

Precision QCD Studies of Semi-Inclusive Deep Inelastic
Scattering at Electron-Ion Collider

By

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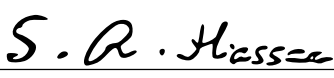
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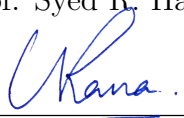
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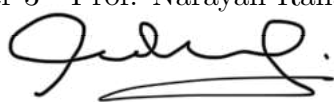

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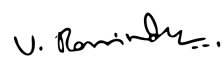

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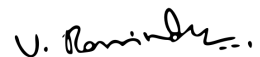


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Saurav Goyal

Dedicated,

*To my family,
whose love, support, and sacrifices
have been my greatest strength.*

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Introduction

The strong interaction is one of the four fundamental forces of nature. It governs the dynamics of quarks and gluons, binds them into hadrons, and ultimately provides the force responsible for holding protons and neutrons together inside atomic nuclei. Quantum Chromodynamics (QCD), the non-Abelian gauge theory based on the local $SU(3)_C$ color symmetry, provides the fundamental description of strong interactions and has been remarkably successful in explaining a wide range of phenomena across vastly different energy scales. At short distances, or equivalently at large momentum transfers, the running of the strong coupling leads to asymptotic freedom, allowing physical observables to be computed systematically using perturbation theory, while at large distances the phenomenon of confinement gives rise to the formation of color-neutral hadrons. Despite the success of QCD as the underlying theory of the strong interaction, understanding how the observed properties of hadrons emerge from the dynamics of quarks and gluons remains one of the central challenges of modern nuclear and particle physics.

Among the most fundamental questions are how the momentum and spin of the nucleon are distributed among its constituents, how different quark flavors contribute to its internal structure, and how colored partons produced in hard-scattering processes hadronize into the color-neutral hadrons observed experimentally. Addressing these questions requires not only a detailed understanding of the non-perturbative structure of hadrons but also highly precise perturbative calculations that connect

experimental measurements with the underlying partonic dynamics. In this sense, high-precision perturbative QCD calculations play an essential role in unraveling the momentum, flavor, and spin structure of the nucleon, together with the mechanisms by which partons hadronize into the observed final-state hadrons.

Deep-Inelastic Scattering (DIS), in which a high-energy lepton is scattered from a hadronic target and only the scattered lepton is detected in the final state, has played a central role in unveiling the partonic structure of hadrons. The pioneering experiments at SLAC established the existence of point-like constituents inside the proton and laid the foundation for the parton model and the subsequent development of QCD. Since then, measurements from fixed-target experiments and high-energy colliders have led to increasingly precise determinations of parton distribution functions (PDFs), which describe the probability of finding a parton carrying a given fraction of the hadron momentum and encode the longitudinal momentum distributions of quarks and gluons inside hadrons. Nevertheless, several important aspects of nucleon structure remain only partially constrained, particularly the flavor decomposition of the sea quark distributions, the polarized parton distributions, and the parton contribution to the nucleon spin. Moreover, the mechanism through which energetic partons produced in hard-scattering processes evolve into observable hadrons is encoded in fragmentation functions (FFs), whose precise determination is equally essential for understanding hadronic final states. Both PDFs and FFs are non-perturbative quantities that connect the partonic description of QCD to experimentally measured hadronic observables.

A major step toward addressing these fundamental questions will be provided by the Electron-Ion Collider (EIC), a future high-luminosity polarized electron-ion collider to be constructed at Brookhaven National Laboratory. The EIC has been designed to explore the structure of nucleons and nuclei with unprecedented precision over a broad kinematic range. It will collide polarized electrons with polarized protons and

light ions, as well as unpolarized nuclei, at center-of-mass energies ranging from approximately 20 to 140 GeV. The combination of high luminosity, polarized beams, variable center-of-mass energies, and excellent detector capabilities will enable measurements with a level of precision far exceeding that of previous facilities.

The scientific program of the EIC extends well beyond improving the precision of existing measurements. One of its principal goals is to determine the 3-dimensional structure of nucleons by simultaneously probing the longitudinal momentum, transverse momentum, spatial distributions, and spin correlations of quarks and gluons. In particular, the EIC aims to provide precise information on flavor-separated quark distributions, polarized quark and gluon densities, and the dynamics of gluons at small Bjorken- x . These measurements are expected to substantially improve our understanding of the origin of nucleon mass and spin, the emergence of hadronic structure from QCD, and the behavior of strongly interacting matter in previously unexplored kinematic regimes.

The unprecedented experimental precision anticipated at the EIC demands equally precise theoretical predictions. The extraction of partonic distributions from experimental observables relies on perturbative QCD calculations through the QCD factorization theorem, where measurable cross sections are expressed as convolutions of universal non-perturbative functions and perturbatively calculable coefficient functions. As experimental uncertainties continue to decrease, theoretical uncertainties originating from missing higher-order perturbative corrections become one of the dominant sources limiting the precision of phenomenological analyses. Consequently, the development of increasingly accurate perturbative predictions has become indispensable for fully exploiting the scientific potential of the EIC.

Among the key processes to be studied at the EIC, Semi-Inclusive Deep-Inelastic Scattering (SIDIS) occupies a particularly important role. In SIDIS, in addition to the scattered lepton, an identified hadron is observed in the final state. This

makes the process more differential than inclusive DIS and provides simultaneous access to the partonic structure of the incoming nucleon and the fragmentation of final-state partons into observed hadrons. The former is described in terms of parton distribution functions, while the latter is encoded in fragmentation functions. SIDIS is therefore an ideal process for studying PDFs and FFs in a unified framework, and plays a central role in flavor separation, spin-dependent studies, and understanding of hadron formation mechanism.

Since SIDIS provides simultaneous access to PDFs and FFs, precise theoretical predictions for this process are essential for the physics program of the EIC. Within QCD factorization, the measured cross-sections are expressed in terms of universal non-perturbative PDFs and FFs convoluted with perturbatively calculable coefficient functions. The inclusion of higher-order QCD corrections is therefore essential for the accuracy of theoretical predictions and hence the PDF and FF extractions from experimental data. While the leading-order calculation captures the basic dynamics of the process, it generally exhibits a significant dependence on unphysical scales like renormalization and factorization scales. This dependence is systematically reduced by including higher-order contributions, thereby improving the stability and reliability of theoretical predictions. In addition, new partonic channels open up beyond leading order and can give sizable contributions to the coefficient functions, making them indispensable for precision phenomenology. Until recently, theoretical predictions for SIDIS were known fully only up to next-to-leading order, with approximate information available at next-to-next-to-leading order in certain limits. The complete NNLO QCD corrections therefore represent an important step toward precision SIDIS phenomenology, providing the accuracy required to match the level of precision expected at the EIC and to reduce the theoretical uncertainties in future phenomenological analyses.

Although the complete NNLO calculation substantially improves the fixed-order de-

scription of SIDIS, the perturbative coefficient functions contain threshold-enhanced logarithmic contributions in the partonic threshold region. These logarithms arise from soft and collinear configurations of QCD radiation and can become dominant when the partonic kinematics approach the threshold limit, thereby spoiling the convergence of the perturbative expansion and significantly reducing the reliability of fixed-order predictions. To obtain stable and precise theoretical results, these dominant logarithmic contributions must be systematically resummed to all orders in the strong coupling. Using QCD factorization and renormalization-group invariance, threshold resummation organizes these enhanced terms systematically to all orders in the strong coupling and provides a natural extension of the fixed-order calculation. It therefore plays an important role in improving theoretical predictions in the kinematic regions that will be explored by the EIC.

Beyond the electromagnetic SIDIS process mediated by a virtual photon exchange, the broad kinematic reach of the EIC will also allow detailed studies of neutral-current and charged-current electroweak SIDIS. Neutral-current interactions receive contributions from both photon and Z boson exchange, while charged-current processes proceed through the exchange of $W^\pm$ bosons. These processes provide complementary information on the flavor structure of the nucleon and offer enhanced sensitivity to specific combinations of quark and anti-quark distributions that cannot be accessed through purely electromagnetic interactions. With polarized beams, they also offer additional access to the spin-dependent structure of the nucleon within the electroweak sector. Precise theoretical predictions for these processes are therefore required for future EIC analyses and form an important part of the precision SIDIS program addressed in this thesis.

