a consistent definition is used for tree-level and one-loop amplitude, one in principle does not have to include the phase factors, however, the results in terms of spinor brackets take particularly simple forms if they are included.

For fermions, let us first consider M_g for simplicity, since it only contains one fermion chain connected to external legs. In this case, our partial amplitudes take the form

$$A = \bar{u}(p_5, \sigma_5) \Gamma v(p_6, \sigma_6), \quad (4.69)$$

which vanishes unless $\sigma_6 = -\sigma_5$. This can be rewritten as the trace of a projector operating on Γ , where we furthermore suppress the arguments of $\bar{u}$ and v for brevity:

$$A = \bar{u}_a \Gamma_{ab} v_b = \text{Tr}[(v \otimes \bar{u}) \Gamma] \equiv \text{Tr}[T_{56, \sigma_5} \Gamma]. \quad (4.70)$$

The projector can be expressed through external momenta by using

$$\begin{aligned} T_{56, \sigma_5} &= \frac{\bar{v} N u}{\bar{v} N u} v \otimes \bar{u} = \frac{1}{\bar{v} N u} (v \otimes \bar{v}) N (u \otimes \bar{u}) = \frac{1}{\bar{v} N u} \frac{1 + \sigma_5 \gamma_5}{2} \not{p}_6 N \not{p}_5 \frac{1 - \sigma_5 \gamma_5}{2} \\ &= \frac{1}{\bar{v} N u} \frac{1}{2} [\not{p}_6 N \not{p}_5 - \sigma_5 \not{p}_6 \gamma_5 N \not{p}_5], \end{aligned} \quad (4.71)$$

where we used the standard identities $\{\gamma_5, \gamma^\mu\} = 0$ and $\gamma_5^2 = 1$. N can be chosen arbitrarily as long as $\bar{v} N u \neq 0$. We choose $N = \not{p}_1$ and use the identity

$$\gamma_5 \not{p}_1 = -\frac{i}{6} \epsilon_{\mu\nu\rho\sigma} \gamma^\mu \gamma^\nu \gamma^\rho p_1^\sigma \quad (4.72)$$

together with the representation (4.6) to obtain

$$T_{56, \sigma_5} = \frac{1}{\bar{v} \not{p}_1 u} \frac{1}{2} \not{p}_6 \left[\not{p}_1 - \frac{2}{3} \frac{\sigma_5}{\text{tr}_5} \sum_{\sigma \in \Sigma_4} \text{sgn}(\sigma) \not{p}_{\sigma(1)} \not{p}_{\sigma(2)} \not{p}_{\sigma(3)} (p_1 \cdot p_{\sigma(4)}) \right] \not{p}_5. \quad (4.73)$$

Due to the trace appearing in Eq. (4.70), we can thus eliminate all Dirac matrices to achieve that the loop momentum in the numerator is always contracted either with itself or external momenta, so that we can apply Eq. (4.61). The normalization is again a simple factor of spinor brackets,

$$\bar{v}(p_6, +\frac{1}{2}) \not{p}_1 u(p_5, -\frac{1}{2}) = -\bar{u}(p_6, -\frac{1}{2}) \not{p}_1 u(p_5, -\frac{1}{2}) = \langle 61 \rangle [15], \quad (4.74)$$

and analogously for flipped helicities. For the calculation of $M_{q'}$, we simply use the additional projector

$$T_{34, \sigma_3} = T_{56, \sigma_5} \big|_{p_5 \rightarrow p_3, p_6 \rightarrow p_4, \sigma_5 \rightarrow \sigma_3} \quad (4.75)$$

for the second fermion line.

4.4.3 Integration-by-Parts Identities

With the methods of Section 4.4.2, we are able to bring all loop integrals into the form

$$I^{(d_0)}(\vec{P}, \vec{n}) \equiv \int d^{d_0-2\epsilon} l \frac{1}{\prod_i ((l + P_i)^2)^{n_i}}, \quad (4.76)$$

where P_i are linear combinations of the external momenta and n_i can be positive or negative integers. To be specific, in our case all integrals belong to the *hexagon integral family*, that is the propagators only contain

$$\vec{P}_6 = \{P_1, \dots, P_6\} = \{0, p_1, p_1 + p_2, \dots, p_1 + p_2 + p_3 + p_4 + p_5\} \quad (4.77)$$

and P_i related by permutation of the external momenta. All occurring integrals are therefore characterized by a member of the permutation group Σ_6 and $\vec{n}_6 = \{n_1, \dots, n_6\}$. For the moment, let us focus on the non-permuted integrals and denote them by $I^{(d_0)}(n_1, n_2, n_3, n_4, n_5, n_6) \equiv I^{(d_0)}(\vec{P}_6, \vec{n}_6)$. In fact, this set of integrals is closed under all *cyclic* permutations of external

momenta, and only members of Σ_6 which are not related by cyclic permutation have to be considered. Alternatively, one can always eliminate p_6 by momentum conservation and restrict the permutations to members of Σ_5 .

It turns out that not all integrals are independent but can be related by *integration-by-parts (IBP) identities* of the form

$$0 = \int d^d l \frac{\partial}{\partial l^\mu} \left[\frac{N_j^\mu}{\prod_i ((l + P_i)^2)^{n_i}} \right], \quad (4.78)$$

where $N_j^\mu \in \{l^\mu, p_1^\mu, \dots, p_5^\mu\}$. Depending on the vectors $\vec{n}$ which one inserts into Eq. (4.78), one gets a system of equations containing different integrals. It turns out that by including more $\vec{n}$, the number of identities grows faster than the number of unknown integrals and one therefore reaches a solvable system of equations. The remaining independent integrals are called *master integrals*. Denoting master integrals as MB_i , the IBP identities arising from the solution of the system of equations then take the form

$$I^{(d_0)}(n_1, n_2, n_3, n_4, n_5, n_6) = \sum_i c_i(\{p_i\}_{i=1}^6, \epsilon) \times \text{MB}_i. \quad (4.79)$$

An algorithm to choose the appropriate vectors $\vec{n}$ given a number of integrals that one wishes to reduce is given by the *Laporta algorithm* [189]. An improved version of this algorithm is implemented in the software package **Kira** [157, 158].

4.4.4 Master Integrals

We choose the basis of master integrals used in Ref. [176] up to modifications of prefactors. To be specific, following the notation from Section 4.4.3, our basis contains

- the six cyclic permutations of

$$\frac{1}{s_{12}(3-2\epsilon)(2-2\epsilon)\epsilon} I^{(4)}(1, 0, 1, 0, 0, 0), \quad (4.80)$$

- the three cyclic permutations of

$$\frac{1}{s_{123}(3-2\epsilon)(2-2\epsilon)\epsilon} I^{(4)}(1, 0, 0, 1, 0, 0), \quad (4.81)$$

- the two cyclic permutations of

$$\frac{1}{(3-2\epsilon)(2-2\epsilon)(1-2\epsilon)} I^{(4)}(1, 0, 1, 0, 1, 0), \quad (4.82)$$

- the six cyclic permutations of

$$\frac{1}{(3-2\epsilon)(1-2\epsilon)} I^{(4)}(1, 1, 1, 1, 0, 0), \quad (4.83)$$

- the six cyclic permutation of

$$\frac{1}{(3-2\epsilon)(1-2\epsilon)} I^{(4)}(1, 1, 1, 0, 1, 0), \quad (4.84)$$

- the three cyclic permutation of

$$\frac{1}{(3-2\epsilon)(1-2\epsilon)} I^{(4)}(1, 1, 0, 1, 1, 0), \quad (4.85)$$

- the six cyclic permutation of the six-dimensional pentagon

$$I^{(6)}(1, 1, 1, 1, 1, 0), \quad (4.86)$$

- the six-dimensional hexagon

$$G_6(12345) I^{(6)}(1, 1, 1, 1, 1, 1). \quad (4.87)$$

The six-dimensional integrals are related to the four-dimensional ones by *dimension-shift relations* [190, 191], which for our case can be conveniently found in Eqs. (3.10)–(3.15) of Ref. [176]. We multiply the six-dimensional hexagon with the Gram determinant to eliminate the latter from the denominator of the respective dimension-shift relation because it vanishes when expressed through spinor variables, see Eq. (4.34). The reason to shift hexagon and pentagon integrals to six dimensions is that this way they do not contribute to the four-dimensional amplitude due to suppression in $\epsilon = (4-d)/2$. Thus, we leverage the well-known fact [192] that one-loop amplitudes in $d = 4$ can always be written as a linear combination of bubble, triangle, and box integrals. Finally, the ϵ -dependent prefactors of those relevant integrals are chosen in such a way that the coefficients c_i in IBP identities (4.79) are polynomials in ϵ , which simplifies some technical steps in Section 4.4.5. Note, however, that due to these factors the integrals no longer have *universal transcendental weight*, a concept introduced in Ref. [193]. One can assign a *transcendental weight* $\mathcal{T}(f)$ to functions or expressions f , most importantly $\mathcal{T}(1) = 0$, $\mathcal{T}(\pi) = 1$, $\mathcal{T}(\log) = 1$, $\mathcal{T}(\text{Li}_n) = n$, and $\mathcal{T}(f_1 f_2) = \mathcal{T}(f_1) + \mathcal{T}(f_2)$. Furthermore, one assigns $\mathcal{T}(\epsilon) = -1$ because ϵ expansions of loop integrals usually come with functions of higher weight the higher the power in ϵ . Then, integrals can have uniform transcendental weight, which can be helpful for solving them, and such an integral basis was chosen in Ref. [176]. Since we only need to substitute known solutions of integrals, sacrificing this property does not pose any problems.

The solutions to all master integrals are conveniently provided in the ancillary files of Ref. [176]. The appearing non-rational functions define the functions F_i from Eq. (4.59), which we sort by their transcendental weight. The only weight-zero “function” is simply the constant $F_1(\vec{s}) = 1$. At weight one, there are the logarithms

$$\log(-s_{ij}), \quad \log(-s_{ijk}), \quad (4.88)$$

which for different i, j, k form 25 independent functions. Note that many of those only appear when taking non-cyclic permutations of external momenta into consideration. Finally, at weight two, there appear

- the constant π^2 ,
- 309 independent products of two logarithms from Eq. (4.88),
- 101 independent dilogarithms of the forms

$$\text{Li}_2\left(1 - \frac{s_{ij}}{s_{ijk}}\right), \quad \text{Li}_2\left(1 - \frac{s_{ij}s_{lm}}{s_{ijk}s_{lmk}}\right), \quad (4.89)$$

- 15 independent normalized *triangle functions*

$$\frac{\text{Tri}(s_{ij}, s_{kl}, s_{mn})}{\sqrt{\Delta_{ij|kl|mn}}}, \quad (4.90)$$

where

$$\begin{aligned} \text{Tri}(s_{ij}, s_{kl}, s_{mn}) \equiv & -\text{Li}_2\left(-\frac{2s_{kl}}{s_{ij} - s_{kl} - s_{mn} - 2\sqrt{\Delta_{ij|kl|mn}}}\right) \\ & -\text{Li}_2\left(-\frac{2s_{mn}}{s_{ij} - s_{kl} - s_{mn} - 2\sqrt{\Delta_{ij|kl|mn}}}\right) \\ & -\frac{\pi^2}{6} - \frac{1}{2}\log\left(\frac{s_{mn}}{s_{kl}}\right)\log\left(\frac{s_{ij} - s_{kl} + s_{mn} - 2\sqrt{\Delta_{ij|kl|mn}}}{s_{ij} + s_{kl} - s_{mn} - 2\sqrt{\Delta_{ij|kl|mn}}}\right) \\ & -\frac{1}{2}\log\left(\frac{2s_{kl}}{s_{ij} - s_{kl} - s_{mn} - 2\sqrt{\Delta_{ij|kl|mn}}}\right)\log\left(\frac{2s_{mn}}{s_{ij} - s_{kl} - s_{mn} - 2\sqrt{\Delta_{ij|kl|mn}}}\right), \end{aligned} \quad (4.91)$$

and $\Delta_{ij|kl|mn} \equiv \frac{1}{4}\lambda(s_{ij}, s_{kl}, s_{mn})$ with the Källén function $\lambda(x, y, z) \equiv x^2 + y^2 + z^2 - 2(xy + yz + zx)$.

Since one-loop integrals never contain poles higher than ϵ^2 , no functions beyond weight two are needed to express the amplitude at ϵ^0 order. Therefore, we now have a complete list of 452 functions over which we sum in Eq. (4.59). Note that this is a valid function basis for all massless six-point one-loop amplitudes. In our specific case, some functions never actually occur, in other words, their corresponding coefficient is always zero.

4.4.5 Implementation

In this section, we describe how we implement a **C++** function taking finite-field values for the spinor brackets as an input and returning the corresponding vector of C_i values of a partial amplitude (4.59). We refer to a call of this function as a *probe* of the amplitude. We describe both the analytic steps that we perform independently of the specific probe in order to build the **C++** function and the numerical steps that are recomputed within **C++** for each probe. For the latter, finite-field variables are implemented using the **FFInt** data type from **FireFly** [184, 185].

The first steps of the amplitude calculation are performed completely analytically. We generate the Feynman diagrams with the private software package **DiaGen**. Using **FORM** [155], we insert Feynman rules and project to the partial amplitudes defined in Section 4.4.1. Furthermore, we insert the fermion projector (4.73) with the helicity as a free variable and perform fermion traces. We write the result of each diagram as a sum of integrals—they can contain standard propagators $((l + P)^2)^{-n}$ as well as numerators $l \cdot Q$, where Q can be a momentum as well as a polarization vector—with coefficients depending on $\text{tr}_5(1234)$ and scalar products between momenta or polarization vectors. This is exported as **C++** code without expressing scalar products through Mandelstam variables or inserting projectors for polarization vectors, since this would lead to the expressions drastically increasing in size.

In **C++**, we can define all scalar products of external momenta, as well as $\text{tr}_5(1234)$, in terms of spinor brackets. This is also possible for scalar products of polarization vectors with external momenta or other polarization vectors by substituting them according to Eq. (4.62). For the loop integrals, on the other hand, we build a custom class which can store any integral $I^{(4)}(n_1, n_2, n_3, n_4, n_5, n_6)$ as defined in Section 4.4.3. To construct objects of this class from the **FORM** output, we implement relations such as Eq. (4.61). This is possible for general linear propagators $l \cdot Q$ as long as Q is a linear combination of external momenta p_i , which is fulfilled for the substituted polarization vectors. Still, if the external momenta attach to the loop in an order that is a non-cyclic permutation of the standard order $\{p_1, p_2, p_3, p_4, p_5, p_6\}$, it is not possible to reach the $I^{(4)}(n_1, n_2, n_3, n_4, n_5, n_6)$ form. As a solution, we classify all diagrams by the permutation necessary to reach the standard form. Since this permutation is not necessarily unique, we choose it such that the overall number of needed permutations is minimal. To achieve this, we always check first if a shift or flip of the loop momentum can be used to prevent a permutation of external momenta. In the end, we find that we need 40 out of the $|\Sigma_5| = 5! = 120$ permutations which in principle could be possible. In practice, we then always work with the standard ordering of momenta, loop over the different permutations, and redefine the numerical finite-field phase-space point to account for the permutation.

The next step is to reduce the occurring integrals to master integrals using IBP reductions, c.f. Section 4.4.3. Conveniently, the software package **Kira** [157, 158] is internally linked to **FireFly** and can perform numerical IBP reductions for any given vector of finite-field values for the Mandelstam variables as well as the dimensional regulator ϵ . We directly access this functionality from within our **C++** implementation. Within **Kira**, we define the hexagon integral family and provide the list of master integrals from Section 4.4.4. Furthermore, we check which integrals appear in our amplitude before reduction, and provide them to **Kira** as well. Given these two lists of integrals, we can write an interface to incorporate the **Kira** output into our **C++** workflow. This interface is called for each of the 40 permutations of external momenta, and for each of these phase-space points for five different numerical values for the dimensional regulator ϵ . With the master integrals from Section 4.4.4 we find that all coefficients c_i in the IBP identities (4.79) are polynomials in ϵ with maximal degree four. Thus, with probes for five different ϵ values, we can infer the coefficients of the polynomials by simple Gaussian elimination.

At this point, we have a representation of the partial amplitudes as a sum of master integrals with prefactors that are polynomials in ϵ . All that remains to do is to insert the solutions of the master integrals, see Section 4.4.4, and extract the ϵ^0 terms that result from multiplying the two ϵ expansions. This concludes the calculation of C_i coefficients which are then returned as a vector.

4.5 Ansätze for Rational Coefficients

In Section 4.4, we have decomposed the amplitude into partial amplitudes, which are furthermore divided into a function basis and rational coefficients. Furthermore, we have described a workflow with which we can obtain finite-field values for the rational coefficients given input values for the spinor-helicity variables. Given such a “black box”, software tools like **FireFly** [184, 185] are in principle able to reconstruct the functional dependence of the rational coefficients on the variables. However, since spinor-helicity variables are not independent but have to be chosen such that they fulfill momentum conservation and Schouten identities, the direct use of such tools is not possible. Of course, one could eliminate all redundant spinor brackets, e.g. with Eq. (A.51). However, as we argue below, this would lead to much more complicated expressions

compared to using the full flexibility of the spinor-helicity formalism. Instead, we build custom ansätze for the rational coefficients using knowledge on how the scattering amplitude must look like. This also allows us to refine the ansätze beyond simple common-denominator rational functions. The methods are based on Refs. [172, 173].

The first property of scattering amplitudes that enables us to create an ansatz is that they have fixed mass dimension and *little-group weight*. For any function A depending on spinor brackets, the mass dimension $[A]$ is defined by

$$A|_{\{|i\rangle \rightarrow \lambda|i\rangle, |j\rangle \rightarrow \lambda|j\rangle\}_{i=1,\dots,n}} = \lambda^{2[A]} A, \quad (4.92)$$

where the notation $|i\rangle \rightarrow \lambda|i\rangle$ should indicate that all spinor brackets of the form $\langle ik\rangle$ or $\langle ki\rangle$ should be rescaled by λ . Since we apply this for all occurring momenta $i = 1, \dots, n$, all spinor brackets are rescaled by λ^2 to obtain the mass dimension. To define the little-group weight, recall that the action of a little-group Lorentz transformation on a spinor amounts to the rescaling with a phase factor, c.f. Appendix A.2. The k th little-group weight $\{A\}_k$ is then defined by the effect of a rescaling of the k th spinor:

$$A|_{|k\rangle \rightarrow \lambda|k\rangle, |k\rangle \rightarrow |k\rangle/\lambda} = \lambda^{\{A\}_k} A. \quad (4.93)$$

The mass dimension and phase-space weights of an n -point amplitude $\mathcal{A}_n$ are well-known (see e.g. Ref. [194] for a pedagogical treatment) to be,

$$[\mathcal{A}_n] = 4 - n, \quad \{\mathcal{A}_n\}_k = -2\sigma_k, \quad (4.94)$$

where σ_k is the helicity of the k th particle and can take the values $\pm\frac{1}{2}$ for fermions and ± 1 for vectors.

With these definitions at hand, assume for a moment that the desired coefficients are polynomials in spinor brackets. Then, those polynomials with fixed mass dimension d and little-group weights ϕ_k give rise to a finite-dimensional vector space over $\mathbb{F}$:

$$\mathcal{M}_{d,\phi} = \{a \in \mathcal{R}_6 : [a] = d \text{ and } \{a\}_k = \phi_k\}. \quad (4.95)$$

If we can construct a basis of this space, we have successfully found a minimal ansatz for the coefficient. We follow Ref. [173] and choose monomials

$$m_{(\alpha,\beta)} \equiv \prod_{j=1}^6 \prod_{i=1}^{j-1} \langle ij \rangle^{\alpha_{ij}} [ij]^{\beta_{ij}} \quad (4.96)$$

as basis elements. First, the exponents (α, β) need to be constrained to be members of $\mathcal{M}_{d,\phi}$:

$$[m_{\alpha,\beta}] = \sum_{j=1}^6 \sum_{i=1}^{j-1} (\alpha_{ij} + \beta_{ij}) \stackrel{!}{=} d, \quad (4.97)$$

$$\{m_{\alpha,\beta}\}_k = \sum_{j=1}^6 \sum_{i=1}^{j-1} (\alpha_{ij} - \beta_{ij})(\delta_{ik} + \delta_{jk}) \stackrel{!}{=} \phi_k. \quad (4.98)$$

Second, we have to ensure linear independence on $\mathcal{R}_6$. This can be done by requiring

$$m_{(\alpha,\beta)} \nmid \text{LM}(g) \quad \forall g \in \mathcal{G}(\mathcal{J}_{\Lambda_6} + \mathcal{K}_{\Lambda_6} + \overline{\mathcal{K}}_{\Lambda_6}). \quad (4.99)$$

Using a computer algebra system, this condition can be translated into conditions on (α, β) .³ The exact conditions depend on the chosen variable ordering. If, for example, for one element $g_i \in \mathcal{G}(\mathcal{J}_{\Lambda_6} + \mathcal{K}_{\Lambda_6} + \overline{\mathcal{K}}_{\Lambda_6})$ there is $\text{LM}(g_i) = \langle 36 \rangle \langle 45 \rangle$, the resulting condition is

$$\alpha_{36} < 1 \text{ or } \alpha_{45} < 1, \quad (4.100)$$

and this has to be repeated for all g_i . Finding all solutions to Eqs. (4.97), (4.98) that fulfill the constraints in Eq. (4.99) leads to a basis of $\mathcal{M}_{d,\phi}$.⁴

Unfortunately, the sought coefficients are not polynomials but rational functions, implying that fixed mass dimension and little-group weight do not suffice for a general ansatz because there remains an infinite number of possibilities by adding factors in both numerator and denominator. Fortunately, we have an additional constraint on the denominator. As pointed out in Ref. [195], the denominators can only contain factors of *letters* of the *function alphabet* of the occurring loop integrals. The letters for six-point integrals are listed in Ref. [176], and when translated to the spinor-helicity formalism, the denominators in our problem can always be written as a product of factors of the following form:

$$\langle ij \rangle, [ij], s_{ijk}, \langle i|j+k|i \rangle, \langle i|j+k|l \rangle, \Delta_{ij|kl|mn}, \quad (4.101)$$

where $\Delta_{ij|kl|mn} \equiv \frac{1}{4}\lambda(s_{ij}, s_{kl}, s_{mn})$ is familiar from the triangle function (4.90). If we have a way to test if a given factor occurs in the denominator of a coefficient, we can thus completely reconstruct its denominator, and the problem of rational reconstruction is reduced to reconstructing the polynomial numerator, whose mass dimension and little-group weights are fixed by the denominator, making it possible to construct an ansatz using Eqs. (4.97)–(4.99). There exist several methods to reconstruct a denominator given a list of potential factors. One approach is the usage of *univariate slices*. The details of this method given spinor-helicity variables are explained in Ref. [196]. In essence, one chooses a reference spinor $|k\rangle$ and shifts all other spinors according to

$$|i\rangle \rightarrow |i\rangle + tc_i |k\rangle, \quad |i] \rightarrow |i]. \quad (4.102)$$

This is called a *holomorphic shift*, whereas the same operation with $|j\rangle \leftrightarrow |j]$ is called *anti-holomorphic shift*. The original spinors $\{|i\rangle, |i]\}_{i=1,\dots,n}$ are chosen on a fixed but random phase-space point, and the variables c_i are random up to the condition that the shifted momentum retain momentum conservation. Now, our coefficients depend only on a single variable t , and the specific dependence can be inferred using e.g. **FireFly**. One can then identify all denominator factors by multiplying with all candidate factors (4.101) expressed through t and checking if the denominator's degree in t decreases. If yes, the candidate is indeed a factor of the denominator. This procedure is repeated for all candidates until the complete t -dependence of the denominator is removed.

In this work, however, we do not use the approach of univariate slices but rather probes on *singular varieties* corresponding to *codimension-1 ideals*. Details, as well as the required concepts from algebraic geometry are discussed in Section 4.5.1.

³In **Mathematica**, the command `MonomialList[gb[[i]], r, DegreeReverseLexicographic]`, where **r** is a polynomial ring, gives a list of monomials contained in the i th element of the Gröbner basis **gb** ordered using degree reverse lexicographic ordering. Thus, its first entry contains the leading monomial.

⁴The solutions can be found in **Mathematica** with the **Solve** command by setting the solution domain to **NonNegativeIntegers**. However, we found that it is possible to obtain the solutions with much less computation time by manually enumerating them using loops with appropriate exit conditions in **C++**.

Finally, considering our approach of reconstructing denominators, it is now clear why we do not simply eliminate all redundant spinor brackets using Eq. (A.51). The resulting denominators would have potentially much more complicated forms because we would have to plug all identities (A.51) into Eq. (4.101) to obtain all allowed denominators. This would lead to less compact final expressions and an oftentimes unclear behavior in singular limits.

4.5.1 Ideals, Varieties, and Partial-Fraction Decomposition

In Section 4.2, we have already introduced the notion of polynomial rings and ideals as subsets of such rings. In this section, which is also based on Ref. [173], we explore further applications of ideals beyond incorporating momentum conservation and Schouten identities. To this end, we work on the quotient ring $\mathcal{R}_6$ from Eq. (4.36) which already incorporates those identities. To be precise, many underlying calculations become computationally less expensive when working on a different quotient ring, R_6 constructed from S_6 , instead of $\mathcal{R}_6$ constructed from $\mathcal{S}_6$. The variables in S_6 are not spinor brackets but rather the components of the underlying Weyl spinors:

$$S_6 \equiv \mathbb{F}[\lambda_{1,0}, \lambda_{1,1}, \dots, \lambda_{6,0}, \lambda_{6,1}, \tilde{\lambda}_{1,\dot{0}}, \tilde{\lambda}_{1,\dot{1}}, \dots, \tilde{\lambda}_{6,\dot{0}}, \tilde{\lambda}_{6,\dot{1}}]. \quad (4.103)$$

Dividing by the momentum-conservation ideal in S_6 defines R_6 :

$$R_6 \equiv S_6/J_{\Lambda_6}, \quad J_{\Lambda_6} = \left\langle \sum_{i=1}^6 \lambda_{i,\alpha} \tilde{\lambda}_{i,\alpha} \right\rangle_{S_6}. \quad (4.104)$$

Other than for $\mathcal{R}_6$, elements of R_6 are not necessarily Lorentz invariant. In fact, it can be shown [173] that the Lorentz-invariant subring of R_6 is isomorphic to $\mathcal{R}_6$:

$$\mathcal{R}_6 \cong \{a \in R_6 : \Lambda(a) = Z_{(\Lambda,a)} a\} \subset R_6, \quad (4.105)$$

where Λ is a Lorentz transformation and $Z_{(\Lambda,a)}$ the effect of the little-group rescaling corresponding to Λ .

Let us start by motivating the concept of ideals on R_6 by sketching the two main applications we use in this work. Recall from Section 4.2 that polynomials belonging to an ideal $\langle p_1, \dots, p_k \rangle_{R_6}$ vanish when $p_i = 0$, $i = 1, \dots, k$. Furthermore, recall the task of reconstructing the denominator of a rational function given a list of factors that could appear. With the concept of ideals, one can reformulate this task as testing whether the denominator of the rational function belongs to the ideal generated by a factor. For example, if we can somehow ascertain that a denominator is a member of $\langle s_{123} \rangle$, we can infer that s_{123} appears as a factor in the denominator. By repeating this for all potential factors, we can fully reconstruct the denominator. For details on how this is implemented, see step 1 of Section 4.5.4.

After this, ideal membership can be used to further refine the ansatz. As a (simplified) example, assume we have found a coefficient to be of the form

$$C_i = \frac{N_i}{s_{123} \langle 12 \rangle [12]}. \quad (4.106)$$

If now $N_i \in \langle \langle 12 \rangle, [12] \rangle$, it makes sense to assume $N_i = N_{i,1}[12] + N_{i,2} \langle 12 \rangle$, and we can therefore choose the partial-fractioned ansatz

$$C_i = \frac{N_{i,1}}{s_{123} \langle 12 \rangle} + \frac{N_{i,2}}{s_{123} [12]}. \quad (4.107)$$

Unfortunately, the translation from ideal membership to partial fractioning is not always that straightforward. To formalize the approach, we need a few more concepts from algebraic geometry.

An *algebraic variety* over a field $\mathbb{F}$ is the subset of $\mathbb{F}^n$ given by the solutions to a system of polynomial equations. It is the natural *geometric* concept related to the *algebraic* concept of ideals: To any ideal $J = \langle p_1, \dots, p_k \rangle_{\mathcal{S}_6}$, we can associate the variety

$$V(J) = \left\{ \vec{b} \in \mathbb{F}^{30} : p_i(\vec{b}) = 0 \ \forall i = 1, \dots, k \right\}. \quad (4.108)$$

Intuitively, all polynomials belonging to the ideal J will vanish for all points that lie on the ideal $V(J)$. For quotient rings like $\mathcal{R}_6$ or R_6 , one has to additionally add the condition that polynomials equivalent to the zero element vanish. For example, the variety $V(\langle \langle 12 \rangle \rangle_{\mathcal{R}_6})$ consists of all vectors of spinor brackets that fulfill momentum conservation, the Schouten identity, and $\langle 12 \rangle = 0$. It is also possible to obtain an ideal in $\mathcal{S}_6$ given a variety in $\mathbb{F}^{30}$ using

$$I(U) = \left\{ p \in \mathcal{S}_6 : p(\vec{b}) = 0 \ \forall \vec{b} \in U \right\}. \quad (4.109)$$

To get some intuition on the relationship between ideals and varieties, notice that the “larger” an ideal, the “smaller” the corresponding variety. For example, the ideal $\langle 1 \rangle_{\mathcal{S}_6}$ contains all polynomials, $\langle 1 \rangle_{\mathcal{S}_6} = \mathcal{S}_6$, because there is no monomial that cannot be written as a multiple of 1. The corresponding variety $V(\langle 1 \rangle_{\mathcal{S}_6})$, on the other hand, is the empty set, $V(\langle 1 \rangle_{\mathcal{S}_6}) = \emptyset$, because there is no point for which $1 = 0$ or for which all polynomials in $\mathcal{S}_6$ vanish. Another example is $\langle 0 \rangle_{\mathcal{S}_6} = \{0\}$ with $V(\langle 0 \rangle_{\mathcal{S}_6}) = \mathbb{F}^{30}$.

Being a geometric concept, it makes sense to associate a dimensionality to varieties. To this end, we first define an *irreducible variety* as a variety U_{irr} which fulfills

$$U_{\text{irr}} = U_1 \cup U_2 \implies U_1 = U_{\text{irr}} \text{ or } U_2 = U_{\text{irr}}. \quad (4.110)$$

The dimension of any variety U is then given by the maximal length d of all chains

$$U_0 \subsetneq U_1 \subsetneq \dots \subsetneq U_d \subseteq U \quad (4.111)$$

of distinct non-empty irreducible subvarieties of U . We carry the concept of dimensionality over to ideals by defining

$$\dim(J) \equiv \dim(V(J)). \quad (4.112)$$

For example, in the case of a polynomial ring R the dimension $\dim(\langle 0 \rangle_R)$ is simply equal to the number of variables in R because the corresponding variety covers the complete space spanned by the variables. For a quotient ring, the dimension of the trivial ideal is given by the dimension of the ideal by which one divides, e.g.

$$\dim(\langle 0 \rangle_{R_6}) = \dim(J_{\Lambda_6}) = 24 - 4 = 20. \quad (4.113)$$

When working with ideals in a ring R , the more intuitive notion is the *codimension* defined as

$$\text{codim}(J) = \dim(\langle 0 \rangle_R) - \dim(J). \quad (4.114)$$

It corresponds to the number of constraints that are imposed when requiring ideal membership. All ideals in R_6 that we use for the denominator reconstruction, that is all ideals with a single

generator given by one of the factors from Eq. (4.101), have codimension one, whereas we use codimension-two ideals to find partial-fractioned ansätze.

The correspondence between ideals and varieties naturally leads to an idea on how to test if a polynomial p belongs to an ideal J . If one can generate a point $\vec{b} \in V(J)$, one could think that checking whether $p(\vec{b}) = 0$ is equivalent to testing $p \in J$. However, this is not true, which can be understood with the following example. Assume, we have a coefficient

$$C_i = \frac{N_i}{\Delta_{12|34|56} \langle 1|3+4|2 \rangle} \quad (4.115)$$

and want to test whether $N_i \in \langle \Delta_{12|34|56}, \langle 1|3+4|2 \rangle \rangle_{R_6}$ by evaluating N_i on points on the associated variety. Because of the identity

$$\Delta_{12|34|56} = \langle 1|3+4|2 \rangle \langle 2|3+4|1 \rangle + \frac{1}{4}(s_{134} - s_{234})^2, \quad (4.116)$$

all points where $s_{134} - s_{234}$ and $\langle 1|3+4|2 \rangle$ vanish automatically lead to $\Delta_{12|34|56}$ also vanishing. In fact, it turns out that

$$V\left(\langle \Delta_{12|34|56}, \langle 1|3+4|2 \rangle \rangle_{R_6}\right) = V\left(\langle s_{134} - s_{234}, \langle 1|3+4|2 \rangle \rangle_{R_6}\right), \quad (4.117)$$

and N_i vanishing on this variety only implies

$$N_i \in \langle s_{134} - s_{234}, \langle 1|3+4|2 \rangle \rangle_{R_6} \supsetneq \langle \Delta_{12|34|56}, \langle 1|3+4|2 \rangle \rangle_{R_6}, \quad (4.118)$$

and we cannot infer a naive partial-fractioned ansatz for C_i . To formalize this notion, one can define the *radical* of an ideal as

$$\sqrt{J} \equiv I(V(J)). \quad (4.119)$$

If $\sqrt{J} = J$, one calls J itself radical, which can be alternatively defined algebraically:

$$J \text{ is radical if } p^k \in J \implies p \in J \quad \forall p \in R, \quad (4.120)$$

where R is the polynomial ring on which J is defined. Coming back to our example, indeed, the relation

$$\sqrt{\langle \Delta_{12|34|56}, \langle 1|3+4|2 \rangle \rangle_{R_6}} = \langle s_{134} - s_{234}, \langle 1|3+4|2 \rangle \rangle_{R_6} \quad (4.121)$$

was found in Ref. [197]. To summarize, in order to test ideal membership by numerical probes on the associated variety, the ideal needs to be radical. For a method to test membership in a non-radical ideal using the corresponding radical, see step 5 of Section 4.5.4.

Unfortunately, restricting oneself to radical ideals is still not sufficient to infer ideal membership and a corresponding partial-fractioned ansatz from probes on the corresponding variety. If the variety U is not irreducible as defined in Eq. (4.110), it *branches* into irreducible sub-varieties U_k :

$$U = \bigcup_k U_k. \quad (4.122)$$

For example, there is

$$V(\langle \langle 12 \rangle, \langle 13 \rangle \rangle_{R_6}) = V(\langle \langle 12 \rangle, \langle 13 \rangle, \langle 23 \rangle \rangle_{R_6}) \cup V(\langle \lambda_{1,\alpha} \rangle_{R_6}). \quad (4.123)$$

If one now probes a numerator N on a point belonging to this variety, it could happen that the point is on the branch $V(\langle\langle 12 \rangle, \langle 13 \rangle, \langle 23 \rangle\rangle_{R_6})$ and for example a numerator $N = N_1 \langle 12 \rangle + N_2 \langle 23 \rangle$ would vanish despite not necessarily belonging to $\langle\langle 12 \rangle, \langle 13 \rangle\rangle_{R_6}$. An ideal corresponding to an irreducible variety is called *prime*, and for any radical ideal J , one can perform a prime decomposition analogously to the branching of the associated variety:

$$J = \bigcap_k J_k. \quad (4.124)$$

Thus, analogously to Eq. (4.123), there is

$$\langle\langle 12 \rangle, \langle 13 \rangle\rangle_{R_6} = \langle\langle 12 \rangle, \langle 13 \rangle, \langle 23 \rangle\rangle_{R_6} \cap \langle\lambda_{1,\alpha}\rangle_{R_6}. \quad (4.125)$$

For non-radical ideals, one can instead perform a *primary decomposition*, where one intersects *primary* ideals J_k , which are non-radical ideals whose radicals are prime.