Motivated by these experimental and theoretical developments, the primary objective of this thesis is to improve the theoretical description of Semi-Inclusive Deep-Inelastic Scattering within the framework of perturbative QCD. The work presented

here includes the computation of complete next-to-next-to-leading-order QCD corrections to polarized SIDIS, the evaluation of the master integrals required for these calculations, the development of a threshold resummation framework beyond fixed-order perturbation theory, and the extension of the NNLO formalism to neutral-current and charged-current electroweak SIDIS. Together, these results contribute toward the level of theoretical precision required to fully exploit the physics potential of the Electron-Ion Collider.

The remainder of this thesis is organized as follows. Chapter 1 introduces the theoretical framework of Quantum Chromodynamics, including the QCD Lagrangian, Feynman rules, the fundamental properties of perturbative QCD, ultraviolet renormalization, and infrared factorization. Chapter 2 presents the theoretical foundations of Deep-Inelastic Scattering, Semi-Inclusive Annihilation, and Semi-Inclusive Deep-Inelastic Scattering, establishing the factorization formalism and kinematic framework relevant to this thesis. Chapter 3 presents the complete next-to-next-to-leading-order QCD calculation of polarized SIDIS with photon exchange, together with the computational framework and phenomenological analysis. Chapter 4 is devoted to the evaluation of the master integrals required for the NNLO calculation. It discusses the master integrals arising from the different contributions, including the new integrals associated with double-real radiation. Their analytic evaluation is described using direct parametrizations, the differential equation method, canonical bases and related techniques for obtaining analytic solutions. Having obtained the fixed-order NNLO coefficient functions, Chapter 5 develops the framework for threshold resummation in SIDIS. It derives the dominant logarithmic contributions beyond fixed-order perturbation theory, organizes them systematically to all orders using QCD factorization and renormalization-group invariance, and provides predictions for the threshold enhanced terms up to fourth order. Chapter 6 extends the NNLO analysis to SIDIS mediated by neutral-current and charged-current electroweak interactions, presenting complete coefficient functions for both polarized

and unpolarized processes and discussing their phenomenological relevance for future EIC studies. Finally, Chapter 7 summarizes the main results of this thesis and outlines possible directions for future research.

Chapter 1

Quantum Chromodynamics

Quantum Chromodynamics provides the theoretical foundation for the study of strong interactions and underlies all perturbative calculations presented in this thesis. In this chapter, we introduce the fundamental concepts of perturbative QCD, including the QCD Lagrangian, the corresponding Feynman rules, and the theoretical framework required for higher-order calculations. Particular emphasis is placed on ultraviolet renormalization and the treatment of infrared singularities through mass factorization, which are indispensable ingredients of perturbative QCD. Collectively, these concepts establish the theoretical basis for perturbative studies of high-energy scattering processes.

1.1 Introduction

Quantum Chromodynamics (QCD) is the fundamental quantum field theory describing the strong interaction, one of the four fundamental forces of nature. It describes the interactions of quarks and gluons, the elementary constituents of hadrons, through the exchange of color charge. Unlike Quantum Electrodynamics (QED), which is based on the Abelian gauge group $U(1)$, QCD is a non-Abelian gauge theory based on the local $SU(3)_C$ color gauge symmetry. As a consequence of its non-Abelian structure, gluons carry color charge and interact with one another, leading to remarkable phenomena such as asymptotic freedom at short distances and color confinement at long distances.

The success of QCD has established it as the fundamental theory of strong interactions over a wide range of energy scales. At sufficiently large momentum transfer, the strong coupling becomes small owing to asymptotic freedom, allowing physical observables to be computed systematically within perturbative QCD. This perturbative framework forms the basis of the higher-order calculations presented in this thesis, including the next-to-next-to leading order (NNLO) corrections and threshold resummation for semi-inclusive deep-inelastic scattering.

In this chapter, we summarize the essential aspects of Quantum Chromodynamics that form the theoretical foundation of the perturbative calculations presented in this thesis. Particular emphasis is placed on the formulation of the QCD Lagrangian, the corresponding Feynman rules, and the perturbative framework required for higher-order calculations. It is not intended to be a complete review of QCD, but a brief introduction to establish the conventions and notations used throughout this thesis. For more details, see for e.g. [4–17] or standard textbooks. The discussion also includes ultraviolet renormalization and the treatment of infrared singularities through mass factorization, which constitute the theoretical basis for the precision studies of Semi-Inclusive Deep-Inelastic Scattering presented in the subsequent chapters.

1.2 QCD Lagrangian and Feynman Rules

The dynamics of the strong interaction are described by a Lagrangian that is invariant under local $SU(3)_C$ gauge transformations. The gauge-invariant QCD Lagrangian is given by

$$\mathcal{L}_{\text{inv}} = -\frac{1}{4}F_{\mu\nu}^a F^{a,\mu\nu} + \sum_f^{n_f} \bar{\psi}_i^{(f)} (i\gamma_\mu D_{ij}^\mu - m_f \delta_{ij}) \psi_j^{(f)}, \quad (1.1)$$

where $\psi_i^{(f)}$ denotes the quark field of flavor f , mass m_f and of color i ($i, j = 1, 2, 3$). The index $a = 1, \dots, 8$ labels the gluon color index. The matrices γ^μ are the Dirac gamma matrices, satisfying the anticommutation relation $\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}$. Note, the repeated color indices are understood to be summed over. The covariant derivative is defined as

$$D_{ij}^\mu = \delta_{ij} \partial^\mu - ig_s T_{ij}^a A^{a,\mu} \quad (1.2)$$

where g_s is the strong coupling constant, T^a are the generators of the $SU(3)_C$ gauge group in the fundamental representation and A^a denotes the gluon gauge field. The gluon field-strength tensor is

$$F_{\mu\nu}^a = \partial_\mu A_\nu^a - \partial_\nu A_\mu^a + g_s f^{abc} A_\mu^b A_\nu^c, \quad (1.3)$$

where f^{abc} are the structure constants of the $SU(3)_C$ gauge group. The first term in Eq. (1.1) describes the dynamics of the gluon fields and through the nonlinear term in $F_{\mu\nu}^a$, generates the characteristic three-gluon and four-gluon self-interactions. The second term contains the kinetic and mass terms of the quark fields together with the quark-gluon interaction arising from the minimal coupling to the gluon fields through the covariant derivative.

The gauge-invariant QCD Lagrangian remains invariant under the local gauge trans-

formations,

$$\psi(x) \rightarrow U(x)\psi(x), \quad A_\mu(x) \rightarrow U(x)A_\mu(x)U^\dagger(x) - \frac{i}{g_s}(\partial_\mu U(x))U^\dagger(x), \quad (1.4)$$

where

$$U(x) = \exp \left[i\theta^a(x)T^a \right] \quad (1.5)$$

is a space-time dependent element of the $SU(3)_C$ gauge group, with $\theta^a(x)$ being the local gauge transformation parameters.

Although local gauge invariance is the fundamental symmetry underlying QCD, it also implies that the gluon field possesses redundant, unphysical degrees of freedom. As a consequence, gauge-field configurations related by a local gauge transformation describe the same physical state, leading to an over-counting of equivalent configurations in the path-integral formulation. Moreover, this redundancy makes the gluon kinetic operator non-invertible, preventing the construction of a well-defined gluon propagator. To remove this redundancy and obtain a consistent perturbative quantization of the theory, a gauge-fixing condition must be imposed.

Throughout the thesis, we employ the covariant Feynman gauge, for which the gauge-fixing term is

$$\mathcal{L}_{\text{GF}} = -\frac{1}{2\xi} \left(\partial^\mu A_\mu^a \right)^2. \quad (1.6)$$

with the gauge parameter chosen as $\xi = 1$ is called Feynman Gauge. However, physical observables are independent of the gauge choice.