All codimension-one ideals that we use for denominator reconstruction are prime, so probes on the associated varieties can be used without any complications. On the other hand, the separation of two denominator factors A, B into different summands in a partial-fractioned ansatz is possible if $\langle A, B \rangle_{R_6}$ is radical and the numerator vanishes for probes on *all* varieties associated to the ideals of the prime decomposition of $\langle A, B \rangle_{R_6}$. Calculations with ideals on R_n , e.g. calculating radicals or testing primary decompositions, can be performed with the software package `lips` [198], which uses the `Python` interface `syngular` [199] to the computer algebra system `Singular` [200]. A list of primary decompositions and radicals of ideals in R_6 is given in Ref. [197].

Finally, let us discuss how one can leverage if a polynomial not just vanishes, but vanishes to a higher order $n > 1$ on a variety. The *ideal power* is simply defined via the ideal product from Eq. (4.27):

$$J^k \equiv J^{k-1}J, \quad J^1 \equiv J. \quad (4.126)$$

However, if a polynomial vanishes to order n on a variety associated to an ideal J , this does not necessarily imply that the polynomial is a member of J^n , but only that it is a member of $J^{(n)}$, where $(\cdot)^{(n)}$ denotes the *symbolic power* of an ideal. While a definition can be found in Ref. [173], for us, it is sufficient to know that if an ideal is of *maximal codimension*, i.e. if its codimension is equal to the (minimal) number of its generators, symbolic power and ideal power coincide. Clearly, this is the case for all codimension-one ideals that we consider. Thus, if we are able to probe to which order a denominator vanishes on a variety, we can not only identify which factors occur in a denominator, but also their power. Furthermore, vanishing to higher order can provide information when working with non-radical ideals, as we explain in step 5 of Section 4.5.4.

4.5.2 p -adic Numbers

When dealing with polynomials, it is possible to test ideal membership by evaluating a polynomial on finite-field points belonging to the corresponding variety. If they vanish there, all finite-field probes will yield zero. However, the numerical tool chain we built in Section 4.4 allows us only to get finite-field probes of the *rational* coefficients C_i , and not of the polynomial numerator or denominator separately. If we now attempt to evaluate these coefficients on varieties on which the denominator vanishes, we run into problems because division by zero is not defined on finite fields. Furthermore, the information that a polynomial vanishes carries no

information on the power to which it vanishes. For example, $\langle 12 \rangle^n$ will evaluate to zero on all points in $V(\langle\langle 12 \rangle\rangle_{R_6})$ regardless of the power $n > 0$.

Due to the aforementioned reasons, it is desirable to perform numerical probes using points that lie close to but not directly on a variety. To do this, we need an absolute value to measure distances, so that we can define which points we consider to be in the vicinity of a variety. However, on finite fields the only absolute value that can be defined is the trivial absolute value:

$$|a|_{\mathbb{F}_p} \equiv \begin{cases} 0, & \text{if } a = 0, \\ 1, & \text{otherwise.} \end{cases} \quad (4.127)$$

This follows from *Fermat's little theorem*, which states

$$a^p \bmod p = a, \quad (4.128)$$

which implies $|a^p|_{\mathbb{F}_p} - |a|_{\mathbb{F}_p} = 0$ and therefore $|a|_{\mathbb{F}_p}(|a|_{\mathbb{F}_p}^{p-1} - 1) = 0$ for all $a \in \mathbb{F}_p$. Hence, it is impossible to define a set of points that lie close to but not on a variety.

A solution is given by *p-adic numbers*. A pedagogical introduction is given in Ref. [179], and their application to rational reconstruction of scattering amplitudes was explored in Refs. [173, 201]. Here, we briefly mention the main ideas. Analogously to a finite field $\mathbb{F}_p$, a *p*-adic field $\mathbb{Q}_p$ is characterized by a prime number *p*. Every element $x \in \mathbb{Q}_p$ is characterized by its coefficients in a power series in this prime number *p*:

$$x = \sum_{i=-l}^{\infty} c_i p^i, \quad (4.129)$$

where *l* can be any finite integer and c_i are integers in the range $0 \leq c_i \leq p-1$. We call the coefficients c_i *digits* of a *p*-adic number. If all digits except c_0 are zero, one can interpret a *p*-adic number just like a finite-field number. However, while any multiple of *p* evaluates to exactly zero in $\mathbb{F}_p$, it only becomes *smaller* in $\mathbb{Q}_p$. Indeed, the *p*-adic absolute value evaluates multiples of *p* according to

$$|cp^n|_{\mathbb{Q}_p} = \frac{1}{p^n}, \quad (4.130)$$

so *larger* powers in *p* correspond to *smaller* absolute values, and the coefficient *c* has no influence. This can be generalized to general *p*-adic numbers by defining the *p*-adic valuation of a number as

$$\nu_p(x) \equiv \min\{k \in \mathbb{Z} : c_i = 0 \ \forall \ i < k\}. \quad (4.131)$$

The absolute value is then defined as

$$|x|_{\mathbb{Q}_p} \equiv \frac{1}{p^{\nu_p(x)}}. \quad (4.132)$$

In other words, the leading non-zero term from Eq. (4.129) defines the absolute value.

With these definitions, it is possible to define phase-space points that lie close to but not on a variety. For example, phase-space points where $\nu_p(\langle 12 \rangle) = 1$ are close to the variety $V(\langle\langle 12 \rangle\rangle_{R_6})$, up to first-order corrections. The generation of *p*-adic phase-space points close to varieties is described in Ref. [173] and implemented in the software package `lips` [198]. If we can perform the numerical probes of the amplitude with *p*-adic instead of finite-field numbers, we can therefore test ideal membership of numerator and denominator of coefficients in a partial amplitude by calculating the *p*-adic valuation of the result. For varieties associated

to codimension-one ideals generated by a single factor f , if $\nu_i(C_i) > 0$, then the numerator is a member of $\langle f \rangle_{R_6}^{\nu_i(C_i)}$, if $\nu_i(C_i) < 0$, the denominator is a member of $\langle f \rangle_{R_6}^{-\nu_i(C_i)}$. It cannot happen that both numerator and denominator belong to the ideal because then the factor could simply cancel. For codimension-two ideals, on the other hand, it could happen that both numerator and denominator vanish when probed on the associated variety. However, for our reconstruction workflow described in Section 4.5.4, testing codimension-two ideal membership is only necessary after the denominator has already been completely reconstructed, so we can directly access the numerator.

It remains to discuss how to perform probes of the amplitude with p -adic numbers. The software `lips` provides phase-space points in the form of digits of p -adic numbers for each spinor bracket. As was pointed out in Ref. [201], one does not need to perform probes in dedicated p -adic arithmetic, but can simply convert the digits to usual integers using regular integer arithmetic on the expansion in Eq. (4.129).⁵ The rational result of the probe then has the correct p -adic expansion, up to the number of digits that were used as input. Converting a rational number to a p -adic number can be done with packages for p -adic arithmetic like `FLINT` [202]. Obtaining this rational result given finite-field probes can be done with the methods from Section 4.3, and is conveniently automatized in `FireFly`. A word of caution is necessary when using this approach. The p -adic points only fulfill Schouten identities and momentum conservation up to the order to which they are generated. Using the corresponding exact integers as input for finite-field probes can lead to problems within our numerical implementation from Section 4.4.5. We therefore only use the generated values for an independent set of spinor brackets and relate the remaining ones within our finite-field implementation using Eq. (A.51). The resulting phase-space point agrees with the generated values up to their p -adic order but receives higher order corrections to fulfill the necessary constraints.

Let us finally mention an application of p -adic numbers beyond testing ideal membership, proposed in Ref. [201]. As mentioned above, the leading digit of a p -adic expansion can be viewed as a regular finite-field number. It can therefore be used to relate or reconstruct polynomials up to higher orders in a given limit. For example, if a coefficient can be written as a partial-fractioned sum of rational functions, only one of which having a $\langle 12 \rangle$ pole, probes on $\langle \langle 12 \rangle \rangle_{R_6}$ will isolate this term. In other words, we can access the residue of the coefficient when expanded in $\langle 12 \rangle$. This can for example be used to check the relations between residues listed in Section 4.5.3.

4.5.3 Spurious Poles

Helpful information for the reconstruction of partial amplitudes can be gained by analyzing *spurious poles*. Since scattering amplitudes are not physical observables, they need not necessarily be finite for all phase-space points. However, their divergent behavior is strictly constrained to infrared, i.e. soft or collinear, phase-space regions, and the leading divergent terms are described by universal functions. Only this way can the divergences cancel when combining amplitudes into a physical observable such as a cross section, as we describe in Chapter 2. All additional divergences that appear in rational coefficients C_i of a partial amplitudes must cancel in the respective limit. This fact can be leveraged during the reconstruction procedure, as we will describe below.

⁵For numbers with negative valuation, the resulting number could be a rational number instead of an integer. However, the phase-space points we use never contain diverging spinor brackets.

From the denominator factors that occur in our partial amplitudes, see Eq. (4.101), single factors of $\langle ij \rangle$, $[ij]$, and s_{ijk} can come from soft or collinear divergences and therefore be non-spurious. On the other hand, higher powers in these factors, as well as the factors $\langle i|j+k|i \rangle$, $\langle i|j+k|l \rangle$, $\Delta_{ij|kl|mn}$ constitute spurious poles when appearing in the denominator.

Let us begin with poles in $\langle i|j+k|i \rangle = s_{ij} + s_{ik}$. Such poles are cancelled when multiplied with the function

$$L_{0,ijk} \equiv \log(-s_{ij}) - \log(-s_{ijk}) = \mathcal{O}(\langle k|i+j|k \rangle). \quad (4.133)$$

The partial amplitude does therefore not diverge in the limit $\langle i|j+k|i \rangle \rightarrow 0$ if the residues of the coefficients of $\log(-s_{ij})$ and $\log(-s_{ijk})$ are equal with opposite sign:

$$\text{Res}(C[\log(-s_{ij})], \langle i|j+k|i \rangle) \stackrel{!}{=} -\text{Res}(C[\log(-s_{ijk})], \langle i|j+k|i \rangle). \quad (4.134)$$

With this information, one can reconstruct the simpler of the two coefficients and subtract the $\langle i|j+k|i \rangle$ pole obtained in this way from the other. Such a handling of $\langle i|j+k|i \rangle$ poles was already done in Refs. [203, 204], where it was furthermore observed that all poles of the form $\langle i|j+k|i \rangle$ decompose into different terms of a partial-fractioned ansatz. This, together with Eq. (4.134), will be used extensively in step 7 of Section 4.5.4. Finally, if a $\langle i|j+k|i \rangle$ pole is not just linear but quadratic, it has to appear as a prefactor to

$$L_{1,ijk} = L_{0,ijk} + \frac{\langle k|i+j|k \rangle}{s_{ijk}} = \mathcal{O}(\langle k|i+j|k \rangle^2), \quad (4.135)$$

connecting quadratic poles occurring in $C[\log(\cdot)]$ with linear poles occurring in $C[1]$.

For poles in $\langle i|j+k|l \rangle$, we make use of the following linear combination of functions:

$$\begin{aligned} & \text{Tri}(s_{ij}, s_{kl}, s_{mn}) + \text{Li}_2\left(1 - \frac{s_{ij}}{s_{ijl}}\right) + \text{Li}_2\left(1 - \frac{s_{mn}}{s_{ijl}}\right) - \log(-s_{kl}) \log(-s_{ijl}) \\ & + \frac{1}{2} \left(\log(-s_{ijl})^2 - \log(-s_{ij}) \log(-s_{mn}) + \log(-s_{kl}) [\log(-s_{ij}) + \log(-s_{mn})] \right) = \mathcal{O}(\langle k|i+j|l \rangle), \end{aligned} \quad (4.136)$$

where it is helpful to remember $\langle k|i+j|l \rangle = -\langle k|m+n|l \rangle$. A function vanishing as $\langle k|i+j|l \rangle$ approaches zero can be obtained by replacing $s_{ijl} \mapsto s_{ijk}$ in Eq. (4.136). Notice further

$$\Delta_{ij|kl|mn} \xrightarrow{\langle k|i+j|l \rangle \rightarrow 0} \frac{(s_{ijk} - s_{ijl})^2}{4}, \quad (4.137)$$

making it possible to rationalize $\sqrt{\Delta_{ij|kl|mn}}$ in this limit. Combining this with Eq. (4.136) leads to the following relation between coefficients:

$$\begin{aligned} \text{Res}\left(C\left[\frac{\text{Tri}(s_{ij}, s_{kl}, s_{mn})}{\sqrt{\Delta_{ij|kl|mn}}}\right], \langle i|j+k|l \rangle\right) = \\ \pm \frac{(s_{ijk} - s_{ijl})}{2} \left[\text{Res}(C[\log(-s_{kl}) \log(-s_{ijl})], \langle i|j+k|l \rangle) \right. \\ \left. - \text{Res}(C[\log(-s_{kl}) \log(-s_{ijk})], \langle i|j+k|l \rangle) \right]. \end{aligned} \quad (4.138)$$

The sign can be obtained by a numerical probe of the residues, which can be done with a p -adic phase-space point where $\langle i|j+k|l \rangle$ vanishes, as described in Section 4.5.2. In our applications,

which are described in detail in step 4 of Section 4.5.4, usually one of the two residues on the right-hand side of Eq. (4.138) is zero.

Finally, information on poles in $\Delta_{ij|kl|mn}^2$ can be obtained with

$$\begin{aligned} & \frac{\text{Tri}(s_{ij}, s_{kl}, s_{mn})}{2\sqrt{\Delta_{ij|kl|mn}}} + \frac{\log(-s_{ij})}{s_{kl} + s_{mn} - s_{ij}} + \frac{\log(-s_{kl})}{s_{ij} + s_{mn} - s_{kl}} + \frac{\log(-s_{mn})}{s_{ij} + s_{kl} - s_{mn}} \\ & + \Delta_{ij|kl|mn} \left(\frac{\log(-s_{ij})}{3(s_{kl} + s_{mn} - s_{ij})^3} + \frac{\log(-s_{kl})}{3(s_{ij} + s_{mn} - s_{kl})^3} + \frac{\log(-s_{mn})}{3(s_{ij} + s_{kl} - s_{mn})^3} + \frac{1}{12s_{ij}s_{kl}s_{mn}} \right) \\ & = \mathcal{O}(\Delta_{ij|kl|mn}^2), \quad (4.139) \end{aligned}$$

implying for example

$$\text{Res}(C[\log(-s_{ij})], \Delta_{ij|kl|mn}) = 2 \text{Res} \left(C \left[\frac{\text{Tri}(s_{ij}, s_{kl}, s_{mn})}{\sqrt{\Delta_{ij|kl|mn}}} \right], \Delta_{ij|kl|mn} \right) / (s_{kl} + s_{mn} - s_{ij}). \quad (4.140)$$

For the practical usage of this formula, see step 6 of Section 4.5.4.

While the above identities were the only ones we ended up using in our reconstruction, we found some additional linear combinations of functions vanishing as $\langle ij \rangle \rightarrow 0$ or $[ij] \rightarrow 0$. Such functions are needed to cancel spurious poles of higher powers in these variables. Functions that vanish to different orders in both $\langle ij \rangle$ and $[ij]$ are

$$\begin{aligned} f_{0,ijk} &= \text{Li}_2 \left(1 - \frac{s_{ik}}{s_{ijk}} \right) + \text{Li}_2 \left(1 - \frac{s_{jk}}{s_{ijk}} \right) + \log(-s_{ijk})^2 + \log(-s_{ik}) \log(-s_{jk}) \\ & - [\log(-s_{ik}) + \log(-s_{jk})] \log(-s_{ijk}) - \frac{\pi^2}{6} = \mathcal{O}(s_{ij}), \end{aligned} \quad (4.141)$$

$$f_{1,ijk} = f_{0,ijk} + s_{ij} \left(\frac{L_{0,ikj}}{\langle j|i+k|j \rangle} + \frac{L_{0,jki}}{\langle i|j+k|i \rangle} \right) = \mathcal{O}(s_{ij}^2), \quad (4.142)$$

$$f_{2,ijk} = f_{1,ijk} + \frac{s_{ij}^2}{2} \left(\frac{L_{1,ikj}}{\langle j|i+k|j \rangle^2} + \frac{L_{1,jki}}{\langle i|j+k|i \rangle^2} \right) = \mathcal{O}(s_{ij}^3). \quad (4.143)$$

Unfortunately, we found that also more intricate combinations of functions vanishing only for either $\langle ij \rangle$ or $[ij]$ can occur:

$$\begin{aligned} g_{0,ijklmn} &= \text{Li}_2 \left(1 - \frac{s_{ij}s_{lm}}{s_{ijk}s_{lmn}} \right) - \text{Li}_2 \left(1 - \frac{s_{ij}}{s_{ijk}} \right) - \text{Li}_2 \left(1 - \frac{s_{lm}}{s_{ijk}} \right) \\ & - \text{Li}_2 \left(1 - \frac{s_{ij}}{s_{lmn}} \right) - \text{Li}_2 \left(1 - \frac{s_{lm}}{s_{lmn}} \right) - \frac{1}{2} (\log(-s_{ijk}) - \log(-s_{lmn}))^2 = \mathcal{O}(\langle mn \rangle), \end{aligned} \quad (4.144)$$

$$\begin{aligned} g_{1,ijklmn} &= g_{0,ijklmn} - \frac{\langle ij \rangle \langle mn \rangle}{\langle im \rangle \langle kn \rangle} \left(\frac{\langle k|n|j \rangle}{\langle n|i+j|n \rangle} L_{0,ijn} - \frac{\langle k|m|j \rangle}{\langle m|i+j|m \rangle} L_{0,ijm} \right) \\ & - \frac{\langle mn \rangle \langle kl \rangle}{\langle im \rangle \langle kn \rangle} \left(\frac{\langle i|n|l \rangle}{\langle n|k+l|n \rangle} L_{0,klm} - \frac{\langle i|m|l \rangle}{\langle m|k+l|m \rangle} L_{0,klm} \right) \\ & - \frac{\langle ik \rangle \langle mn \rangle}{\langle im \rangle \langle kn \rangle} (\log(-s_{ijn}) - \log(-s_{ijm})) = \mathcal{O}(\langle mn \rangle^2), \end{aligned} \quad (4.145)$$

$$g_{2,ijklmn} = g_{1,ijklmn} - \frac{1}{2} \left(\frac{\langle ij \rangle \langle mn \rangle}{\langle im \rangle \langle kn \rangle} \right)^2 \left(\frac{\langle k|n|j \rangle^2}{\langle n|i+j|n \rangle^2} L_{1,ijn} + \frac{\langle k|m|j \rangle^2}{\langle m|i+j|m \rangle^2} L_{1,ijm} \right)$$

$$\begin{aligned}
& -\frac{1}{2} \left(\frac{\langle mn \rangle \langle kl \rangle}{\langle im \rangle \langle kn \rangle} \right)^2 \left(\frac{\langle i|n|l \rangle^2}{\langle n|k+l|n \rangle^2} L_{1,kl n} + \frac{\langle i|m|l \rangle^2}{\langle m|k+l|m \rangle^2} L_{1,kl m} \right) \\
& -\frac{1}{2} \left(\frac{\langle ik \rangle \langle mn \rangle}{\langle im \rangle \langle kn \rangle} \right)^2 (\log(-s_{ijn}) - \log(-s_{ijm})) \\
& + \langle mn \rangle^2 \left(\frac{\langle ij \rangle \langle ik \rangle}{(\langle im \rangle \langle kn \rangle)^2} \frac{\langle k|m|j \rangle}{\langle m|i+j|m \rangle} L_{0,ijm} - \frac{\langle kl \rangle \langle ik \rangle}{(\langle im \rangle \langle kn \rangle)^2} \frac{\langle i|n|l \rangle}{\langle n|k+l|n \rangle} L_{0,kl n} \right) \\
& = \mathcal{O}(\langle mn \rangle^3),
\end{aligned} \tag{4.146}$$

where the relations vanishing as $[ij] \rightarrow 0$ can be obtained by complex conjugation. While we believe that such relations can in principle be helpful to obtain more compact expressions for an amplitude, it is unclear how to use them in an automated manner. They are therefore not used in our workflow for the reconstruction which we describe in Section 4.5.4.

4.5.4 Workflow of the Reconstruction

With all the tools from the previous sections at hand, let us describe the workflow that was employed for the reconstruction. For each partial amplitude, we follow this step-by-step procedure:

1. Reconstruct (denominator) factors using p -adic probes on varieties associated to codimension-one ideals.
2. Find a linearly independent set of coefficients such that the unknown numerators have minimal mass dimension.
3. Reconstruct the numerators of all coefficients of functions with transcendental weight two except triangle functions.
4. Where necessary, infer the leading poles of triangle coefficients in $\langle i|j+k|l \rangle$ and subtract them.
5. Reconstruct the triangle coefficients. If necessary, refine the ansatz using heuristic rules and probes on varieties associated to codimension-two ideals.
6. Infer the leading $\Delta_{ij|kl|mn}$ poles of coefficients of functions with transcendental weight one or zero and subtract them.
7. Reconstruct poles of $\log(-s_{ijk})$ functions using heuristic partial-fractioning rules. Use the results to remove all $\langle i|j+k|i \rangle$ poles in the remaining coefficients.
8. Reconstruct the remaining coefficients, if necessary using heuristic partial-fractioning rules.

Let us give some more details on the individual steps.

1. Codimension-one ideals As described in Section 4.5.1, codimension-one ideal membership reveals factors of a polynomial. Following Section 4.5.2, we generate p -adic phase-space points lying on 205 varieties associated to the codimension-one ideals generated by the factors (4.101) and permutations thereof. To be specific, we use the software package `lips` [198] and generate two-digit p -adic numbers with $p \sim 10^3$. The resulting integer values for the spinor brackets are used as input values to `FireFly`, which can then reconstruct the rational result. The p -adic valuation of the result are then computed using `FLINT` [202] when needed within `C++` or in `Mathematica` using a package for p -adic arithmetic [205]. In order to avoid accidental

cancellations due to the relatively small prime numbers, we generate four different phase-space points per variety and demand the valuation of the probes to agree among at least three of them. With the resulting valuations $\nu_{i,j}$, we can then infer the form of the rational coefficients of the partial amplitudes:

$$C_i = \left[\prod_{j=1}^{205} f_j^{\nu_{i,j}} \right] N_i, \quad (4.147)$$

where the factors contain all denominator factors of C_i ($\nu_{i,j} < 0$) and potentially some numerator factors ($\nu_{i,j} > 0$). The missing factors N_i are unknown polynomials in spinor brackets with fixed mass dimension and phase-space weight. The objective of the following steps is to obtain them. Even though the factors $f_j^{\nu_{i,j}}$ may also contain some numerator factors, we will use the term *numerators* to refer to N_i for the remainder of this section.

2. Linear relations between coefficients It turns out that in partial amplitudes

$$A(\{p_i\}_{i=1,\dots,6}) = \sum_{i=1}^n C_i(\vec{b}) \times F_i(\vec{s}), \quad (4.148)$$

not all coefficients C_i are linearly independent. It is therefore sufficient to reconstruct the coefficients contained in a linearly independent subset $\{C_i\}_{i \in B}$, where $B \subset \{1, \dots, n\}$ and obtain the remaining ones via linear combination. Linear dependencies can be found by numerically computing the nullspace

$$K((C_i(\vec{b}_j))_{ji}) = \left\{ \vec{k} : \sum_{i=1}^n C_i(\vec{b}_j) k_i = 0 \ \forall j = \{1, \dots, n\} \right\} \quad (4.149)$$

where we can obtain the matrix $(C_i(\vec{b}_j))_{ji}$ by performing probes on n random phase-space points $\vec{b}_j$. For efficiency, we reuse n distinct rational probes from step one, when we calculated codimension-one ideal membership. By using the full rational result, the nullspace is not impacted by poles or zeros on $\mathbb{Q}_p$.⁶ Any coefficient C_l for which there exists a $\vec{k} \in K((C_i(\vec{b}_j))_{ji})$ with $k_l \neq 0$ could be removed from the list of coefficients we need to reconstruct, and we choose the one where the numerator has the largest mass dimension. This procedure is repeated with $n \mapsto n - 1$ and C_l removed from the list of coefficients until the nullspace is empty. The remaining coefficients form the independent subset $\{C_i\}_{i \in B}$ where the coefficients have minimal numerator mass dimension. These are the coefficients we wish to reconstruct in the following steps. The partial amplitude then takes the form

$$A(\{p_i\}_{i=1,\dots,6}) = \sum_{i \in B} \sum_{j=1}^n C_i(\vec{b}) M_{ij} F_j(\vec{s}) \quad (4.150)$$

The matrix M_{ij} has rational numbers as entries and can, like B itself, be obtained with linear-algebra methods. For example, in **Mathematica**, we can reorder the columns of $(C_i(\vec{b}_j))_{ji}$ such that for all $i \in B$, $i' \notin B$, there is $i > i'$. Then, the command `NullSpace[NullSpace[C]]` returns M .

⁶For computational efficiency, it is still advisable to compute the nullspace on a finite field $\mathbb{F}_{p'}$ with $p' \gg p$. Mapping rational numbers to $\mathbb{F}_{p'}$ is straightforward with the concepts introduced in Section 4.3, and computing the nullspace can e.g. be done in **Mathematica** using `NullSpace[matrix, Modulus -> prime]`.

Note that in Ref. [195], a further reduction in the numerator mass dimension was achieved by an additional basis change

$$\tilde{C}_i = \sum_{j \in B} a_{ij} C_j, \quad (4.151)$$

where a_{ij} is a matrix of rational numbers. A refined algorithm for such basis improvement was described in Ref. [197] based on the analysis of spurious poles. We, however, find no significant improvement in this way, indicating that the function basis from Section 4.4.4 might already be close to optimal. To leverage the vanishing of spurious poles, we instead make use of the analysis described in Section 4.5.3 and in the steps hereafter.

3. Reconstruction of simple numerators For all our partial amplitudes, the numerators of coefficients of functions with transcendental weight two, with the exception of triangle functions, are simple enough to be reconstructed in common-denominator form. To that end, we first generate a basis of allowed monomials in N_i according to Eqs. (4.97)–(4.99). We then perform as many probes on random finite-field phase-space points as there are unknowns in the ansatz.⁷ The random phase-space points are generated as described in Appendix A.3. The finite-field coefficients in the ansatz are then obtained by Gaussian elimination and checked by testing them on one additional probe. The rational coefficients can then be obtained as explained in Section 4.3, using the Euclidean algorithm and, if necessary, the Chinese Remainder Theorem.

4. $\langle i|j+k|l \rangle$ poles The triangle functions often have numerators whose mass dimension is too large for them to be reconstructed in common-denominator form. As a first step to simplify them, we use Eq. (4.138) to eliminate the highest-power poles of the form $\langle i|j+k|l \rangle$. Specifically, assume that we are in the special case

$$\text{Res} \left(C \left[\frac{\text{Tri}(s_{ij}, s_{kl}, s_{mn})}{\sqrt{\Delta_{ij|kl|mn}}} \right], \langle i|j+k|l \rangle \right) = \frac{(s_{ijk} - s_{ijl})}{2} \text{Res}(C[\log(-s_{kl}) \log(-s_{ijk})], \langle i|j+k|l \rangle). \quad (4.152)$$

Subtracting $(s_{ijk} - s_{ijl}) C[\log(-s_{kl}) \log(-s_{ijk})]/2$ from the triangle coefficient removes the highest $\langle i|j+k|l \rangle$ pole. However, it can happen that $C[\log(-s_{kl}) \log(-s_{ijk})]$ contains some denominator factors that are not contained in the triangle coefficient, implying that such a naive approach would again introduce new denominator factors and therefore not decrease the mass dimension of the numerator. Instead, let N_l and D_l denote numerator and denominator of $C[\log(-s_{kl}) \log(-s_{ijk})]$, $\mathcal{D}_l$ the product of denominator factors appearing in $C[\log(-s_{kl}) \log(-s_{ijk})]$ but not in $C[\text{Tri}(s_{ij}, s_{kl}, s_{mn})/\sqrt{\Delta_{ij|kl|mn}}]$, and $\mathcal{D}_t$ those appearing in the latter but not the former. It must then be possible to write

$$N_l \mathcal{D}_t = N_t \mathcal{D}_l + R \langle i|j+k|l \rangle. \quad (4.153)$$

If we can find N_t (knowing the exact form of R is not necessary), then subtracting

$$\frac{s_{ijk} - s_{ijl}}{2} \frac{N_t \mathcal{D}_l}{D_l \mathcal{D}_t} \quad (4.154)$$

⁷As described in Section 4.4, we obtain a result for all coefficients C_i for each probe. Thus, we of course do not perform new probes for each coefficient but perform once as many probes as needed for the most complicated numerator, save the results, and use as many as needed per coefficient.

from the triangle coefficient removes the highest $\langle i|j+k|l \rangle$ pole without introducing new denominator factors. To find N_t , one can use the polynomial reduction techniques from Section 4.2 with the Gröbner basis $\langle \mathcal{D}_l, \langle i|j+k|l \rangle \rangle_{R_6}$. However, this can quickly become computationally expensive for complicated N_l . Instead, we again invoke numerical reconstruction on finite fields. Since their mass dimensions and little-group weights are known, we can build ansätze for N_t and R using Eqs. (4.97)–(4.99) and reconstruct them using random probes of the analytically known $N_l \mathcal{D}_l$. This can be improved even further by using finite-field probes on points where $\langle i|j+k|l \rangle$ vanishes because this way, R does not need to be reconstructed. The generation of such points is discussed in Appendix A.3.

5. Reconstruct triangle coefficients Even after performing the previous step, the mass dimension of numerators of triangle coefficients is often too large to reconstruct them in common-denominator form, and even if doing so, the result contains rational numbers with very large numerators and denominators, requiring to perform the reconstruction on many different prime fields and leading to numerically less stable amplitudes. Therefore, we improve the ansatz using partial fractioning, see Section 4.5.1. To this end, we first find that coefficients of $\text{Tri}(s_{ij}, s_{kl}, s_{mn})/\sqrt{\Delta_{ij|kl|mn}}$ never contain denominator factors other than

$$\langle ij \rangle, \langle kl \rangle, \langle mn \rangle, \langle i|k+l|j \rangle, \langle k|m+n|l \rangle, \langle m|i+j|n \rangle, \Delta_{ij|kl|mn}, \quad (4.155)$$

and factors obtained from those by parity. Keep in mind that momentum conservation implies relations of the form $\langle k|m+n|l \rangle = -\langle k|i+j|l \rangle$. Then, we build a partial-fractioned ansatz by imposing the following heuristic rules on the denominators in each term:

- If the denominator contains $\Delta_{ij|kl|mn}$, do not include any factors $\langle ab \rangle, [ab]$.
- If the denominator contains $\Delta_{ij|kl|mn}^2$, no factor $\langle a|c+d|b \rangle$ has a higher power than one.
- If the denominator contains $\Delta_{ij|kl|mn}$, at most one factor $\langle a|c+d|b \rangle$ has a power two, all others have a lower power.

While we cannot give a definitive statement on how fundamental these rules are, they can be tested for any partial amplitude before its reconstruction by using probes on varieties corresponding to the prime ideals

$$\langle s_{ikl} - s_{jkl}, \langle i|k+l|j \rangle \rangle_{R_6} = \sqrt{\langle \Delta_{ij|kl|mn}, \langle i|k+l|j \rangle \rangle_{R_6}} \quad (\text{c.f. Eqs. (4.116), (4.121)}), \quad (4.156)$$

$$\langle s_{kl} - s_{mn}, \langle ij \rangle \rangle_{R_6} = \sqrt{\langle \Delta_{ij|kl|mn}, \langle ij \rangle \rangle_{R_6}}, \quad (4.157)$$

and ideals related by permutation and parity. Eq. (4.157) was found in Ref. [197] and can be intuitively understood with the relation

$$4\Delta_{ij|kl|mn} = (s_{kl} - s_{mn})^2 + s_{ij}(s_{ij} - 2(s_{kl} + s_{mn})). \quad (4.158)$$

It is particularly useful to perform probes on p -adic points where $\langle i|k+l|j \rangle = \mathcal{O}(p^2)$ and $s_{ikl} - s_{jkl} = \mathcal{O}(p)$, i.e. the latter vanishes linearly as usual but the former vanishes to squared order instead. This way, if we find $N = \mathcal{O}(p^2)$, we know directly that we can write

$$N = N_1 \langle i|k+l|j \rangle + N_2 (s_{ikl} - s_{jkl})^2 = \tilde{N}_1 \langle i|k+l|j \rangle + \tilde{N}_2 \Delta_{ij|kl|mn}, \quad (4.159)$$

leading to a valid partial-fraction decomposition. Probes with $\langle ij \rangle = \mathcal{O}(p^2)$, $s_{kl} - s_{mn} = \mathcal{O}(p)$ are useful analogously.

Probes on such varieties can not only be used to validate the heuristic rules from above, but also to identify further partial-fractioning possibilities or numerator factors. Additional ansatz improvements can be made by testing membership to the two prime ideals from the decomposition [197]

$$\langle \langle i|k+l|j \rangle, \langle k|i+j|l \rangle \rangle_{R_6} = \langle \langle ik \rangle, [jl] \rangle_{R_6} \cap \langle \langle i|k+l|j \rangle, \langle k|i+j|l \rangle, s_{il} - s_{jk} \rangle_{R_6} \quad (4.160)$$

and ideals related by permutation.

Given a partial-fractioned ansatz, we can reconstruct the numerators analogously to step 3. The only difference is that the coefficients of the numerators of the different summands are not necessarily all linearly independent. In Ref. [197], they describe a way to first numerically eliminate all redundant coefficients and then solve the system of equations to obtain the remaining ones, however, we simply use the overcomplete ansatz and remove the redundant coefficients during Gaussian elimination.

6. $\Delta_{ij|kl|mn}$ poles Having reconstructed all triangle coefficient, we can use Eq. (4.139) to remove the leading $\Delta_{ij|kl|mn}$ poles from the remaining weight-one and weight-zero coefficients. This is done analogously to step 4. The differences are that here also the denominators from Eq. (4.139) have to be included into the $\mathcal{D}_l$ factor, and that we do not use custom phase-space points where $\Delta_{ij|kl|mn}$ vanishes for the reconstruction because we find that N_l is simple enough due to the measures in step 5.

7. $\log(-s_{ijk})$ coefficients The main guidance for reconstructing logarithm coefficients are denominator factors of the form $\langle c|a+b|c \rangle$. It was observed in Refs. [196, 203, 204] that it is always possible to separate them by partial fractioning without introducing new, spurious, denominators. With Eq. (4.133) we can furthermore relate terms in $C[\log(-s_{ijk})]$ which are divergent as $\langle c|a+b|c \rangle \rightarrow 0$ with terms in $C[\log(-s_{ab})]$.⁸ We observe that the numerator mass dimensions of $\log(-s_{ijk})$ coefficients are usually smaller than those of $\log(-s_{ab})$ coefficients, which is why we start by reconstructing the former and using the result to eliminate $\langle c|a+b|c \rangle$ poles from the latter. Fortunately, we find that unlike for other spurious poles, it is possible to bring terms with $\langle c|a+b|c \rangle$ poles into exactly the same form in both $C[\log(-s_{ijk})]$ and $C[\log(-s_{ab})]$, such that these terms contain only denominator factors which are already present in their common-denominator form. This has two convenient implications: First, we can simply add such terms to $C[\log(-s_{ab})]$ once we have reconstructed them in $C[\log(-s_{ijk})]$ without additional calculations akin to those in step 4. Second, we can infer a particularly compact partial-fractioned ansatz for $C[\log(-s_{ijk})]$. To be explicit, we proceed in the following way:

- a. For every $\langle c|a+b|c \rangle$ factor in the denominator of $\log(-s_{ijk})$, identify all denominator factors that are present in both $C[\log(-s_{ijk})]$ and $C[\log(-s_{ab})]$. We denote the product of these factors as $D_{ijk|ab}$.
- b. Reconstruct the numerators in the ansatz

$$\sum_{(ab)} \frac{N_{ijk|ab}}{D_{ijk|ab}} + \frac{N_{ijk|\text{rest}}}{D_{ijk|\text{rest}}}, \quad (4.161)$$

⁸Note that either $\{a, b, c\} = \{i, j, k\}$ or $\{a, b, c\} = \{1, 2, 3, 4, 5, 6\} \setminus \{i, j, k\}$, for which $s_{ijk} = s_{abc}$ due to momentum conservation.

where $D_{ijk|\text{rest}}$ is the denominator of $C[\log(-s_{ijk})]$ without all $\langle c|a+b|c \rangle$ factors.

c. Add $N_{ijk|ab}/D_{ijk|ab}$ to $C[\log(-s_{ab})]$.