The covariant gauge-fixing procedure in a non-Abelian gauge theory is more subtle than in QED. Since the gauge transformations of QCD are nonlinear in the gluon fields, imposing a gauge condition modifies the path-integral measure by a field-

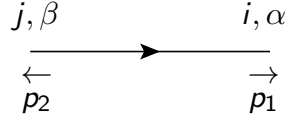
dependent Jacobian, known as the Faddeev-Popov determinant. It is represented by introducing anticommuting scalar fields, called the Faddeev-Popov (FP) ghost fields, which are spin-0 particles but obeying fermionic statistics. From a physical point of view, enforcing a covariant gauge condition leaves unphysical polarization states in the gluon propagator that do not automatically decouple from physical amplitudes. The ghost fields contribute only through closed loops and exactly cancel the contributions from the unphysical gluon polarizations. Although, FP ghosts are not physical particles and never appear as external states, they are essential for preserving gauge invariance, unitarity, and the consistency of perturbative QCD. Their dynamics are described by the Faddeev-Popov ghost Lagrangian,

$$\mathcal{L}_{\text{FP}} = \partial^\mu \bar{c}^a \left(\delta^{ab} \partial_\mu + g_s f^{abc} A_\mu^b \right) c^c, \quad (1.7)$$

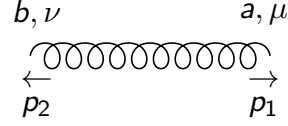
where c^a and $\bar{c}^a$ denote the ghost and anti-ghost fields, respectively, transforming under the adjoint representation of the gauge group. The complete gauge-fixed QCD Lagrangian is therefore given by

$$\mathcal{L}_{\text{QCD}} = \mathcal{L}_{\text{inv}} + \mathcal{L}_{\text{GF}} + \mathcal{L}_{\text{FP}}. \quad (1.8)$$

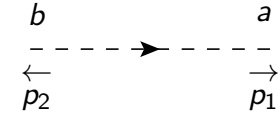
The Feynman rules of QCD are obtained directly from the complete gauge-fixed Lagrangian. Throughout this thesis, quarks are represented by straight lines, gluons by curly lines, and Faddeev-Popov ghosts by dotted lines. The momentum-space Feynman rules for the quark, gluon, and ghost propagators, together with the quark-gluon, ghost-gluon, three-gluon, and four-gluon interaction vertices, constitute the basic ingredients for constructing scattering amplitudes order-by-order in perturbative QCD. The complete set of Feynman rules for an $\text{SU}(N_c)$ gauge theory is summarized in Figs. [1.1](#) and [1.2](#).



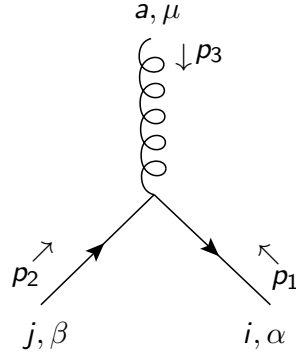
$$i(2\pi)^4 \delta^4(p_1 + p_2) \delta_{ij} \left(\frac{1}{\not{p}_1 - m_f} \right)_{\alpha\beta}$$



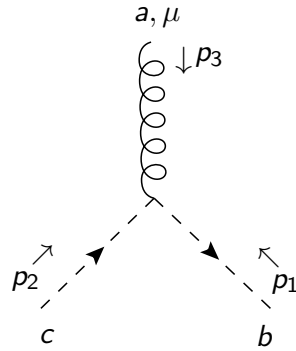
$$i(2\pi)^4 \delta^4(p_1 + p_2) \delta^{ab} \frac{1}{p_1^2} \times \left(-g_{\mu\nu} + (1 - \xi) \frac{p_1^\mu p_1^\nu}{p_1^2} \right)$$



$$i(2\pi)^4 \delta^4(p_1 + p_2) \delta^{ab} \frac{1}{p_1^2}$$

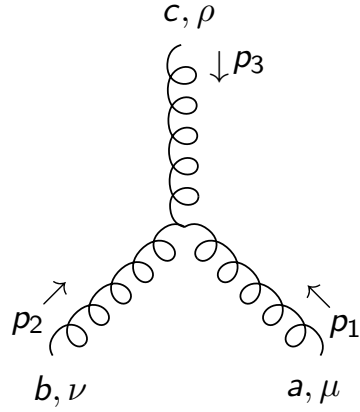


$$ig_s(2\pi)^4 \delta^4(p_1 + p_2 + p_3) T_{ij}^a (\gamma^\mu)_{\alpha\beta}$$

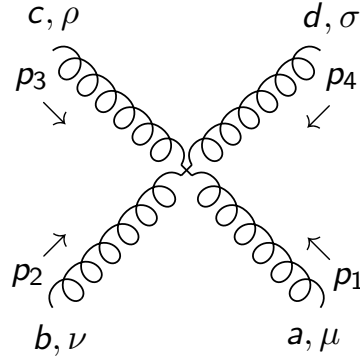


$$-g_s(2\pi)^4 \delta^4(p_1 + p_2 + p_3) f^{abc} p_1^\mu$$

Figure 1.1: Momentum-space Feynman rules for the quark, gluon, and ghost propagators, together with the quark-gluon and ghost-gluon interaction vertices, in a general covariant gauge.



$$\begin{aligned} & \frac{g_s}{3!} (2\pi)^4 \delta^4(p_1 + p_2 + p_3) f^{abc} \\ & \times \left[g^{\mu\nu} (p_1 - p_2)^\rho + g^{\nu\rho} (p_2 - p_3)^\mu \right. \\ & \left. + g^{\rho\mu} (p_3 - p_1)^\nu \right] \end{aligned}$$



$$\begin{aligned} & -\frac{g_s^2}{4!} (2\pi)^4 \delta^4(p_1 + p_2 + p_3 + p_4) \\ & \times \left[(f^{ace} f^{bde} - f^{ade} f^{bce}) g^{\mu\nu} g^{\rho\sigma} \right. \\ & + (f^{abe} f^{cde} - f^{ade} f^{bce}) g^{\mu\rho} g^{\nu\sigma} \\ & \left. + (f^{ace} f^{dbe} - f^{ade} f^{cde}) g^{\mu\sigma} g^{\nu\rho} \right] \end{aligned}$$

Figure 1.2: Momentum-space Feynman rules for the gluon self-interaction vertices.

In the above Feynman rules, the indices are defined as follows:

- $a, b, \dots$ denote color indices in the adjoint representation, taking values $1, \dots, N_c^2 - 1$.
- $i, j, \dots$ denote color indices in the fundamental representation, taking values $1, \dots, N_c$.
- $\alpha, \beta, \dots$ denote Dirac spinor indices.
- $\mu, \nu, \dots$ denote Lorentz indices.

The quantities f^{abc} are the totally antisymmetric structure constants of the $SU(N_c)$ gauge group. They are related to the generators T^a of the fundamental representation through the commutation relation

$$[T^a, T^b] = if^{abc}T^c. \quad (1.9)$$

The generators T^a are traceless, Hermitian matrices which are normalized according to

$$\text{Tr}(T^a T^b) = T_F \delta^{ab}, \quad (1.10)$$

where, $T_F = \frac{1}{2}$. The generators satisfy the completeness relation

$$T_{ij}^a T_{kl}^a = \frac{1}{2} \left(\delta_{il} \delta_{kj} - \frac{1}{N_c} \delta_{ij} \delta_{kl} \right). \quad (1.11)$$

Note, repeated color indices are understood to be summed over. The following identities are used in simplifying the color algebra:

$$T_{ik}^a T_{kj}^a = C_F \delta_{ij}, \quad f^{acd} f^{bcd} = C_A \delta^{ab}, \quad (1.12)$$

where the quadratic Casimir operators in the fundamental and adjoint representations are given by

$$C_F = \frac{N_c^2 - 1}{2N_c}, \quad C_A = N_c. \quad (1.13)$$

For QCD, corresponding to the gauge group $SU(3)$, one has

$$N_c = 3, \quad C_F = \frac{4}{3}, \quad C_A = 3, \quad T_F = \frac{1}{2}, \quad (1.14)$$

with n_f denoting the number of active quark flavors.

1.3 Perturbative Calculation in QCD

Quantum Chromodynamics exhibits two remarkable and complementary properties: color confinement and asymptotic freedom. Together, they govern the behavior of the strong interaction over different distance and energy scales.

At large distances, corresponding to low momentum transfer, quarks and gluons (collectively called partons) are confined within color neutral hadrons such as protons, neutrons, and mesons. Unlike the electromagnetic interaction, the attractive force between colored particles does not diminish as they are separated, instead, it increases with distance. Consequently, attempting to pull a quark out of a hadron requires an ever-increasing amount of energy. Once this energy exceeds the threshold for quark-antiquark pair production, new colored particles are created from the vacuum and combine with the original partons to form new color-singlet hadrons, rather than allowing isolated quarks or gluons to exist. Although a rigorous analytical proof of confinement is still lacking, it is strongly supported by experimental observations, as no free quarks or gluons have ever been detected.

In contrast, at sufficiently short distances or equivalently at high momentum transfer, the interaction between quarks and gluons becomes asymptotically weak. This remarkable property, known as asymptotic freedom, was discovered independently by [18] and by [19] in 1973, a discovery recognized with the 2004 Nobel Prize in Physics, see also [20–22]. Asymptotic freedom implies that quarks and gluons behave asymptotically free particles in high-energy scattering processes, thereby providing the theoretical foundation for perturbative Quantum Chromodynamics (pQCD).