8. Remaining coefficients There remain the coefficients $C[\log(-s_{ab})]$ and $C[1]$. The leading $\Delta_{ij|kl|mn}$ poles have been removed from them in step 6, and the $\langle c|a+b|c \rangle$ poles have already been removed from the $\log(-s_{ab})$ coefficients in step 7c. To also eliminate the $\langle c|a+b|c \rangle$ poles in the $C[1]$ coefficient, we can use the known $\langle c|a+b|c \rangle^2$ poles from the $\log(-s_{ijk})$ coefficients together with Eq. (4.135), analogously to step 4. The numerator of the remainder of $C[1]$ is then reconstructed in common-denominator form. For $C[\log(-s_{ab})]$, we again apply heuristic partial-fractioning rules. After subtracting $\langle c|a+b|c \rangle$ and $\Delta_{ij|kl|mn}$ poles individually, we already have parts of the coefficient in a partial-fractioned form

$$C[\log(-s_{ab})] = \sum_{(ijk)} \frac{N_{ijk|ab}}{D_{ijk|ab}} + \frac{N_{ij|kl|mn}}{D_{ij|kl|mn}} + \frac{N_{ab|\text{rest}}}{D_{ab|\text{rest}}}, \quad (4.162)$$

where only $N_{ab|\text{rest}}$ is unknown. To obtain it, we use an ansatz

$$\frac{N_{ab|\text{rest}}}{D_{ab|\text{rest}}} = \sum_i \frac{N_{ab|\text{rest},i}}{D_{ab|\text{rest},i}}, \quad (4.163)$$

where we assume that all factors which never appear together in any of the denominators $D_{ijk|ab}$ and $D_{ij|kl|mn}$ can also be separated into different $D_{ab|\text{rest},i}$ denominators. In a few cases, this ambitious partial-fractioning ansatz turns out incorrect, which gets automatically noticed when testing the coefficients obtained by Gaussian elimination on one additional finite-field point, as mentioned in step 3. In this case, we relax some separation assumptions in an ad-hoc manner on a case-to-case basis. This could in principle be refined by testing membership to additional codimension-2 ideals listed in Ref. [197], however, we find this not necessary for our purposes.

This completes the reconstruction of analytic expressions of the amplitudes. The obtained expressions have been made publicly available in Ref. [206], which contains ancillary files to Ref. [3].

4.6 Numerical Implementation

The analytic expressions are implemented as C++ code, which then numerically calculates the squared amplitudes according to Eqs. (4.45) and (4.46). This implementation can then be used for the numerical cross section calculation presented in Chapter 5 and Ref. [3]. Since in the cross section two of the partons are incoming, we need to perform an analytic continuation of the functions listed in Section 4.4.4. The necessary prescriptions can be found in Ref. [207].

To improve the efficiency, we use FORM output optimization for the numerators of individual terms after partial fractioning. We find that this approach of direct compilation of all expressions leads to an implementation which is about a factor five faster than an alternative implementation where the analytic amplitude results are parsed during runtime. Using the qd library [208], we compile the code up to octuple precision to achieve the desired accuracy. This is necessary for our application within a slicing method as outlined in Chapter 5. To test the precision, the amplitude is evaluated a second time for every phase-space point after rescaling all dimensionful quantities by a factor 10. We expect this to simply correspond to a rescaling of the result according to the known mass dimension of the amplitude, c.f. Eq. (4.94). A comparison to

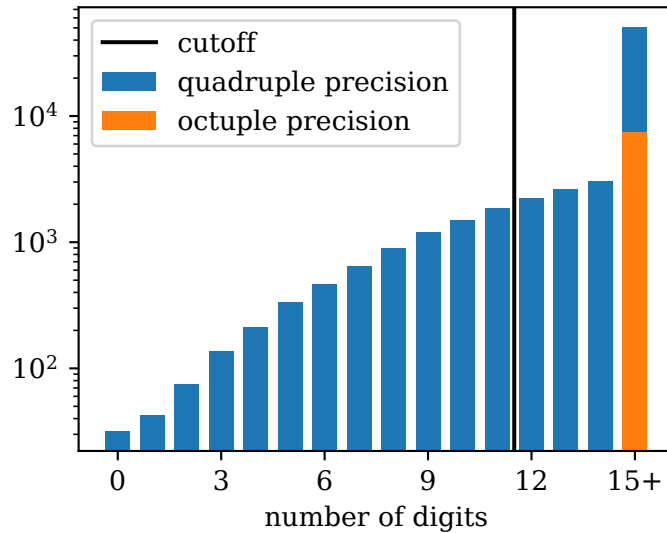


Figure 4.1: Distribution of the number of corrects digits provided by our implementation. Data corresponds a sample of phase-space points used in the cross section calculation described in Chapter 5. Thus, the majority of points lie in infrared regions of the phase space. The points to the left of the vertical bar have less than 12 correct digits and are reevaluated in octuple precision, where they always have at least 15 correct digits. Figure taken from Ref. [3].

this expectation then yields an estimate for the number of correct digits. Figure 4.1 shows this estimate for a sample of phase-space points during the cross section calculation. These are usually infrared phase-space points, which is why we use quadruple precision as the default for all evaluations. If we estimate less than 12 correct digits, we reevaluate the amplitude in octuple precision. We find the average evaluation time per phase-space point, including the rescaled evaluation and potential evaluations in octuple precision, to be 0.5 seconds for the sample of Fig. 4.1. In comparison, the tool *NJet* [209], which also allows evaluations in octuple precision and can provide a precision comparable to our implementation, has an evaluation time which is approximately 100 times longer.

Chapter 5

Photon-Pair Production at N³LO in QCD

As alluded to multiple times throughout the thesis, we finally present the main phenomenological result of this work, the cross section $\sigma_{pp \rightarrow \gamma\gamma}^{\text{N}^3\text{LO}}$ for the production of a photon pair at N³LO in QCD, in this chapter. The results shown here have already been published in Ref. [3].¹ While N³LO calculations of $2 \rightarrow 1$ processes have been achieved with reverse unitarity and q_T slicing, see Chapter 2, our work constitutes the first calculation of a hadron-collider process with $2 \rightarrow 2$ kinematics at this order, marking a milestone in perturbative QCD calculations.

Following the discussion in Chapter 2, the production of a photon pair is the ideal process for making this advancement because they are not colored, which is, at this point in time, a prerequisite in order to use available methods for N³LO calculations for hadron colliders. Apart from this theoretical motivation, photons are an integral part of the physics program of the LHC. While they directly couple to quarks and can therefore probe hard QCD processes, they are observable final-state particles, unlike the colored partons which evolve to form jets. They are detected in the so-called *electromagnetic calorimeters* of the LHC experiments [210, 211]. Thus, they can provide simple signatures with comparatively small systematic uncertainties. Unfortunately, photons are not only produced in the hard process, as shown in Fig. 5.1. They can also stem from collinear radiation off charged partons while a jet is formed, so-called *fragmentation*. Other, so-called *non-prompt* photons can occur after hadronization of partons by hadronic decays. In order to formulate observables which are mostly described by the hard process of interest, one can use *photon isolation*, where one sets a limit on partonic/hadronic activity around photons. This significantly reduces the contribution of the other photon sources, for which the photons oftentimes appear in the vicinity of jets. The simplest realization of such a photon isolation which comes to mind is to simply forbid all partons in a certain radius R around photons. However, such a requirement is not *infrared safe*, i.e. an observable defined this way does not fulfill the requirements of the KLN theorem discussed in Chapter 2. Excluding

¹A note on the author's personal contribution to Ref. [3]. Besides the calculation of the one-loop six-point amplitudes described in Chapter 4, I have performed the complete numerical calculation for the $q\bar{q}$ production channel, the other channels have been calculated by R. Poncelet. For the implementation of the slicing procedure in STRIPPER as described in Section 2.2, I have debugged the implementation provided by T. Generet and performed checks with example calculations of the Drell-Yan production cross section. The implementation of hybrid floating-point precision and updated selector function was done by T. Generet and R. Poncelet. Besides his many preceding contributions to STRIPPER, the software package used here, M. Czakon has coordinated and supervised the project. Note that because I have also written most of the text of Ref. [3], parts of the description of the calculation in this chapter are parallel to the presentation there.

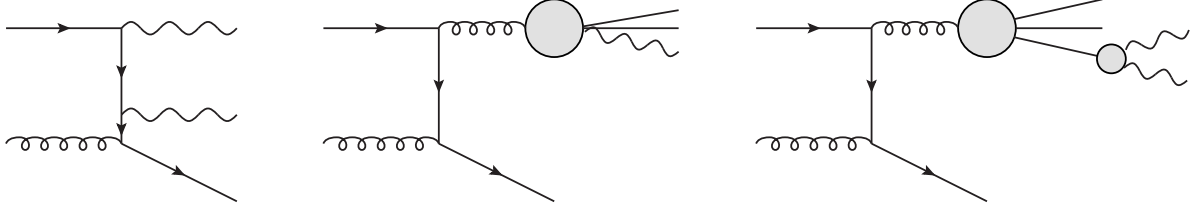


Figure 5.1: Diagrams representing different origins of photons at hadron colliders. While we are usually interested in photons originating in the hard process (left), they can also occur from electromagnetic radiation from charged particles within jets, so-called *fragmentation* (center), or hadronic decays (right).

partonic radiation around photons also forbids the radiation of soft gluons into this phase space, leading to an incomplete cancellation of infrared poles.

To discuss different approaches to tackle this problem, let us first define common parametrizations of the final-state momenta of particles measured at collider experiments. One can define their direction in the laboratory frame using the polar angle θ relative to the beam axis and the azimuthal angle ϕ in the transverse plane. Then, the *pseudorapidity* of a particle is given by

$$\eta \equiv -\log \left[\tan \left(\frac{\theta}{2} \right) \right], \quad (5.1)$$

and the angular distance between particle i and a photon γ reads

$$r_i \equiv \sqrt{(\eta_i - \eta_\gamma)^2 + (\phi_i - \phi_\gamma)^2}. \quad (5.2)$$

With these definitions, we can define a possible theoretical prescription for photon isolation, the so-called *hard-cone* (sometimes called *fixed-cone*) isolation. Instead of forbidding all partonic activity around photons, one limits the summed transverse energy of partons within a fixed radius R_{max}^h . To this end, we define

$$E_T(r) \equiv \sum_{\substack{i \\ r_i < r}} E_{T,i}, \quad (5.3)$$

i.e. the sum of transverse energies $E_{T,i}$ of all partons i within the radius r . We then impose

$$E_T(r) < E_T^{\text{max}} = \epsilon_h E_{T,\gamma}, \quad \text{for } r < R_{\text{max}}^h, \quad (5.4)$$

where $E_{T,\gamma}$ is the transverse energy of the photon and $\epsilon_h = \mathcal{O}(0.1)$ some small parameter. This way, soft radiation is allowed and infrared safety of QCD radiation is restored. However, by allowing some partonic activity up to a radius $r = 0$, it is required to include exact-collinear photon radiation within fragmentation, c.f. the center diagram of Fig. 5.1. This can only be described through non-perturbative *fragmentation functions*, in analogy to the initial state PDFs which describe exact-collinear production of partons from protons. This complicates the theoretical description, making the calculation more complicated. To avoid this, an alternative *smooth-cone* isolation prescription has been proposed in Ref. [212]. There, the condition on partonic transverse energies reads

$$E_T(r) < E_T^{\text{max}}(r) = \epsilon_s E_{T,\gamma} \left(\frac{1 - \cos(r)}{1 - \cos(R_{\text{max}}^s)} \right)^n, \quad \text{for } r < R_{\text{max}}^s, \quad (5.5)$$

which again contains a small parameter $\epsilon_s = \mathcal{O}(0.1)$ and the additional parameter $n > 0$. Because $E_T^{\max}(r) \rightarrow 0$ as $r \rightarrow 0$, there is no need for the inclusion of photon fragmentation, while still maintaining infrared safety. While appealing from a theoretical standpoint, imposing smooth-cone isolation in experimental measurements is not realistic due to finite detector granularity. Instead, hard-cone isolation is the default prescription used in experimental observations of isolated photons, see e.g. Ref. [213] for an experimental study of photon isolation. To combine the theoretical merits of smooth-cone isolation with the experimentally accessible hard-cone condition, a hybrid prescription has been proposed in Refs. [214, 215], where both conditions, Eqs. (5.4) and (5.5), are imposed with $R_{\max}^s < R_{\max}^h$. This way, the larger hard cone is in agreement with the experimental procedure, while the removal of fragmentation has a smaller effect due to the smaller smooth cone. Still, for an accurate incorporation of the experimental photon-isolation criteria, the most desirable procedure is using only a hard-cone condition while incorporating fragmentation functions, as was done in Ref. [216] for single-photon production at NNLO. However, with no such fragmentation function available at N³LO, we will use the aforementioned hybrid prescription.

Having discussed photons-production at hadron colliders in general, let us now move specifically to the production of a photon pair, $pp \rightarrow \gamma\gamma$. Arguably the most famous occurrence of photon-pair measurements at the LHC was during the Higgs discovery [8, 9], where one of the most important decay channels was $H \rightarrow \gamma\gamma$. It combines a simple topology with a fully visible final state and comparatively small systematic uncertainties. However, for Higgs measurements, the non-resonant background contributions, which include prompt photon-pair production, $pp \rightarrow \gamma\gamma$, as well as processes with one or two non-prompt photons, are usually not modeled with theoretical Monte Carlo simulations but with data-driven methods. While an N³LO prediction of $\sigma_{pp \rightarrow \gamma\gamma}$ improves the theoretical modeling, this alone is not sufficient to completely replace data-driven techniques. For this, improvements in parton showers, hadronization models, and other theoretical tools would be necessary, which is beyond the scope of this thesis.

Still, the measurement of the production cross section of $pp \rightarrow \gamma\gamma$ in itself serves as a precision probe of the SM and has been performed by CMS [217] and ATLAS [218]. There has also been previous interest from the theory side with first NNLO predictions obtained using q_T slicing in Refs. [219, 220]. The results of Ref. [220] for the fiducial cross section for different center-of-mass energies are shown in Fig. 5.2. One immediately notices that the theoretical predictions vastly differ between the different orders in perturbation theory. This is not in line with the expectation of perturbative convergence at lower orders discussed in Chapter 2. There, we have also discussed the method of scale variation to estimate the theoretical uncertainty due to missing higher-order corrections. Again, we see in Fig. 5.2 that this does not seem reliable, with every higher order lying far outside the uncertainty band of the previous order. Also, the size of the uncertainty band increases with higher order. When comparing the predictions to data, one can see that an agreement is observed at NNLO for the first time, while lower orders do not provide reliable predictions.

A possible explanation for this poor convergence is the appearance of new partonic production channels at higher orders. Example diagrams of different partonic channels are shown in Fig. 5.3. While at LO, the only way to produce a photon pair is given by the process $q\bar{q} \rightarrow \gamma\gamma$, different partonic initial states are possible when including real radiation. At NLO, the processes $qg \rightarrow \gamma\gamma q$ and $\bar{q}g \rightarrow \gamma\gamma \bar{q}$ start to contribute, while at NNLO, there are different quark channels such as $qq' \rightarrow \gamma\gamma qq'$ as well as the gluon-gluon channel $gg \rightarrow \gamma\gamma q\bar{q}$. The latter also starts to contribute as a loop-induced contribution $gg \rightarrow \gamma\gamma$. While the loop-induced contribution is a one-loop diagram which is relevant starting at NNLO, it is effectively an LO calculation from

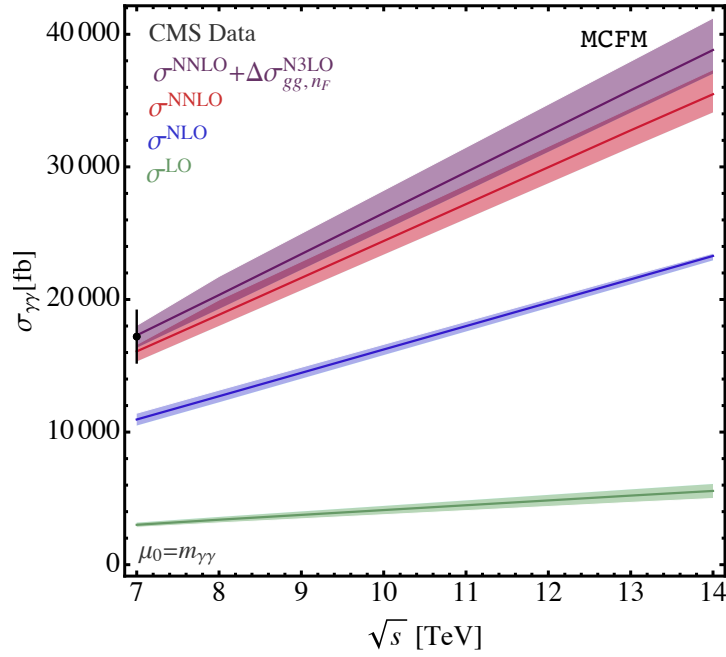


Figure 5.2: Fiducial cross section for photon-pair production as a function of the center-of-mass energy $\sqrt{s}$ through NNLO as calculated in Ref. [220]. A partial $N^3\text{LO}$ result from including corrections to the loop-induced $gg \rightarrow \gamma\gamma$ contribution is also shown. The shaded bands indicate the error estimated through scale variation, c.f. Eq. (2.14). The phase-space cuts were chosen in agreement with a CMS measurement at 7 TeV [217], whose data point is included in the plot. Figure taken from Ref. [220].

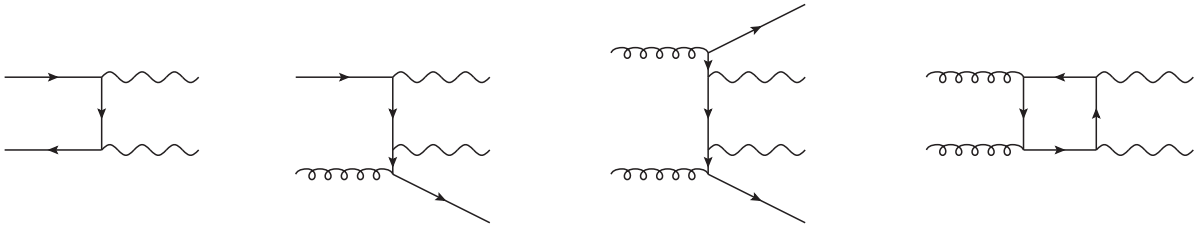


Figure 5.3: Example Feynman diagrams for the production of a photon pair through different partonic channels. From left to right, they contribute starting at LO ($q\bar{q}$), NLO (qg), and NNLO (gg). The rightmost diagram shows the production in the gg channel through the loop-induced process $gg \rightarrow \gamma\gamma$.

the cross-section point of view, without the need to cancel infrared divergences. Therefore, the N³LO contributions from the effective NLO correction to $gg \rightarrow \gamma\gamma$ can be calculated without the need for an N³LO subtraction or slicing method. This has also been done in Ref. [220] and is shown in Fig. 5.2. While the deviation from the NNLO prediction is small, one still observes an increase in the scale-uncertainty band. For these reasons, a full N³LO calculation, which we present hereafter, is highly desirable from a theoretical point of view in order to study the convergence behavior.

We use the q_T -slicing method described in Section 2.2 for the calculation of $\sigma_{pp \rightarrow \gamma\gamma}^{\text{N}^3\text{LO}}$. For the first term of Eq. (2.32), we use the outlined implementation of Eq. (2.37) within **STRIPPER**. For the hard function H_{ab} , we require virtual corrections to $q\bar{q} \rightarrow \gamma\gamma$ through three-loop order, which are taken from Refs. [221, 222]. The second term of Eq. (2.32) corresponds to an NNLO calculation of $pp \rightarrow \gamma\gamma j$, which has already been performed in Refs. [63, 69]. While we can in principle reuse the **STRIPPER** implementation of Ref. [63], major improvements in precision are necessary in order to apply it to a slicing procedure with small $q_{T,\text{cut}}$. To achieve that, we reimplement the complete **STRIPPER** library to also work in quadruple precision, implemented with the **qd** library [208], on top of the existing double-precision implementation. Depending on how infrared the generated phase-space point is, we choose the faster double precision or the more precise quadruple precision. Furthermore, we update the selector functions, c.f. Eq. (2.21), of the subtraction scheme. In particular, we replace Eq. (18) of Ref. [53] by

$$d_{ij,k} = \frac{E_i}{\sqrt{s}} \frac{E_j}{\sqrt{s}} (1 - \cos \theta_{\min})(1 - \cos \theta_{\max}), \quad \theta_{\min/\max} = \min / \max\{\theta_{ij}, \theta_{ik}, \theta_{jk}\} \quad (5.6)$$

in order to reduce the appearing angular hierarchies. Finally, the precision of the used amplitudes is of highest importance. While we can keep using the tree-level amplitudes from the **avhlib** library [170, 171] which were used in Ref. [63], the two-loop amplitudes need to be updated to those of Ref. [223] to include full-color information. The amplitudes observed to be most crucial to the stability of the calculation are the one-loop six-point amplitudes. Because we find that the **OpenLoops** library [224, 225], which provided these amplitudes for the calculation in Ref. [63], is not sufficient in that regard, and the implementation in **NJet** [209] is too computationally intensive, we employ our custom implementation described in detail in Chapter 4. The only one-loop amplitudes for which we use **OpenLoops** are ones needed for the loop-induced $gg \rightarrow \gamma\gamma$ contributions already calculated in Ref. [220] as discussed above. It is worth noting that similarly to Ref. [220], it would now be possible to include partial N⁴LO results with an effective NNLO calculation of loop-induced contributions because the necessary three-loop $gg \rightarrow \gamma\gamma$ [226] and two-loop $gg \rightarrow \gamma\gamma g$ [227] amplitudes are available. However, we leave this to future work and concentrate on obtaining a pure N³LO prediction.

In order to compare our calculation to the latest ATLAS measurement

$$\sigma_{pp \rightarrow \gamma\gamma}^{\text{ATLAS}} = 31.4 \pm 0.1 \text{ (stat.)} \pm 2.4 \text{ (syst.) pb} \quad (5.7)$$

published in Ref. [218], we adopt the parameters used there. It should be noted that our fixed-order N³LO calculation contains at most five particles in the final state, with up to three radiated partons in addition to the photon pair. This is not a realistic description of the final states measured at the LHC, where usually many more particles are reconstructed from the data. These particles can be produced through soft or collinear splittings of the hard partons. To theoretically simulate this transition from *parton level* to *particle level*, a parton shower, which to some extent resums collinear radiation to all orders in α_s , can be employed. Alternatively, the experi-

mental measurements can be unfolded to parton level by inverting the detector response as well as the parton shower and hadronization. This often introduces further uncertainties, but allows for a direct comparison to fixed-order predictions. In Ref. [218], no such unfolding to parton level was performed. On the other hand, no parton showers that can retain the correctness of the calculation at N³LO are available. Nevertheless, Ref. [218] uses their particle-level results to compare with a fixed-order NNLO calculation obtained with NNLOJET (c.f. Section 2.1). Therefore, we try to reproduce this comparison, while increasing the order to N³LO, by using the same parameters which had been used for the NNLOJET calculation. To be explicit, we work in QCD+QED, see Eq. (1.3), with $n_f = 5$ massless quarks and no top-quark contributions to fermionic loops. We set the QED coupling to $\alpha = 1/137$ and extract the QCD coupling α_s from the NNPDF3.0 PDF set [228] with the LHAPDF software package [229]. This is also used for the values of the PDFs. While the usage of N³LO PDFs would be desirable, only approximate-N³LO sets [230, 231] are available at this point. While there has been remarkable recent progress in the calculations of four-loop splitting functions [232], complete results necessary for exact N³LO PDFs are not available yet. Therefore, we decide to instead employ the aforementioned PDF set in order to maintain comparability with the calculation used in Ref. [218]. We work at the center-of-mass energy $\sqrt{s} = 13$ TeV and employ the following phase-space cuts:

- The transverse momentum of the photon with larger transverse momentum is required to fulfill $p_{T,\gamma_1} > 40$ GeV. The other photon is required to have $p_{T,\gamma_2} > 30$ GeV. Note that this does not set a cut on the transverse momentum of the photon pair, $q_T \equiv p_{T,\gamma\gamma}$, which we use as the slicing variable below.
- The pseudorapidities of the photons are subject to the cuts $|\eta_\gamma| < 2.37$, excluding $1.37 < |\eta_\gamma| < 1.52$.
- The angular separation between the two photons, $\Delta R_{\gamma\gamma} \equiv \sqrt{(\eta_{\gamma_1} - \eta_{\gamma_2})^2 + (\phi_{\gamma_1} - \phi_{\gamma_2})^2}$, is required to be greater than 0.4.
- We use the hybrid photon-isolation prescription outlined above, with the parameters of Eqs. (5.4) and (5.5) set to $\epsilon_h = 0.09$, $R_{\max}^h = 0.2$, $\epsilon_s = 0.15$, $R_{\max}^s = 0.1$, $n = 1$.

Let us note again that the possibility to include such fiducial cuts without theoretical complications is one of the appealing features of subtraction and slicing methods, where the phase-space integration is performed with Monte Carlo methods. Finally, we set the renormalization and factorization scales, c.f. Chapter 2, to the invariant mass of the photon pair, $\mu_R = \mu_F = m_{\gamma\gamma}$. Scale uncertainties are obtained with seven-point scale variation (2.14).

The requirement of very high numerical precision emphasized above can be understood by looking at the first results presented in Fig. 5.4. We show the different contributions to $\sigma_{pp \rightarrow \gamma\gamma j}^{\text{NNLO}}$ within the sector-improved residue subtraction scheme, c.f. Section 2.1, as a function of the slicing parameter

$$r_{\text{cut}} \equiv \frac{q_{T,\text{cut}}}{m_{\gamma\gamma}}. \quad (5.8)$$

Clearly, there are large numerical cancellations between the contributions, especially for small r_{cut} . However, a small r_{cut} is necessary in order to be able to sensibly approximate the first term of Eq. (2.32). Therefore, we require large computational resources to decrease the statistical uncertainty introduced through Monte Carlo integration. In particular, contributions requiring a lot of computation time (resources used for this calculation are given in parentheses in million CPU hours) are σ_F^{RV} (2.7), σ_F^{RR} (2.3), σ_{SU}^{RR} (2.4), σ_{DU}^{RR} (0.5), and σ_F^{VV} (0.6). The

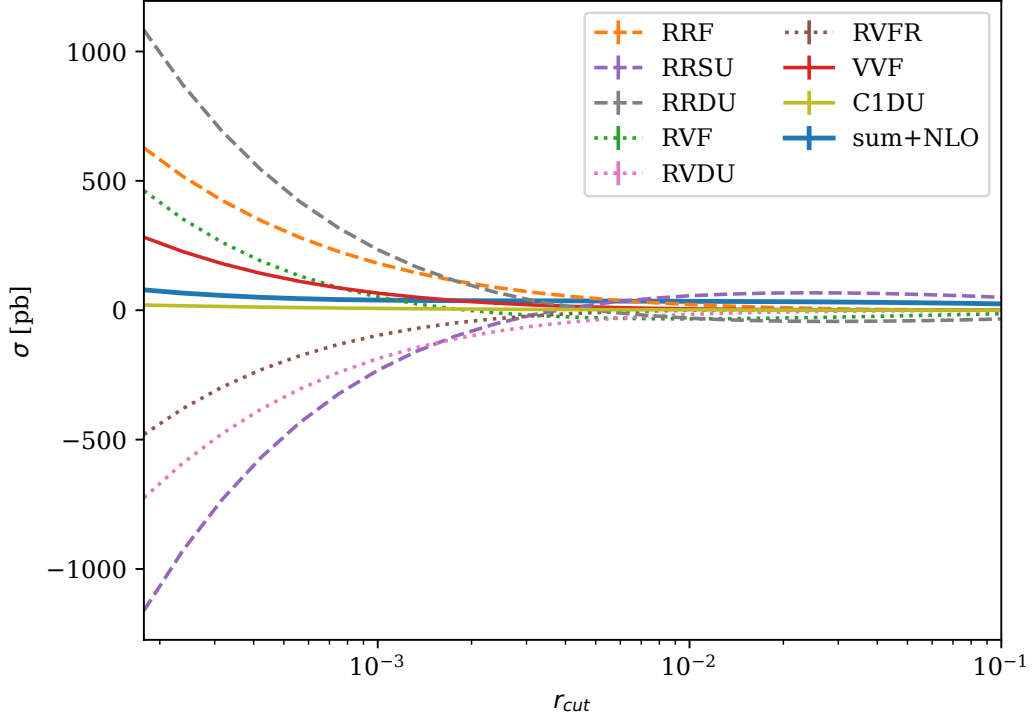


Figure 5.4: Size of the different contributions defined in Eq. (2.31) to the cross section $\sigma_{pp \rightarrow \gamma\gamma j}^{\text{NNLO}}$. We only include those terms of Eq. (2.31) which are non-zero at $\mathcal{O}(\epsilon^0)$. They are shown as a function of the slicing parameter r_{cut} . Figure corresponding to the left plot of Fig. 2 of Ref. [3].

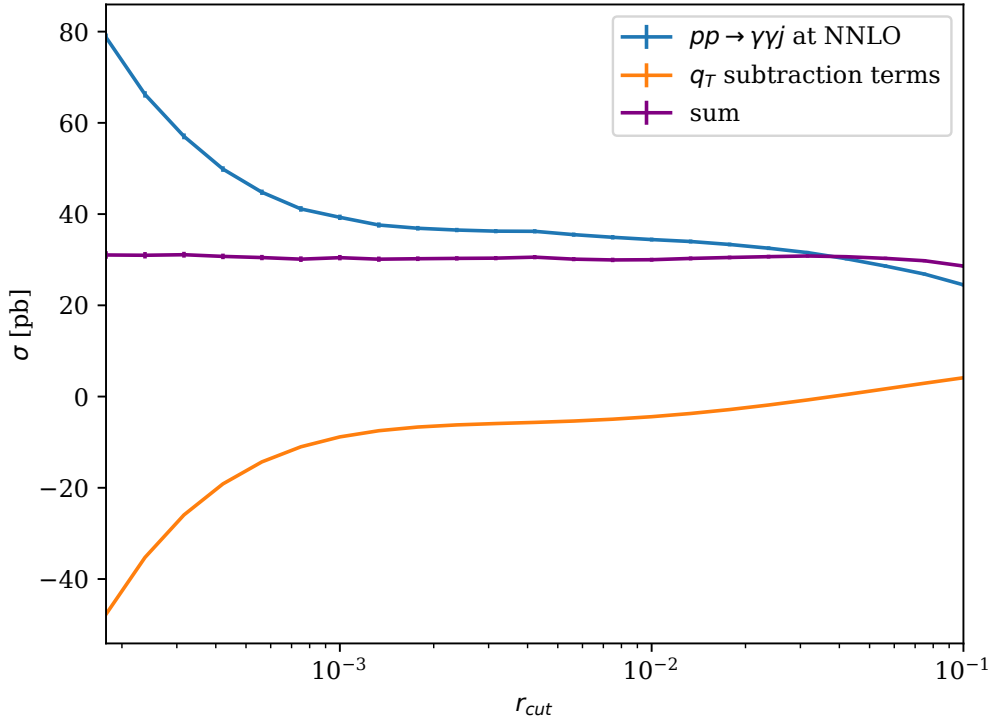


Figure 5.5: Cancellation of the two contributions to q_T slicing, c.f. Eq. (2.32), where we denote the terms approximated with the factorization theorem (2.33) as q_T subtraction terms. Figure corresponding to the center plot of Fig. 2 of Ref. [3].

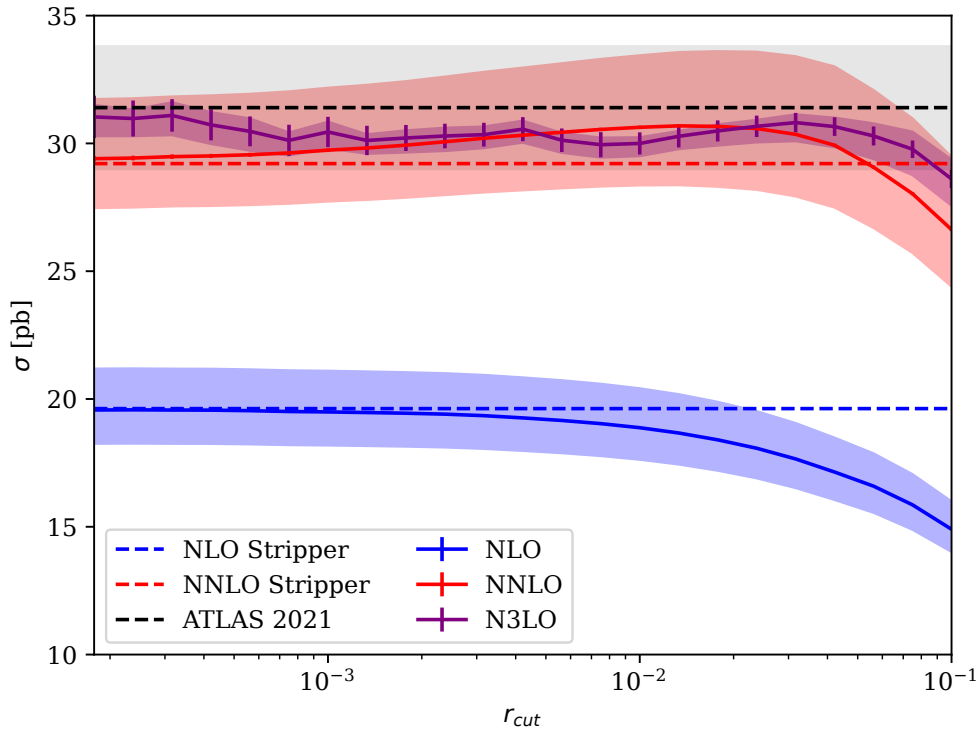


Figure 5.6: NLO, NNLO, and N³LO predictions for the $pp \rightarrow \gamma\gamma$ cross section obtained with the q_T -slicing method, as a function of the slicing parameter r_{cut} . The statistical Monte Carlo uncertainties are displayed as error bars, the shaded bands correspond to the theoretical uncertainty estimated through seven-point scale variation (2.14). The dashed lines show the results of direct cross section calculations with the sector-improved residue subtraction scheme and the experimental result by ATLAS [218]. The uncertainty associated to the latter is also shown as a shaded band. Figure corresponding to the right plot of Fig. 2 of Ref. [3]. Numerical values to reproduce this figure are given in Appendix B.

large cost associated to the computation of σ_F^{RV} emphasizes the necessity of a highly-efficient implementation of the six-point one-loop amplitudes described in Section 4.6.