In this regime, the strong coupling constant is sufficiently small that physical observables can be computed systematically as a perturbative expansion in powers of the strong coupling $\alpha_s = g_s^2/(4\pi)$, with successive terms representing higher-order radiative corrections. A generic perturbative expansion for a physical observable (σ)

can be written as

$$\sigma = \sigma^{(0)} + \alpha_s \sigma^{(1)} + \alpha_s^2 \sigma^{(2)} + \cdots, \quad (1.15)$$

where $\sigma^{(0)}$ denotes the leading-order (LO) contribution, while $\sigma^{(1)}$, and the subsequent terms correspond to the next-to-leading-order (NLO) and higher-order corrections, respectively. The inclusion of higher-order contributions systematically improves the precision of theoretical predictions and reduces their dependence on the unphysical scales like renormalization and factorization scales. Beyond leading order, the calculations receive contributions from both virtual (loop) diagrams and real-emission processes. These higher-order corrections introduce ultraviolet (UV) and infrared (IR) divergences in intermediate stages of the calculation. Ultraviolet divergences arise from the short-distance behavior of loop integrals, whereas infrared divergences are associated with soft and collinear parton emissions. Throughout this thesis, both these divergences are regulated using dimensional regularization [23–25], in which the space-time dimensions is analytically continued to $d = 4 + \epsilon$. Within this framework, the divergences manifest themselves as poles in the dimensional regularization parameter ϵ . They are systematically treated within perturbative QCD through renormalization and factorization, respectively. We briefly discuss these aspects in the following sections.

1.3.1 Ultraviolet Renormalization

Virtual loop integrals in perturbative QCD contain ultraviolet (UV) divergences arising from the large-momentum region of the loop integrals. These divergences are regulated using dimensional regularization, in which they appear as poles in the dimensional regularization parameter ϵ , allowing them to be identified and isolated in a systematic and gauge-invariant manner.

The ultraviolet divergences are removed by redefining the parameters and fields appearing in the QCD Lagrangian. Since all quarks are treated as massless throughout the thesis, ultraviolet divergences are removed solely through the renormalization of the QCD coupling constant. The bare coupling $\hat{a}_s = \hat{g}_s^2/(16\pi^2)$ is related to the renormalized coupling $a_s(\mu_R^2)$ by

$$\hat{a}_s S_\epsilon = Z_{a_s}(\mu_R^2) a_s(\mu_R^2) \left(\frac{\mu^2}{\mu_R^2} \right)^{\frac{\epsilon}{2}}, \quad (1.16)$$

where Z_{a_s} is the coupling renormalization constant, μ is the dimensional-regularization scale, μ_R is the renormalization scale, and

$$S_\epsilon = \exp \left(\frac{\epsilon}{2} (\gamma_E - \ln(4\pi)) \right). \quad (1.17)$$

Throughout this thesis, UV renormalization is performed in the modified minimal subtraction ($\overline{\text{MS}}$) scheme, in which the renormalization constant Z_{a_s} absorbs only the poles in the dimensional regularization parameter ϵ , together with the associated universal constants contained in S_ϵ . An important consequence of renormalization is that the strong coupling becomes dependent on the renormalization scale. Its evolution is governed by the renormalization group equation,

$$\mu_R^2 \frac{da_s(\mu_R^2)}{d\mu_R^2} = \frac{\epsilon}{2} a_s(\mu_R^2) + \beta(a_s(\mu_R^2)), \quad (1.18)$$

where $\beta(a_s)$ is the QCD β -function. It admits a perturbative expansion of the form

$$\beta(a_s) = - \sum_{i=0}^{\infty} a_s^{i+2}(\mu_R^2) \beta_i. \quad (1.19)$$

which is known to five loops [26–29], the first two coefficients given by

$$\beta_0 = \frac{11}{3} C_A - \frac{4}{3} T_F n_f, \quad \beta_1 = \frac{34}{3} C_A^2 - \frac{20}{3} C_A T_F n_f - 4 C_F T_F n_f. \quad (1.20)$$

For QCD, $C_A = 3$, $C_F = 4/3$, and $T_F = 1/2$, giving $\beta_0 > 0$ for the physically relevant number of active quark flavors. Consequently, at leading order, the running coupling decreases logarithmically with increasing energy scale, giving rise to the phenomenon of asymptotic freedom. The running of the strong coupling is illustrated in Fig. 1.3. At high energies, the coupling becomes sufficiently small for perturbative calculations to be reliable.

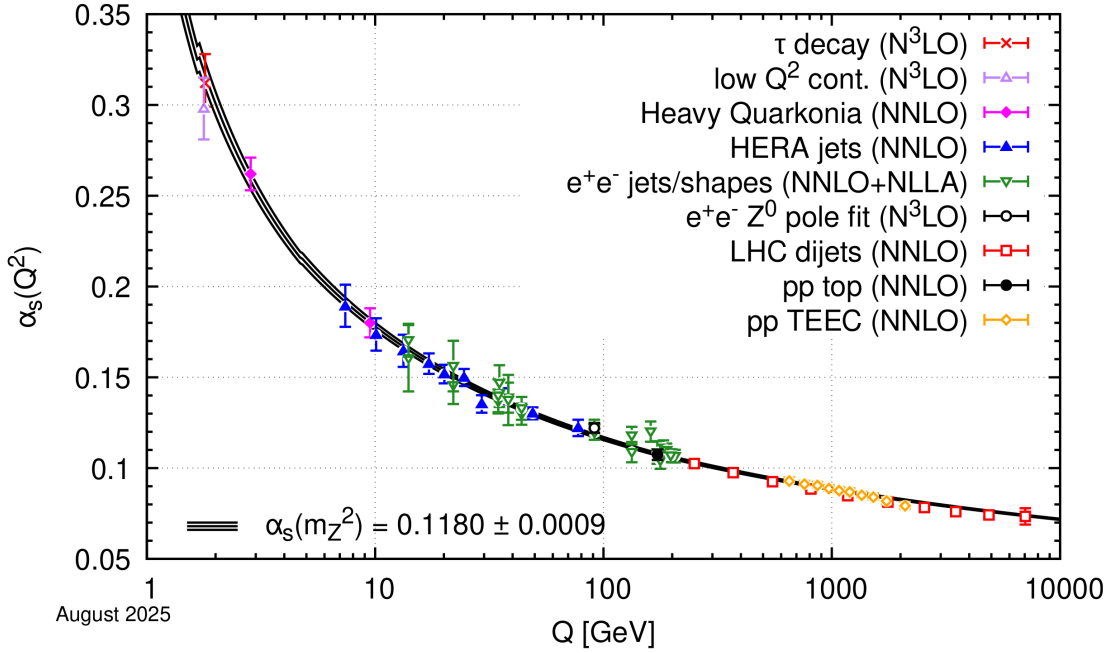


Figure 1.3: Measurements of strong coupling constant $\alpha_s = g_s^2/(4\pi)$ as a function of the energy scale Q compared to the running of the coupling computed at five loops taking as an input the current PDG average, $\alpha_s(m_Z^2) = 0.1180 \pm 0.0009$. Pictures taken from [1].

1.3.2 Infrared Singularities and Factorization

Physical observables, such as scattering cross sections and structure functions, are computed in perturbative QCD as expansions in the strong coupling constant. At large momentum transfers, the internal structure of hadrons is resolved, and the hard interaction occurs between their constituent quarks and gluons. This picture is well described by the so-called parton model, in which the hadron is treated as a collec-

tion of quasi-free, point-like constituents called partons. Within the parton model, the incident probe interacts incoherently with a single parton carrying a fraction of the parent hadron’s momentum. The probability of finding a parton of a given type carrying a momentum fraction of the hadron is encoded in the parton distribution function. The hadronic cross section can then be expressed as a convolution of the perturbatively calculable partonic cross section with the non-perturbative parton distribution functions. For semi-inclusive processes in which a particular hadron is identified in the final state, the factorization formula additionally involves a fragmentation function describing the transition of a final state parton into the observed hadron.

The partonic cross sections are calculated order-by-order in perturbative QCD. After ultraviolet renormalization, the partonic amplitudes and cross sections are, in general, still not finite (in $\epsilon \rightarrow 0$) due to the presence of infrared (IR) singularities. In perturbative QCD with massless quarks and gluons, these divergences arise from two distinct kinematic configurations. Soft divergences occur when the momentum of an emitted parton approaches zero, whereas collinear divergences arise when a massless parton becomes collinear to another massless parton. To obtain physically meaningful predictions, the virtual corrections must be combined with the corresponding real-emission contributions. The latter also contain soft and collinear singularities with the same universal structure as those appearing in the virtual corrections. Upon combining the virtual and real contributions these soft and collinear singularities cancel according to the Kinoshita-Lee-Nauenberg (KLN) theorem [30, 31], which states that the transition rates obtained after summing over all experimentally indistinguishable degenerate initial and final states, the infrared divergences cancel order by order in perturbation theory.

For processes involving hadronic initial states, however, the initial-state collinear singularities do not cancel. Instead, they are universal and are absorbed into the

bare parton distribution functions (PDFs) through the procedure of mass factorization [32–38]. Likewise, in semi-inclusive processes involving identified hadrons in the final state, the remaining collinear singularities associated with the fragmentation process are absorbed into the bare fragmentation functions (FFs).

The universality of PDFs and FFs is a consequence of the QCD factorization theorem, which states that hard-scattering processes involving hadrons can be factorized into a perturbatively calculable short-distance part and universal non-perturbative functions describing the hadronic structure and fragmentation. The short-distance part is process dependent and can be computed order by order in perturbative QCD, whereas the long-distance functions are universal and can be extracted from experimental data [39–83]. This separation forms the theoretical foundation for precision QCD predictions involving hadronic processes.

Similar to UV renormalization, mass factorization is performed at an arbitrary scale, known as the factorization scale, μ_F . Together with the renormalization scale μ_R , it represents an unphysical scale introduced by the perturbative framework. At any finite order in perturbation theory, physical predictions retain a residual dependence on these scales. This dependence is an artifact of truncating the perturbative expansion and is progressively reduced as higher-order corrections are included.

1.4 Summary

In this chapter, we have reviewed the basic theoretical framework of Quantum Chromodynamics relevant to the perturbative calculations presented in this thesis. We introduced the QCD Lagrangian together with the gauge-fixing and Faddeev-Popov ghost terms required for the consistent quantization of the theory, followed by the corresponding Feynman rules that form the building blocks of perturbative QCD calculations.

The distinctive properties of QCD, namely confinement and asymptotic freedom, determine its behavior at different energy scales. While confinement prevents the observation of isolated quarks and gluons, asymptotic freedom ensures that the strong coupling becomes sufficiently small at high energies, thereby enabling reliable perturbative calculations.

We also briefly introduced the parton model description of high-energy hadronic scattering, in which a hard probe interacts with the quarks and gluons (collectively called partons) inside a hadron. Within the QCD factorization framework, hadronic observables are expressed as convolutions of perturbatively calculable partonic cross sections with universal non-perturbative distribution functions.

The treatment of ultraviolet and infrared divergences arising in higher-order calculations was briefly reviewed. Ultraviolet divergences are removed through the renormalization of the strong coupling constant, whereas the remaining collinear singularities are absorbed into universal parton distribution and fragmentation functions through the procedure of mass factorization. This separation of short-distance perturbative dynamics from long-distance non-perturbative physics constitutes the basis of the QCD factorization theorem and underlies precision predictions for hard-scattering processes involving hadrons.

The concepts presented in this chapter constitute the theoretical foundation for the perturbative QCD calculations and phenomenological analyses carried out throughout this thesis.

Chapter 2

Semi-Inclusive Deep-Inelastic Scattering: Theoretical Preliminaries

This chapter provides the theoretical background required for the study of Semi-Inclusive Deep-Inelastic Scattering (SIDIS) within perturbative Quantum Chromodynamics (QCD). It introduces the key concepts of factorization, partonic structure, and QCD evolution that form the basis of all subsequent analysis in this thesis. We begin by reviewing Deep Inelastic Scattering (DIS), the process that played a central role in establishing the partonic structure of hadrons and the development of the QCD improved parton model. This is followed by a brief discussion of semi inclusive annihilation and fragmentation functions, which are essential for describing hadron production in the final state. These ingredients are then combined in the framework of SIDIS. We discuss its theoretical description within the QCD improved parton model, emphasizing the factorization of the cross section into perturbatively calculable coefficient functions and universal parton distribution and fragmentation functions.

2.1 Introduction

Understanding the internal structure of hadrons and the dynamics of their constituents remains one of the central goals of high-energy physics. Since quarks and gluons are confined within hadrons, they cannot be observed as free particles. Instead, information about their properties, interaction and their dynamics must be inferred through high-energy scattering experiments that probe hadronic matter at increasingly shorter distance scales. Building on the QCD framework introduced in the previous chapter, we now discuss the high-energy scattering processes that provide experimental access to the internal structure of hadrons.

The modern understanding of hadron structure originated from Deep Inelastic Scattering (DIS) experiments performed at the Stanford Linear Accelerator Center (SLAC) in the late 1960s [84, 85]. These experiments provided the first evidence that protons possess an internal substructure and led to the development of the parton model. The subsequent formulation of QCD and the discovery of asymptotic freedom established the theoretical foundation for describing the strong interactions of quarks and gluons.

Today, a variety of scattering processes are used to investigate different aspects of hadron structure. DIS provides access to the partonic content of hadrons, while electron-positron annihilation offers direct information on the hadronization of partons. Combining these two perspectives naturally leads to Semi-Inclusive Deep-Inelastic Scattering (SIDIS), which simultaneously probes both the initial-state partonic structure and the fragmentation process in the final state. Each of these processes plays a complementary role in understanding QCD dynamics.

In this chapter, we review the theoretical foundations relevant for the study of SIDIS. We begin with inclusive DIS and the QCD-improved parton model, followed by a discussion of Semi-Inclusive Annihilation and fragmentation functions. These

ingredients are then combined in the framework of SIDIS, which forms the basis of the calculations presented in this thesis.

2.2 Deep-Inelastic Scattering

Deep-Inelastic Scattering (DIS) has played a fundamental role in uncovering the internal structure of hadrons and establishing the modern description of strong interactions [86]. The process involves the scattering of a high-energy lepton from a hadronic target through the exchange of a highly virtual electroweak gauge boson. The large momentum transfer associated with the exchanged boson provides a short-distance probe capable of resolving the constituents of the hadron.

The first DIS experiments were carried out at the Stanford Linear Accelerator Center (SLAC) in collaboration with MIT during the late 1960s [84, 85]. In these experiments, high-energy electrons were scattered off proton and deuteron targets. The measured cross sections differed significantly from those expected for a point-like proton, indicating the presence of internal constituents. Even more remarkably, the extracted structure functions exhibited an approximate scaling behavior, suggesting that the scattering occurred from nearly free point-like objects within the proton.

In DIS, high-energy electron off a proton target via the exchange of a highly virtual photon, the process is given as

$$e^-(k) + P(P_H) \rightarrow e^-(k') + X, \quad (2.1)$$

where $k(k')$ denote the momenta of incoming (outgoing) leptons, P_H is the momentum of the target proton, and X represents the inclusive hadronic final state. Since only the scattered lepton is observed, all hadronic final states are summed over inclusively. The momentum transferred $q = k - k'$ with $Q^2 = -q^2 > 0$ measuring the

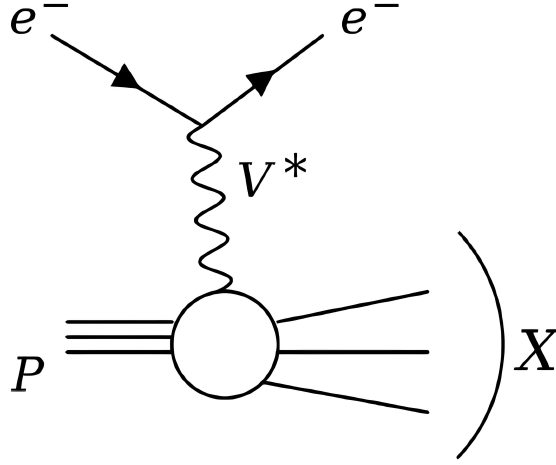


Figure 2.1: Schematic diagram of Deep-Inelastic Scattering (DIS), $e^- + P \rightarrow e^- + X$, mediated by the exchange of a virtual gauge boson V .

resolving power of the probe and the dimensionless variable $x = Q^2/(2P_H \cdot q)$, called Bjorken variable. The deep-inelastic regime is characterized by large Q^2 or large energy transfer at fixed x which probes the internal constituents of the proton.