Besides the cancellation within the NNLO calculation, its result has to further cancel against the low- q_T approximation (2.33). This is displayed in Fig. 5.5. One clearly sees the separately diverging terms for $r_{\text{cut}} < 10^{-3}$ and the convergence of the sum for $r_{\text{cut}} \rightarrow 0$, as expected from Eq. (2.32). This sum constitutes the final prediction for the fiducial cross section $\sigma_{pp \rightarrow \gamma\gamma}^{\text{N}^3\text{LO}}$. We display it again in Fig. 5.6, together with the scale uncertainties, lower-order predictions, and the experimental result by ATLAS. At NLO and NNLO, the result can be obtained both through q_T slicing and with a subtraction scheme. Comparing the two methods, we see that slicing converges to the correct value as $r_{\text{cut}} \rightarrow 0$. The difference between the slicing result for a given r_{cut} and the correct $r_{\text{cut}} \rightarrow 0$ value is referred to as *power corrections*. For the N³LO result, we observe that the central value lies within the scale-uncertainty band of the NNLO result, for the first time indicating perturbative convergence for this process. Furthermore, we see that despite the enormous computational resources that were used, there remains a relatively large Monte Carlo uncertainty of about 2%. However, the uncertainty obtained through scale variation is also about 2%, much smaller than the approximately 8% at NNLO, another sign of perturbative convergence. In view of the small NLO and NNLO power corrections, the relatively large Monte

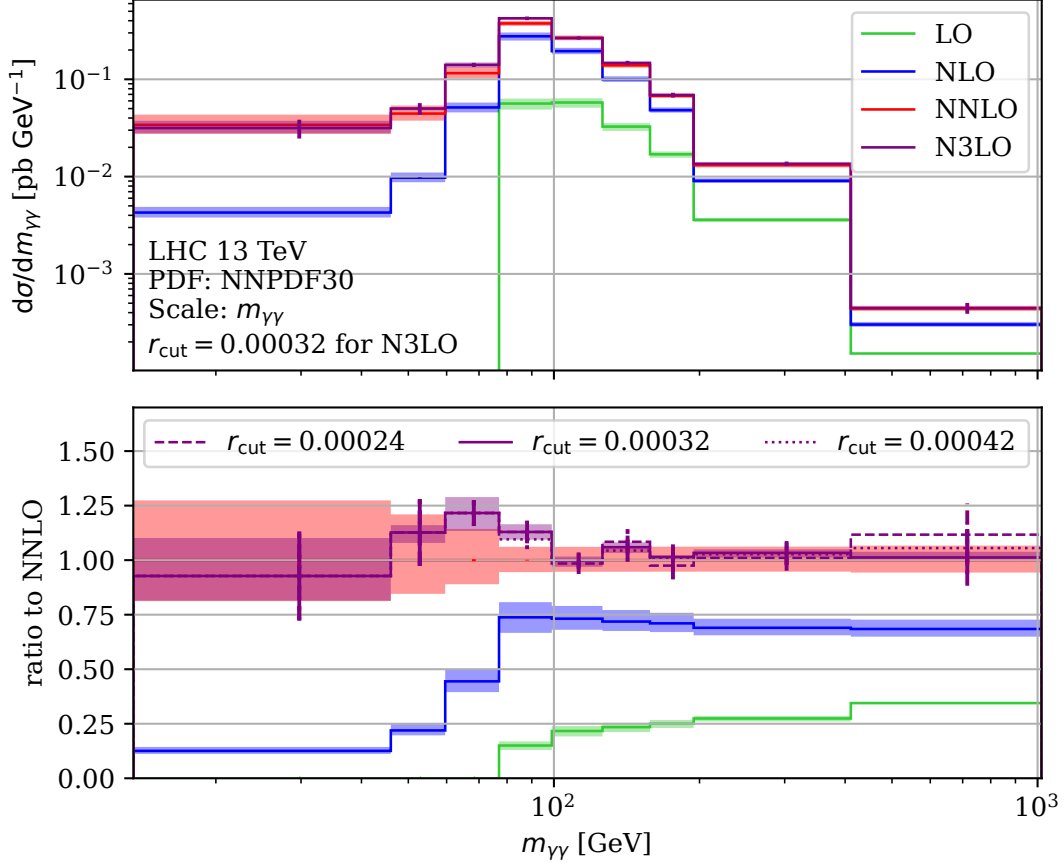


Figure 5.7: Differential cross section $d\sigma_{pp \rightarrow \gamma\gamma}/dm_{\gamma\gamma}$ through N³LO. Up to NNLO, the results are obtained with the subtraction scheme implemented in **STRIPPER**. At N³LO, q_T slicing is used, where we indicate the remaining dependence on the slicing parameter r_{cut} by showing the result for multiple r_{cut} values in the lower panel, where the ratio of all results the NNLO prediction is shown. Figure taken from Ref. [3].

Carlo uncertainty, and the observed convergence of the N³LO result as $r_{\text{cut}} \rightarrow 0$, we decide to quote the value at $r_{\text{cut}} = 3.2 \times 10^{-4}$ as the final result, which then reads

$$\sigma_{pp \rightarrow \gamma\gamma}^{\text{N}^3\text{LO}} = 31.2(6)_{-0.7}^{+0.5} \text{ pb}, \quad (5.9)$$

where the value in parentheses indicates the Monte Carlo uncertainty of 0.6 pb, and $_{-0.7}^{+0.5}$ pb the uncertainty estimated through scale variation. Taken together, the previous 8% uncertainty could be reduced to about 3%. The result is in agreement with the ATLAS measurement of 31.4 ± 2.4 pb ($\sim 8\%$ uncertainty). For future measurements with improved precision, our result provides the necessary reduction of theoretical uncertainty.

Finally, since the q_T -slicing method used here gives access to fully-differential information, we are able to produce the $m_{\gamma\gamma}$ distribution of the cross section through N³LO, shown in Fig. 5.7. Again, we observe perturbative convergence and a negligible dependence on r_{cut} . However, due to the optimization of the Monte Carlo integration to minimize the statistical uncertainty of the total cross section, larger Monte Carlo uncertainties are present in less dominant $m_{\gamma\gamma}$ regions, of comparable size to the scale uncertainty of the NNLO result.

Chapter 6

Conclusions

In this thesis, we have presented results for the fiducial production cross section of a photon pair at the LHC at N³LO. With the fiducial cuts listed in Chapter 5, the final result reads

$$\sigma_{pp \rightarrow \gamma\gamma}^{\text{N}^3\text{LO}} = 31.2(6)^{+0.5}_{-0.7} \text{ pb}, \quad (6.1)$$

with an uncertainty of about 3%. This constitutes the first calculation of a hadron-collider process with $2 \rightarrow 2$ kinematics at this order in perturbation theory. We observed perturbative convergence and a reduction in the scale uncertainty compared to the NNLO result, which had an uncertainty of about 8%. In contrast, no convergence and increasing scale uncertainties had been observed up to NNLO.

To achieve this result, we have performed a calculation with the q_T -slicing method. This calculation required a numerical calculation with very high numerical stability. Among other things, we have performed an analytic calculation with an efficient numerical implementation of the necessary six-point one-loop amplitude using modern techniques for amplitude computations.

Additionally, we have gained insights into the structure of general QCD amplitudes by studying their behavior at next-to-leading power in infrared limits. In particular, we have presented expansions valid at NLP for the collinear limit of tree-level amplitudes as well as for the soft-gluon limit of one-loop amplitudes, which may include both massless and massive particles.

There exist many possible future directions for NLP calculations. There are the obvious extensions of our results to higher loop orders or to the radiation of multiple infrared particles. Additionally, while we have presented results for both massive and massless amplitudes in the soft expansion, the massless case is not simply the smooth $m \rightarrow 0$ limit of the massive result. In particular, the collinear region described in Section 3.4.3 must be included for massless particles while being unnecessary in the massive case. This can lead to problems if the emitted gluon is soft compared to the momenta of all other particles, but some particles have a mass of comparable size to the gluon momentum. To study this case, a separate expansion in the small mass is necessary. Such an expansion has recently been studied in the QED case in Ref. [123]. There, they still include a so-called $J_{f\partial\gamma}$ jet function, where derivatives of the Born amplitude need to be included, which we have shown to be unnecessary for the soft-gluon expansion in Section 3.4.3. An extension to QCD and a study of the necessity of this $J_{f\partial\gamma}$ function are interesting future problems.

Regarding cross section calculations, the obvious next step is the calculation of a hadron-collider cross section with a resolved jet in the final state at N³LO in QCD. This might shed light on the interesting question of factorization-breaking effects discussed in Chapter 2. This is because such effects start to be potentially relevant at N³LO when massless colored particles

appear in both initial and final state. A possible road to such a calculation is the usage of N -jettiness slicing, see Section 2.2. With very recent progress in the calculation of N -jettiness soft functions [233, 234], obtaining the necessary one-jettiness soft function at $N^3\text{LO}$ might be achievable in the near future. On the other hand, the enormous computational resources needed for the calculation presented in this thesis show that relying purely on slicing methods might not be a sustainable path. For example, Fig. 5.4 impressively shows the reduced numerical cancellations within a **STRIPPER** calculation if phase-space points farther away from infrared divergences are calculated. Therefore, it can be concluded from the results of this thesis that the long-term future objective should be the construction of a subtraction scheme applicable to $N^3\text{LO}$ hadron-collider cross sections.

Appendix A

Ingredients for Amplitudes at Higher Order in QCD

In this appendix, we summarize basic ingredients necessary for the computation of QCD amplitudes. In particular, they are relevant for the calculations in Chapters 3 and 4.

A.1 Feynman Rules

The most important building blocks for amplitude calculations are Feynman diagrams with the corresponding Feynman rules. In this section, we summarize these rules for QCD including massless and massive fermions. Additionally, we include the interactions of quarks with photons within QED.

Quark propagators have the value

$$i \xrightarrow{p} j = i\delta_{ij} \frac{\not{p} + m}{p^2 - m^2 + i0^+}, \quad (\text{A.1})$$

which is also valid for massive quarks with $m = 0$. Gluon propagators depend on the gauge choice. In a physical gauge, also called light-cone gauge,

$$a, \mu \xrightarrow{p} b, \mu = i\delta^{ab} \frac{1}{p^2 + i0^+} \left(-g_{\mu\nu} + \frac{p_\mu n_\nu + p_\nu n_\mu}{p \cdot n} \right), \quad (\text{A.2})$$

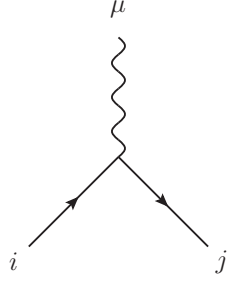
with an arbitrary light-like reference vector n^μ , whose dependence cancels when calculating physical gauge-invariant quantities. Alternatively, one can use a covariant gauge, where

$$a, \mu \xrightarrow{p} b, \mu = i\delta^{ab} \frac{1}{p^2 + i0^+} \left(-g_{\mu\nu} + (1 - \xi) \frac{p_\mu p_\nu}{p^2 + i0^+} \right), \quad (\text{A.3})$$

with arbitrary ξ . The value $\xi = 1$ corresponds to Feynman gauge. In case of covariant gauges, one also needs to introduce ghosts as internal particles. The ghost propagator reads

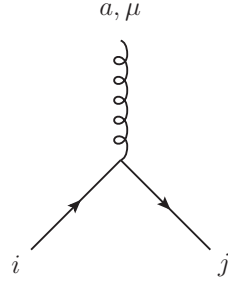
$$a \xrightarrow{p} b = i\delta^{ab} \frac{1}{p^2 + i0^+}. \quad (\text{A.4})$$

The Feynman rules for vertices are

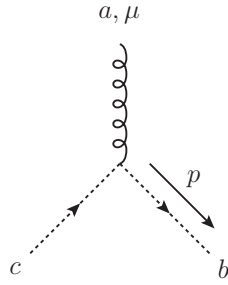


$$= ieQ\gamma^\mu, \quad (\text{A.5})$$

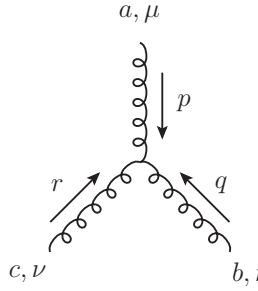
Q being the charge of the quark,



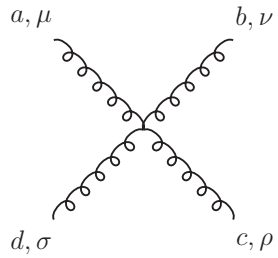
$$= ig_s\gamma^\mu T_{ij}^a, \quad (\text{A.6})$$



$$= g_s f^{abc} p^\mu, \quad (\text{A.7})$$



$$= g_s f^{abc} ((p-q)^\rho g^{\mu\nu} + (q-r)^\mu g^{\nu\rho} + (r-p)^\mu g^{\rho\mu}), \quad (\text{A.8})$$



$$= -ig_s^2 (f^{abe} f^{cde} (g^{\mu\rho} g^{\nu\sigma} - g^{\mu\sigma} g^{\nu\rho}) \\ + f^{ace} f^{bde} (g^{\mu\nu} g^{\rho\sigma} - g^{\mu\sigma} g^{\nu\rho}) \\ + f^{ade} f^{bce} (g^{\mu\nu} g^{\rho\sigma} - g^{\mu\rho} g^{\nu\sigma})). \quad (\text{A.9})$$

We do not print Feynman rules related to the counterterm Lagrangian $\mathcal{L}^{CT}$ for wave function and coupling counterterms. The reason is that amplitudes are always polynomial in these quantities, and multiplicative renormalization, e.g. $g_s^B = Z_g g_s^R$, can easily be performed without

attention to the details of the internal interactions in Feynman diagrams. Masses, however, appear non-polynomially as can be seen in Eq. (A.1). It can therefore be useful to perform mass renormalization by means of Feynman rules with the two-point vertex

$$\longrightarrow \text{---} \times \text{---} \longrightarrow = -i(Z_m - 1)m, \quad (\text{A.10})$$

with the mass renormalization constant Z_m in $\overline{\text{MS}}$ renormalization given by

$$Z_m^{\overline{\text{MS}}} = 1 - \frac{3\alpha_s}{4\pi} \frac{1}{\epsilon} + \mathcal{O}(\alpha_s^2). \quad (\text{A.11})$$

In this thesis, the mass counterterm is only relevant in Section 3.4.1.

A.2 Spinors and Polarization Vectors

External particles in scattering amplitudes are not associated with a propagator from Feynman rules, which would be exactly divergent. Instead, the Lehmann-Symanzik-Zimmermann (LSZ) reduction formula [235] dictates that only *amputated* diagrams without external propagator lines contribute. These are then contracted with the external wave functions, spinors in case of fermions and polarization vectors in case of vector bosons, and multiplied with LSZ normalization constants. For massless particles, these LSZ constants cancel the wave function renormalization constants, therefore both of them are of little relevance in practical calculations.

In this section, we summarize relevant formulae regarding the external wave functions. They correspond to different representations of Lorentz transformations and furthermore depend on the momentum of the external particle. Due to this, representations in the space of the wave functions correspond to the *little group* of Lorentz transformations where this momentum remains unchanged. Before discussing the little group, recall that general elements of the Lorentz group,¹

$$\Lambda(\omega) = e^\omega, \quad (\text{A.12})$$

correspond to elements of the universal cover $\text{SL}(2, \mathbb{C})$. In particular,

$$A(\omega) = e^{-\frac{i}{2}\omega_{\mu\nu}[\frac{i}{4}(\sigma^\mu\bar{\sigma}^\nu - \sigma^\nu\bar{\sigma}^\mu)]} \in \text{SL}(2, \mathbb{C}), \quad (\text{A.13})$$

where

$$\sigma^0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (\text{A.14})$$

are the Pauli matrices and $\bar{\sigma}^\mu \equiv (\sigma^0, -\sigma^1, -\sigma^2, -\sigma^3)$. In the case of massless particles, the little group elements for the momentum $p_0^\mu = (E, 0, 0, E)$ can now be written as elements of $\text{SL}(2, \mathbb{C})$:

$$A(z, \theta) = \begin{pmatrix} e^{-\frac{i}{2}\theta} & 0 \\ e^{-\frac{i}{2}\theta} z & e^{\frac{i}{2}\theta} \end{pmatrix}, \quad z \in \mathbb{C}, \quad \theta \in [0, 4\pi). \quad (\text{A.15})$$

The representations $\mathcal{D}(A) = A$ and $\mathcal{D}(A) = (A^{-1})^\dagger$ correspond to left-handed and right-handed Weyl spinor representations, respectively. The wave functions which transform with respect to

¹To be precise, we only consider the proper orthochronous Lorentz group throughout this section.

these representations are called Weyl spinors and read

$$\lambda_\alpha(p) \equiv \frac{1}{\sqrt{p^0 + p^3}} \begin{pmatrix} p^0 + p^3 \\ p^1 + ip^2 \end{pmatrix}, \quad \tilde{\lambda}^{\dot{\alpha}} = \frac{1}{\sqrt{p^0 + p^3}} \begin{pmatrix} p^0 + p^3 & p^1 - ip^2 \end{pmatrix}, \quad (\text{A.16})$$

respectively. They fulfill the Weyl equation

$$\hat{p} \lambda(p) = 0, \quad \tilde{\lambda}(p) \hat{p} = 0 \quad (\text{A.17})$$

with

$$\hat{p} \equiv p_\mu \sigma^\mu, \quad \hat{p}_{\alpha\dot{\beta}} = \lambda_\alpha(p) \tilde{\lambda}_{\dot{\beta}}(p), \quad (\text{A.18})$$

where indices are raised with the metric

$$\epsilon^{\alpha\beta} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad \epsilon^{\dot{\alpha}\dot{\beta}} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \quad (\text{A.19})$$

and lowered with

$$\epsilon_{\alpha\beta} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad \epsilon_{\dot{\alpha}\dot{\beta}} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \quad (\text{A.20})$$