The hadronic structure probed in DIS is encoded in the structure functions. For unpolarized DIS, the leading structure functions are conventionally denoted by $F_1(x, Q^2)$ and $F_2(x, Q^2)$. One of the most remarkable observations from the SLAC experiments was that these structure functions depended predominantly on the variable x , and only weakly on Q^2 . This behavior, known as Bjorken scaling, i.e. at $Q^2 \rightarrow \infty$ and $P_H \cdot q \rightarrow \infty$ keeping x fixed, the structure functions become independent of Q^2 i.e. $F_i(x, Q^2) \approx F_i(x)$, suggested that the proton contains point-like constituents that behave approximately as free particles during the interaction.

Using current algebra [87], J.D. Bjorken proposed that such scaling should emerge naturally at asymptotically large momentum transfer. Shortly after, R.P. Feynman, James Bjorken and Emmanuel A. Paschos introduced the parton model [88–90], which gave a physical interpretation of this result. He proposed fast-moving hadron is described as a collection of quasi-free, point-like constituents called partons. At very high energy, the interaction time of the virtual photon is much shorter than the

typical QCD interaction time between partons. As a result, the photon effectively probes a frozen snapshot of the proton. The scattering can therefore be interpreted as an incoherent sum of elastic scatterings off individual partons.

Within this framework, the structure functions acquire a simple probabilistic interpretation in terms of parton distribution functions. An important consequence is the Callan–Gross relation, $F_2(x) = 2xF_1(x)$, which follows from the assumption that the struck constituents are spin $\frac{1}{2}$ particles. The experimental verification of this relation provided strong evidence that the proton constituents observed in DIS behave like spin $\frac{1}{2}$ particles, consistent with the quark model proposed by Gell-Mann and Zweig [91, 92].

The identification of these constituents with quarks was further established during the 1970s through deep-inelastic neutrino-nucleon scattering experiments at CERN and Fermilab. Unlike electromagnetic interactions, charged-current weak interactions are sensitive to the flavor of the struck quark, enabling detailed investigations of the flavor structure of the nucleon. These measurements not only strengthened the quark-parton picture but also provided important tests of the electroweak sector of the Standard Model. Together with the earlier SLAC measurements, these experiments firmly established deep-inelastic scattering as a powerful tool for probing hadron structure. As discussed in Chapter 1, the theoretical description of strong interactions is provided by Quantum Chromodynamics (QCD). In particular, the discovery of asymptotic freedom in 1973 established that the strong coupling decreases at short distances, allowing quarks to behave as nearly free particles when probed at large momentum transfer. This remarkable property provides the theoretical explanation for the approximate Bjorken scaling observed in the SLAC experiments and forms the theoretical foundation for the modern description of DIS.

As experimental precision improved, it became clear that Bjorken scaling is not exact. Instead, the structure functions exhibit a mild dependence on Q^2 , known

as scaling violations. This is best seen in plots of $F_i(x, Q^2)$ as a function of Q^2 for fixed values of x , see Fig (2.2). If Bjorken scaling were exact, F_2 at fixed x would be independent of Q^2 , and each curve would therefore be horizontal, but instead the figure exhibits logarithmic scaling violations. This behaviour indicates that the structure of the proton resolved in DIS changes with the probing scale.

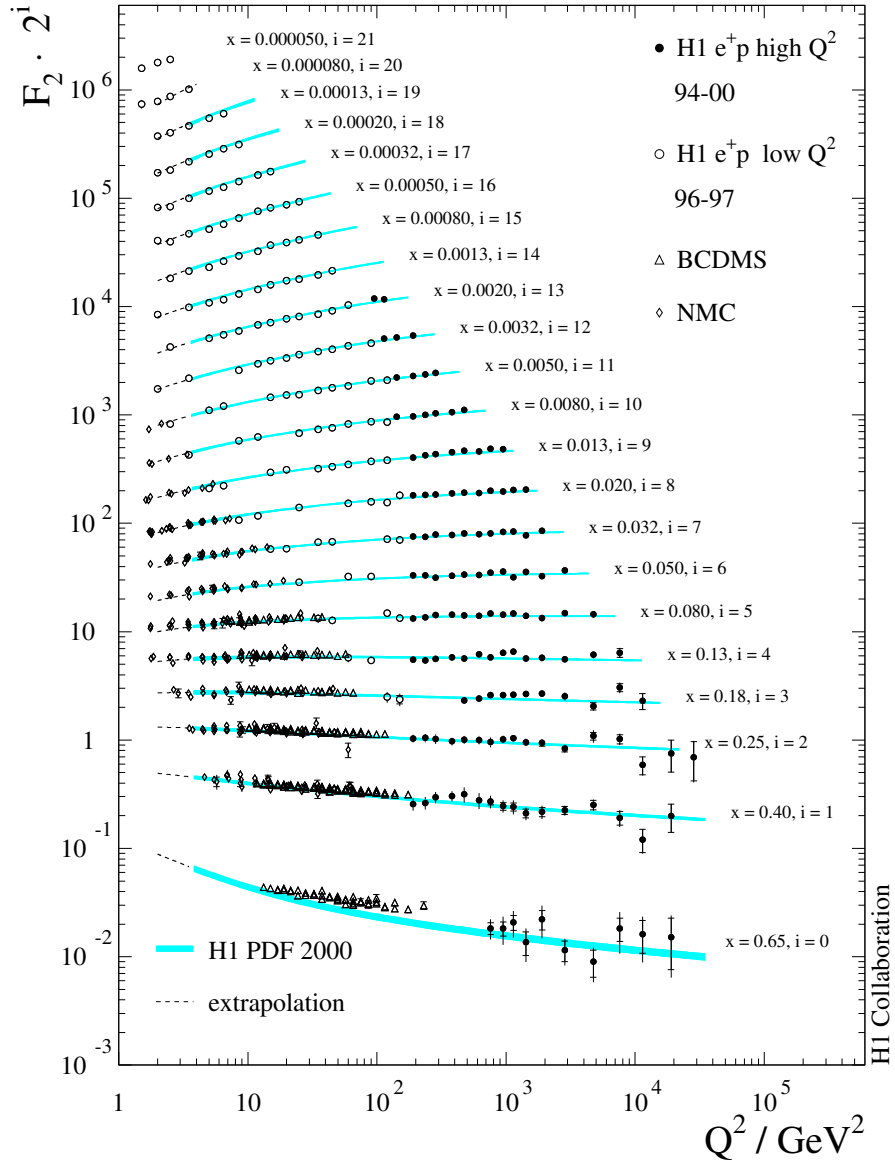


Figure 2.2: F_2 structure function as a function of the momentum transfer scale Q^2 , here values of F_2 in successive x bins are multiplied by factors of 2^i , as indicated on the vertical axis, plot take from [2], see also [3].

A major advance came in the 1990s with the HERA electron-proton collider at

DESY, which explored an unprecedented kinematic range in Bjorken- x and Q^2 . The precise measurements from HERA significantly improved the determination of parton distribution functions, especially the gluon distribution, and enabled precision tests of QCD evolution over a wide range of energy scales.

The modern description of DIS is based on the QCD factorization theorem, which separates short-distance perturbative dynamics from long-distance non-perturbative hadronic structure [32, 33, 37, 93–97]. In this framework, the structure functions can be expressed schematically as (eg. see [98, 99])

$$F_i(x, Q^2) = \sum_a \int_x^1 \frac{dx_1}{x_1} f_{a/P}(x_1, \mu_F^2) \mathcal{C}_{i,a} \left(\frac{x}{x_1}, Q^2, \mu_F^2 \right), \quad (2.2)$$

where the coefficient functions (CFs) $\mathcal{C}_{i,a}$ are calculable in perturbative QCD which describes the hard scattering process, while $f_{a/P}$ are universal parton distribution functions (PDFs) which encode the non-perturbative structure of the hadron. Here a is summed over quark, anti-quark and gluon degree of freedom. μ_F is the factorization scale separating short and long distances physics.

Both the parton distribution functions and the coefficient functions depend on the factorization scale μ_F . The μ_F dependence of the PDFs is governed by the Dokshitzer–Gribov–Lipatov–Altarelli–Parisi (DGLAP) evolution equations [100–104], while the corresponding dependence of the CFs is constrained by renormalization-group invariance. These μ_F dependences cancel in the structure functions when all perturbative orders are included.

A convenient choice is $\mu_F^2 = Q^2$, for which the explicit logarithms of Q^2/μ_F^2 in the coefficient functions vanish. However, the structure functions retain a physical dependence on Q^2 , since the PDFs are then evaluated at the scale Q^2 and evolve with this scale according to the DGLAP equations. This evolution originates from parton radiation and splitting processes, which modify the partonic content resolved by a

probe as its resolution scale changes. In addition, the coefficient functions depend on Q^2 through the running strong coupling $a_s(Q^2)$, governed by the renormalization of the coupling constant, and through their renormalization group evolution. Together with the evolution of the PDFs, these effects produce the logarithmic violations of Bjorken scaling observed in deep-inelastic scattering.

This factorization framework forms the foundation of modern QCD phenomenology and enables the extraction of universal parton distributions from experimental data. The universality of PDFs allows them to be extracted from experimental data and applied to a wide range of high-energy scattering processes.

The concepts developed through DIS provide the basis for understanding a broad class of high-energy scattering processes. In the following section, we discuss semi-inclusive annihilation, which introduces fragmentation functions and complements the information obtained from DIS.

2.3 Towards Semi-Inclusive Process

DIS is an inclusive process, meaning that only the scattered lepton is measured while all hadronic final states are summed over. This inclusive nature makes DIS particularly suitable for extracting parton distribution functions, which describe the momentum distributions of quarks and gluons inside hadrons. However, DIS provides only partial information about strong interaction dynamics. While it reveals how partons are distributed within a hadron before the hard scattering, it does not directly address how energetic quarks and gluons form the hadrons observed in experiments. This non-perturbative process, known as hadronization, is an essential aspect of QCD phenomenology.

To gain access to hadronization dynamics, one must consider semi-inclusive processes, in which a specific hadron in the final state is identified. The observation

of a final-state hadron provides additional information beyond that available in inclusive measurements and introduces fragmentation functions, which quantify the probability for a parton to produce a given hadron carrying a fraction of its momentum.

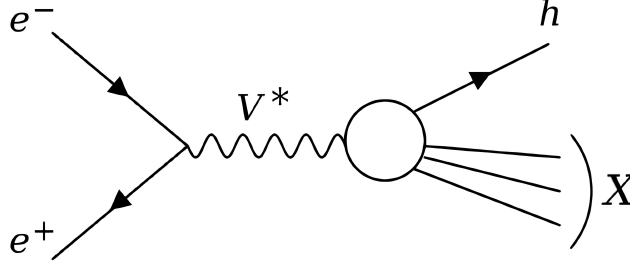


Figure 2.3: Schematic diagram of single-inclusive annihilation (SIA), $e^+e^- \rightarrow h + X$, where a virtual vector boson V , where h is the identified hadron and X denotes the inclusive hadronic remnant.

The study of hadronization, requires processes that are sensitive to the fragmentation of partons into identified hadrons. The cleanest environment for such investigations is provided by electron–positron annihilation [105],

$$e^+(k) + e^-(k') \rightarrow h(P_h) + X \quad (2.3)$$

where an electron and positron annihilate into a virtual electroweak boson, which subsequently produces a quark–antiquark pair. The observed hadron h originates from the fragmentation of one of the final-state partons, while the remaining hadrons are summed over inclusively. This process, known as Semi-Inclusive Annihilation (SIA), provides direct access to fragmentation functions and complements the information obtained from DIS.

Unlike DIS, where the hadron appears in the initial state, electron–positron annihilation involves no hadrons in the incoming state. Consequently, the process is free from parton distribution functions and provides a particularly clean laboratory for studying the hadronization mechanism. The non-perturbative information is

encoded entirely in fragmentation functions (FFs), which describe the probability for a parton to fragment into a hadron carrying a given fraction of its momentum [62, 97, 106–111]. FFs therefore play a role analogous to that of parton distribution functions.

Analogous to Bjorken variable x in DIS, the scaling variable associated with the identified hadron h in SIA is defined as $z = (2P_h \cdot q)/Q^2$, where P_h is the momentum of the observed hadron and $q = k + k'$ is the momentum of the exchanged boson, with $q^2 = Q^2 > 0$. The differential cross section can be expressed in terms of fragmentation functions $D_{h/a}$, where a labels the fragmenting parton and h the observed hadron. In the parton model, fragmentation functions admit a probabilistic interpretation analogous to that of parton distribution functions in DIS. While PDFs describe the probability of finding a parton inside a hadron, fragmentation functions describe the probability of observing a hadron in the fragmentation products of a parton. They therefore provide complementary information about the non-perturbative dynamics of QCD. As in DIS, QCD predicts logarithmic violations of the Bjorken scaling behavior. Partons produced in the hard scattering can radiate additional gluons and undergo successive branching processes before hadronization. As a consequence, fragmentation functions become dependent on the hard scale Q^2 . Their evolution is governed by time-like DGLAP equations, which are the counterparts of the space-like evolution equations for parton distribution functions.

The hadronic dynamics in SIA are encoded in fragmentation structure functions F_i^h , which admit a factorized representation in perturbative QCD, see e.g. [99], see also [112–120]. The QCD factorization theorem allows these structure functions to be written as a convolution of perturbatively calculable coefficient functions and universal fragmentation functions,

$$F_i^h = \sum_a \int_z^1 \frac{dz_1}{z_1} D_{h/a}(z_1, \mu_F^2) C_{i,a}^h \left(\frac{z}{z_1}, Q^2, \mu_F^2 \right), \quad (2.4)$$

where $\mathcal{C}_{i,a}^h$ denote the hard-scattering coefficient functions and $D_{h/a}$ are the fragmentation functions. This factorized framework provides a systematic description of hadron production in electron-positron annihilation and enables the extraction of universal fragmentation functions from experimental data.

Together, deep-inelastic scattering and semi-inclusive hadron production in e^+e^- annihilation provide complementary information about hadronic structure: DIS probes the distribution of partons inside hadrons, while SIA probes the fragmentation of partons into hadrons. A natural process that combines both aspects is Semi-Inclusive Deep-Inelastic Scattering (SIDIS), where a hadron is observed in the final-state in addition to the scattered lepton. SIDIS therefore provides simultaneous sensitivity to both the structure of the incoming hadron and the hadronization of the outgoing parton.

2.4 Semi-Inclusive Deep-Inelastic Scattering

Semi-Inclusive Deep-Inelastic Scattering (SIDIS) provides a unique framework for investigating both the partonic structure of hadrons and the hadronization of partons within QCD. By detecting an identified hadron in the final-state in addition to the scattered lepton, SIDIS simultaneously probes parton distribution functions (PDFs) and fragmentation functions (FFs). This unique combination of initial- and final-state information makes SIDIS an essential process for exploring hadron structure, parton fragmentation mechanism and underlying dynamics of QCD.

Experimentally, SIDIS has been extensively studied at facilities such as HERMES [121] and COMPASS [122] yielding valuable information on nucleon structure and hadronization mechanisms. Looking forward, the future Electron-Ion Collider (EIC) at BNL [123, 124], as well as the proposed Electron-Ion Collider in China (EicC) [125] will significantly extend the kinematic reach and precision of SIDIS

measurements, making accurate theoretical predictions increasingly important.

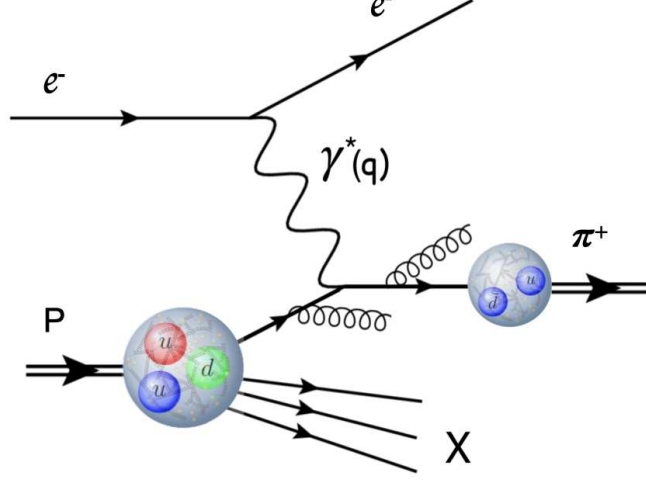


Figure 2.4: Schematic representation of π^+ production in SIDIS process.