Instead of two-dimensional Weyl spinors, one oftentimes works with four-dimensional Dirac spinors, which can be chosen in the massless case as

$$u(p, +\tfrac{1}{2}) \equiv \begin{pmatrix} \lambda_0(p) \\ \lambda_1(p) \\ 0 \\ 0 \end{pmatrix}, \quad u(p, -\tfrac{1}{2}) \equiv \begin{pmatrix} 0 \\ 0 \\ \tilde{\lambda}^{\dot{0}}(p) \\ \tilde{\lambda}^{\dot{1}}(p) \end{pmatrix} \quad (\text{A.21})$$

for particles, with the Dirac spinors of antiparticles defined by

$$v(p, \sigma) \equiv -u(p, -\sigma). \quad (\text{A.22})$$

They fulfill the Dirac equation

$$\not{p} u(p, \sigma) = 0, \quad \bar{u}(p, \sigma) \not{p} = 0, \quad (\text{A.23})$$

where

$$\bar{u}(p, \sigma) \equiv u^\dagger(p, \sigma) \gamma^0 \quad (\text{A.24})$$

is the natural conjugate of $u(p, \sigma)$ and

$$\not{p} \equiv p_\mu \gamma^\mu, \quad (\text{A.25})$$

with the Weyl representation of γ matrices

$$\gamma^\mu = \begin{pmatrix} \mathbb{0}_{2 \times 2} & \sigma^\mu \\ \bar{\sigma}^\mu & \mathbb{0}_{2 \times 2} \end{pmatrix}. \quad (\text{A.26})$$

The representations of general Lorentz transformations in Dirac space are

$$S(\omega) = e^{-\frac{i}{4} \omega_{\mu\nu} \sigma^{\mu\nu}} \quad (\text{A.27})$$

with $\sigma^{\mu\nu} \equiv \frac{i}{2}[\gamma^\mu, \gamma^\nu]$. This leads to the expected property

$$S(\omega)\gamma^\mu S^{-1}(\omega) = (\Lambda(\omega)^{-1})^\mu{}_\nu \gamma^\nu. \quad (\text{A.28})$$

Furthermore, the Lorentz transformations A_p which transform the reference momentum p_0 to the momentum p ,

$$A_p = \frac{1}{\sqrt{2E(p^0 + p^3)}} \begin{pmatrix} \frac{E}{p^0}(p^0 + p^3) & -p^1 + ip^2 \\ \frac{E}{p^0}(p^1 + ip^2) & p^0 + p^3 \end{pmatrix}, \quad p = \Lambda(A_p)p_0, \quad (\text{A.29})$$

acts as

$$S(A_p)u(p_0, \sigma) = u(p, \sigma), \quad (\text{A.30})$$

where we use the notations $\Lambda(A_p)$ and $S(A_p)$ to refer to the elements of the different representations corresponding to the ω defined by $A(\omega) = A_p$. A little group element acts as

$$S(A(z, \theta))u(p_0, \sigma) = e^{-i\theta\sigma}u(p_0, \sigma). \quad (\text{A.31})$$

After noticing that the Lorentz transformation

$$\Lambda(A_{\Lambda p})^{-1}\Lambda\Lambda(A_p) \quad (\text{A.32})$$

is a little group transformation for any Λ and p , one can write the action of an arbitrary Lorentz transformation Λ on a massless Dirac spinor as

$$\begin{aligned} S(\Lambda)u(p, \sigma) &= S(A_{\Lambda p})S(A_{\Lambda p}^{-1})S(\Lambda)S(A_p)S(A_p^{-1})u(p, \sigma) \\ &= S(A_{\Lambda p})S(A(z, \theta))S(A_p^{-1})u(p, \sigma) = e^{-i\theta\sigma}u(\Lambda p, \sigma), \end{aligned} \quad (\text{A.33})$$

where z and θ are defined by

$$S(A(z, \theta)) \equiv S(A_{\Lambda p}^{-1})S(\Lambda)S(A_p). \quad (\text{A.34})$$

The advantage of Dirac space is that intrinsically four-dimensional massive spinors can be treated within the same space. For massive particles, the little group for a particle at rest with momentum $p_0^\mu = (m, 0, 0, 0)$ is given by the standard $\text{SU}(2)$ group of rotations in quantum mechanics. To transform p_0 to an arbitrary momentum p , the Lorentz transformation reads

$$A_p = \frac{\sigma \cdot p + m}{\sqrt{2m(p^0 + m)}}, \quad p = \Lambda(A_p)p_0. \quad (\text{A.35})$$

Accordingly, one can obtain from the Dirac spinors for particles at rest, which can be defined as

$$u(p_0, +\tfrac{1}{2}) \equiv \sqrt{m} \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad u(p_0, -\tfrac{1}{2}) \equiv \sqrt{m} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix}, \quad v(p_0, +\tfrac{1}{2}) \equiv \sqrt{m} \begin{pmatrix} 0 \\ -1 \\ 0 \\ -1 \end{pmatrix}, \quad v(p_0, -\tfrac{1}{2}) \equiv \sqrt{m} \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad (\text{A.36})$$

the spinors at arbitrary momenta with

$$u(p, \sigma) \equiv \frac{\not{p} + m}{\sqrt{2m(E + m)}} u(p_0, \sigma), \quad v(p, \sigma) \equiv \frac{-\not{p} + m}{\sqrt{2m(E + m)}} v(p_0, \sigma). \quad (\text{A.37})$$

Now, the Dirac equation reads

$$(\not{p} - m)u(p, \sigma) = 0, \quad (\not{p} + m)v(p, \sigma) = 0. \quad (\text{A.38})$$

As expected, the action of A_p in spinor space is again

$$S(A_p)u(p_0, \sigma) = u(p, \sigma). \quad (\text{A.39})$$

A little group element $U \in \text{SU}(2)$ acts as

$$S(U)u(p_0, \sigma) = \sum_{\sigma'} \mathcal{D}_{\sigma'\sigma}^{(1/2)}(U)u(p_0, \sigma'), \quad (\text{A.40})$$

with the Wigner rotation matrices $\mathcal{D}_{\sigma'\sigma}^{(1/2)}(U)$. In analogy to the massless case, one obtains for general Lorentz transformations:

$$S(\Lambda)u(p, \sigma) = \sum_{\sigma'} \mathcal{D}_{\sigma'\sigma}^{(1/2)}(U)u(\Lambda p_i, \sigma'), \quad (\text{A.41})$$

where U is defined by

$$S(U) \equiv S(A_{\Lambda p}^{-1})S(\Lambda)S(A_p). \quad (\text{A.42})$$

Finally, let us consider wave functions in the case of massless vector bosons. As the name suggests, they can conveniently be written in four-dimensional Minkowski space, in equivalence to ordinary vectors. An explicit representation are the polarization vectors

$$\varepsilon_\mu(p, \pm 1) = \frac{\pm 1}{\sqrt{2}p^0(p^1 \mp ip^2)} \begin{pmatrix} 0 \\ p^1 p^3 \mp ip^0 p^2 \\ p^2 p^3 \pm ip^0 p^1 \\ (p^3)^2 - (p^0)^2 \end{pmatrix}, \quad (\text{A.43})$$

which fulfill $p \cdot \varepsilon(p, \sigma) = \bar{p} \cdot \varepsilon(p, \sigma) = 0$, with $\bar{p}^\mu = (p^0, -p^1, -p^2, -p^3)$, and

$$\sum_\sigma \varepsilon_\mu(p, \sigma) \varepsilon_\nu^*(p, \sigma) = -g_{\mu\nu} + \frac{p_\mu \bar{p}_\nu + p_\nu \bar{p}_\mu}{p \cdot \bar{p}}. \quad (\text{A.44})$$

The little group is identical to the case of massless quarks. With a , b , and θ defined by

$$\Lambda(A(a + ib, \theta)) \equiv \Lambda(A_{\Lambda p}^{-1})\Lambda\Lambda(A_p), \quad (\text{A.45})$$

in analogy to Eq. (A.34), arbitrary Lorentz transformations act as

$$\Lambda_\mu^\nu \varepsilon_\nu(p, \sigma) = e^{-i\theta\sigma} \left(\varepsilon_\mu(\Lambda p, \sigma) + \frac{\sigma a + ib}{\sqrt{2}E} (\Lambda p)_\mu \right). \quad (\text{A.46})$$

The second term appears to be a potential problem to the Lorentz invariance of scattering amplitudes. This is prevented by the fact that an amplitude M fulfills the *Ward identity*

$$M_{\varepsilon(p, \sigma) \rightarrow p} = 0. \quad (\text{A.47})$$

An alternative representation for polarization vectors is used in spinor-helicity formalism introduced in Section 4.1. It reads

$$\varepsilon_\mu^*(p, r, +1) \equiv \frac{[p|\gamma_\mu|r\rangle}{\sqrt{2}\langle rp\rangle}, \quad \varepsilon_\mu^*(p, r, -1) \equiv -\frac{\langle p|\gamma_\mu|r\rangle}{\sqrt{2}[rp]}, \quad (\text{A.48})$$

with an arbitrary reference momentum r . In this case, $p \cdot \varepsilon(p, r, \sigma) = r \cdot \varepsilon(p, r, \sigma)$ and

$$\sum_\sigma \varepsilon_\mu(p, r, \sigma) \varepsilon_\nu^*(p, r, \sigma) = -g_{\mu\nu} + \frac{p_\mu r_\nu + p_\nu r_\mu}{p \cdot r}. \quad (\text{A.49})$$

A.3 Six-Particle Spinor-Helicity Phase-Space Points

In this section, we discuss an ingredient for the specific amplitude calculation in Chapter 4. There, we work in the spinor-helicity formalism and need to generate random values for spinor brackets. When doing so, we need to make sure that they fulfill Schouten and momentum-conservation identities, Eqs. (4.17), (4.18). To achieve this, one can randomly sample values for the brackets

$$\langle 34 \rangle, \langle 35 \rangle, \langle 45 \rangle, \langle 46 \rangle, \langle 56 \rangle, [21], [31], [41], [51], [61], [62], [63], [64], [65]. \quad (\text{A.50})$$

The number of 14 independent variables can be understood by the eight independent variables appearing when working with six-point momentum-twistor variables and the additional six phase factors associated to the spinors, one for each particle. The remaining variables can then be obtained using the relations

$$\begin{aligned} [54] &= \frac{[51][64] - [41][65]}{[61]} \\ [53] &= \frac{[51][63] - [31][65]}{[61]} \\ [43] &= \frac{[41][63] - [31][64]}{[61]} \\ [52] &= \frac{[51][62] - [21][65]}{[61]} \\ [42] &= \frac{[41][62] - [21][64]}{[61]} \\ [32] &= \frac{[31][62] - [21][63]}{[61]} \\ \langle 25 \rangle &= \frac{\langle 35 \rangle [31] + \langle 45 \rangle [41] - \langle 56 \rangle [61]}{-[21]} \\ \langle 24 \rangle &= \frac{\langle 34 \rangle [31] - \langle 45 \rangle [51] - \langle 46 \rangle [61]}{-[21]} \\ \langle 36 \rangle &= \frac{\langle 35 \rangle \langle 46 \rangle - \langle 34 \rangle \langle 56 \rangle}{\langle 45 \rangle} \\ \langle 15 \rangle &= \frac{\langle 25 \rangle [62] + \langle 35 \rangle [63] + \langle 45 \rangle [64]}{-[61]} \\ \langle 14 \rangle &= \frac{\langle 24 \rangle [62] + \langle 34 \rangle [63] - \langle 45 \rangle [65]}{-[61]} \end{aligned} \quad (\text{A.51})$$

$$\begin{aligned}
\langle 26 \rangle &= \frac{\langle 36 \rangle [31] + \langle 46 \rangle [41] + \langle 56 \rangle [51]}{-[21]} \\
\langle 23 \rangle &= \frac{-(\langle 34 \rangle [41]) - \langle 35 \rangle [51] - \langle 36 \rangle [61]}{-[21]} \\
\langle 16 \rangle &= \frac{-(\langle 36 \rangle [32]) - \langle 46 \rangle [42] - \langle 56 \rangle [52]}{-[21]} \\
\langle 13 \rangle &= \frac{\langle 34 \rangle [42] + \langle 35 \rangle [52] + \langle 36 \rangle [62]}{-[21]} \\
\langle 12 \rangle &= \frac{-(\langle 34 \rangle [43]) - \langle 35 \rangle [53] - \langle 45 \rangle [54] - \langle 36 \rangle [63] - \langle 46 \rangle [64] - \langle 56 \rangle [65]}{-[21]}
\end{aligned}$$

which embed Schouten identities and momentum conservation.

In order to generate phase-space points that lie on specific varieties, one has to further reduce the number of randomly sampled variables. For the variety $V(\langle\langle 5|3+4|6 \rangle\rangle_{R_6})$, one can set

$$[64] = -\frac{\langle 35 \rangle [63]}{\langle 45 \rangle} \quad (\text{A.52})$$

instead of sampling it randomly, and then proceed as for any phase-space point. Phase-space points on any variety of the form $V(\langle\langle i|j+k|l \rangle\rangle_{R_6})$ can then be obtained by appropriate permutation of spinor brackets. In analogy, points lying on $V(\langle\langle i|j+k|i \rangle\rangle_{R_6})$ can be generated by permutation of spinor brackets on $V(\langle\langle 6|4+5|6 \rangle\rangle_{R_6})$ obtained by setting

$$[65] = -\frac{\langle 46 \rangle [64]}{\langle 56 \rangle}. \quad (\text{A.53})$$

Appendix B

Detailed Numerical Results of the Photon-Pair Production Cross Section

In this appendix, we report the numerical values to reproduce Fig. 5.6. They have already been published as supplementary material to Ref. [3]. The direct **STRIPPER** calculations at NLO and NNLO have produced the values $\sigma^{\text{NLO}} = 19.62^{+1.62}_{-1.32}$ and $\sigma^{\text{NNLO}} = 29.21(5)^{+2.28}_{-1.89}$. In Table B.1, we present the values obtained with the q_T -slicing method as a function of the slicing parameter r_{cut} .

Table B.1: Values obtained with q_T slicing that are displayed in Fig. 5.6. Table taken from the supplementary material of Ref. [3].

r_{cut}	σ^{NLO}	σ^{NNLO}	$\sigma^{\text{N}^3\text{LO}}$
0.000178	$19.57(3)^{+1.62}_{-1.32}$	$29.40(9)^{+2.33}_{-1.93}$	$31.14(83)^{+0.43}_{-0.72}$
0.000237	$19.58(3)^{+1.62}_{-1.32}$	$29.43(9)^{+2.33}_{-1.93}$	$31.07(70)^{+0.31}_{-0.66}$
0.000316	$19.57(3)^{+1.62}_{-1.32}$	$29.48(8)^{+2.35}_{-1.94}$	$31.19(64)^{+0.48}_{-0.74}$
0.000422	$19.56(2)^{+1.62}_{-1.32}$	$29.51(7)^{+2.36}_{-1.95}$	$30.81(61)^{+0.46}_{-0.72}$
0.000562	$19.54(2)^{+1.61}_{-1.31}$	$29.56(7)^{+2.38}_{-1.96}$	$30.56(58)^{+0.46}_{-0.73}$
0.000750	$19.51(2)^{+1.61}_{-1.31}$	$29.63(7)^{+2.41}_{-1.98}$	$30.12(60)^{+0.30}_{-0.57}$
0.001000	$19.49(2)^{+1.61}_{-1.31}$	$29.74(7)^{+2.44}_{-2.01}$	$30.45(59)^{+0.40}_{-0.62}$
0.001334	$19.47(2)^{+1.60}_{-1.31}$	$29.82(7)^{+2.47}_{-2.03}$	$30.11(57)^{+0.24}_{-0.49}$
0.001778	$19.44(2)^{+1.60}_{-1.30}$	$29.93(7)^{+2.50}_{-2.05}$	$30.21(50)^{+0.29}_{-0.54}$
0.002371	$19.41(2)^{+1.60}_{-1.30}$	$30.06(7)^{+2.54}_{-2.08}$	$30.29(47)^{+0.32}_{-0.56}$
0.003162	$19.35(2)^{+1.59}_{-1.30}$	$30.20(6)^{+2.59}_{-2.12}$	$30.34(46)^{+0.31}_{-0.50}$
0.004217	$19.26(2)^{+1.58}_{-1.29}$	$30.32(6)^{+2.64}_{-2.15}$	$30.55(46)^{+0.33}_{-0.50}$
0.005623	$19.16(2)^{+1.57}_{-1.28}$	$30.44(6)^{+2.70}_{-2.19}$	$30.13(45)^{+0.28}_{-0.47}$
0.007499	$19.04(2)^{+1.56}_{-1.26}$	$30.55(6)^{+2.75}_{-2.23}$	$29.95(49)^{+0.27}_{-0.48}$
0.010000	$18.88(2)^{+1.54}_{-1.25}$	$30.63(6)^{+2.81}_{-2.27}$	$30.00(43)^{+0.24}_{-0.47}$
0.013335	$18.67(2)^{+1.51}_{-1.23}$	$30.69(6)^{+2.88}_{-2.32}$	$30.28(43)^{+0.21}_{-0.48}$
0.017783	$18.40(2)^{+1.48}_{-1.20}$	$30.66(6)^{+2.94}_{-2.36}$	$30.49(41)^{+0.25}_{-0.55}$
0.023714	$18.07(1)^{+1.45}_{-1.17}$	$30.58(6)^{+3.00}_{-2.39}$	$30.67(41)^{+0.25}_{-0.61}$
0.031623	$17.65(1)^{+1.40}_{-1.14}$	$30.35(6)^{+3.05}_{-2.43}$	$30.80(37)^{+0.32}_{-0.71}$
0.042170	$17.14(1)^{+1.34}_{-1.09}$	$29.93(5)^{+3.08}_{-2.43}$	$30.65(36)^{+0.34}_{-0.80}$
0.056234	$16.59(1)^{+1.28}_{-1.04}$	$29.07(5)^{+3.01}_{-2.38}$	$30.28(37)^{+0.47}_{-0.89}$
0.074989	$15.86(1)^{+1.20}_{-0.97}$	$28.03(5)^{+2.94}_{-2.31}$	$29.76(34)^{+0.67}_{-1.00}$
0.100000	$14.90(1)^{+1.09}_{-0.88}$	$26.63(5)^{+2.85}_{-2.23}$	$28.61(36)^{+0.74}_{-1.04}$

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