The SIDIS process is described by

$$l(k_l, \lambda_l) + H(P, \lambda_H) \rightarrow l'(k'_l) + H'(P_H) + X, \quad (2.5)$$

where l (l') and H (H') denote the incoming (outgoing) lepton and hadron respectively. For neutral current (NC) processes, we have $l' = l$ and the intermediate virtual particles are γ^* , Z^* and interference between them. For the charged current (CC) processes, the intermediate vector boson is either W^+ or W^- depending on the charge of l' ($l' \neq l$). Here k_l (k'_l) and P (P_H) are momenta of incoming (outgoing) lepton and hadron respectively and $q = k_l - k'_l$ is the momentum transfer between incoming leptons and hadrons. We define, $q^2 = -Q^2$, defines the hard scale of the process. λ_l and λ_H are the helicity of incoming lepton and hadron respectively. More on these processes can be found in [126–134].

The SIDIS kinematics is described by the variables

$$x = \frac{Q^2}{2P \cdot q}, \quad y = \frac{P \cdot q}{P \cdot k_l}, \quad z = \frac{P \cdot P_H}{P \cdot q}, \quad (2.6)$$

along with the center-of-mass energy $s = (P + k_l)^2$. The variable x corresponds to the Bjorken scaling variable, y denotes the inelasticity, and z is the fraction of the initial energy transferred to the observed hadron. In the single-vector-boson exchange approximation, the differential hadronic cross section factorizes into a leptonic tensor $L_{j,\lambda_l}^{\mu\nu}$ and a hadronic tensor $W_{\mu\nu,\lambda_H}^j$ [83]:

$$\frac{d^3\sigma_{l_{\lambda_l}H_{\lambda_H}\rightarrow l'H'X}}{dxdydz} = 2\pi y M_H \alpha_e^2 \sum_j D_j L_{j,\lambda_l}^{\mu\nu}(k_l, k_{l'}, q) W_{\mu\nu,\lambda_H}^j(P, P_H, S, q). \quad (2.7)$$

Here, M_H and S are the mass and spin of the incoming hadron. α_e is the fine structure constant, $\alpha_e = g_e^2/(4\pi)$ and g_e is the electromagnetic coupling. For NC processes the sum includes contributions from $j = \gamma\gamma, ZZ$, and $j = \gamma Z$ intermediate vector bosons, while for CC processes $j = W^\pm$. Here,

$$\begin{aligned} D_{\gamma\gamma} &= \frac{1}{(Q^2)^2}, & D_{\gamma Z} &= \frac{(Q^2 + M_Z^2)}{Q^2((Q^2 + M_Z^2)^2 + \Gamma_Z^2)}, \\ D_{ZZ} &= \frac{1}{((Q^2 + M_Z^2)^2 + \Gamma_Z^2)}, & D_{W^\pm} &= \frac{1}{((Q^2 + M_W^2)^2 + \Gamma_W^2)}, \end{aligned} \quad (2.8)$$

where M_V and Γ_V ($V = Z, W$) are the mass and width of the intermediate vector boson V .

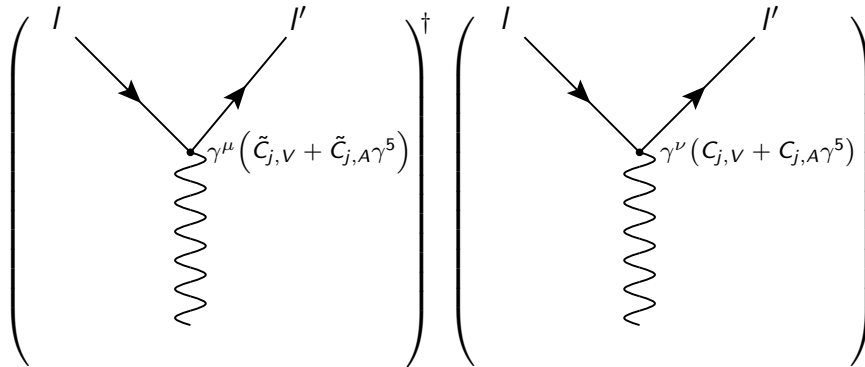


Figure 2.5: Leptonic tensor with a general vector and axial-vector coupling structure.

For a massless fermion with polarization λ_l , the leptonic tensor $L_{j,\lambda_l}^{\mu\nu}$, corresponding to a generic vector-axial vertex is given as, see Fig. (2.5),

$$L_{j,\lambda_l}^{\mu\nu} = \sum_{\lambda_{l'}} \left(\bar{u}(k_{l'}, \lambda_{l'}) \gamma^\mu (\tilde{C}_{j,V} + \tilde{C}_{j,A} \gamma^5) u(k_l, \lambda_l) \right)^\dagger \times \left(\bar{u}(k_{l'}, \lambda_{l'}) \gamma^\nu (C_{j,V} + C_{j,A} \gamma^5) u(k_l, \lambda_l) \right) \quad (2.9)$$

Similar expression is written for initial anti-fermion. To incorporate generic lepton of lepton number l_l and helicity λ_l ,

$$L_{j,\lambda_l}^{\mu\nu} = \text{Tr} \left[\not{k}_{l'} \gamma^\nu (C_{j,V} + C_{j,A} \gamma^5) \not{k}_l \left(\frac{1 - l_l \lambda_l \gamma^5}{2} \right) \gamma^\mu (\tilde{C}_{j,V}^* + \tilde{C}_{j,A}^* \gamma^5) \right] \quad (2.10)$$

To define the helicity of fermions ($l_l = +1$) we have used the relation,

$$u(p, \lambda) \bar{u}(p, \lambda) = \not{p} \left(\frac{1 - \lambda \gamma^5}{2} \right), \quad (2.11)$$

for fermions with $\lambda = 1$ for $+$ or $\uparrow$ helicity and $\lambda = -1$ for $-$ or $\downarrow$ helicity. Here, $C_{j,V}$ ($C_{j,A}$) and $\tilde{C}_{j,V}$ ($\tilde{C}_{j,A}$) denotes the general vector (axial-vector) couplings associated with the two leptonic currents entering the tensor [116, 135–138]. In general, the two sets of couplings may be identical or different, allowing the expression to describe both squared amplitudes and interference contributions.

For NC interactions, γ and Z couple to a fermion of flavor f through the vertex

$$-ig_e e_f \gamma^\mu, \quad ig_e \gamma^\mu (\bar{g}_{V_f} - \bar{g}_{A_f} \gamma^5), \quad (2.12)$$

receptively, where

$$\bar{g}_{V_f} = \frac{g_{V_f}}{2 \sin \theta_W \cos \theta_W}, \quad \bar{g}_{A_f} = \frac{g_{A_f}}{2 \sin \theta_W \cos \theta_W}. \quad (2.13)$$

Here θ_W is the Weinberg mixing angle, and the vector (g_{V_f}) and axial-vector (g_{A_f})

couplings are given by

$$g_{V_f} = T_f^3 - 2e_f \sin^2 \theta_W, \quad g_{A_f} = T_f^3. \quad (2.14)$$

T_f^3 denotes the third component of the weak isospin of the fermion f , and e_f is the electric charge of the fermion f in units of the electron charge [83].

For CC interactions, the vector bosons W^+ and W^- couple to fermions through the vertices

$$ig_e \gamma^\mu (1 - \gamma^5) \bar{V}_{ff'}, \quad ig_e \gamma^\mu (1 - \gamma^5) \bar{V}_{ff'}^* \quad (2.15)$$

respectively, $\bar{V}_{ff'} = \frac{V_{ff'}}{2\sqrt{2}\sin\theta_W}$ where f and f' denote the members of a weak isospin doublet. In the leptonic sector, $f = l$ and $f' = \nu_l$ correspond to a charged lepton and its associated neutrino ($l = e, \mu, \tau$), respectively. However, since the flavor of the incoming lepton is fixed, the PMNS mixing typically does not appear explicitly in the cross section. In the quark sector, $f = \mathbf{u}$ represents an up-type quark (u, c) and $f' = \mathbf{b}$ represents a down-type quark (d, s), with $V_{\mathbf{ub}}$ being the corresponding element of the Cabibbo-Kobayashi-Maskawa (CKM) matrix.

The leptonic tensors $L_{j,\lambda_l}^{\mu\nu}$ corresponding to exchanges of different electroweak bosons, $j = \gamma\gamma, \gamma Z, ZZ, W^\pm$, are found to be

$$\begin{aligned} L_{\gamma\gamma,\lambda_l}^{\mu\nu} &= 2k_l^\mu k_l'^\nu + 2k_l'^\mu k_l^\nu - Q^2 g^{\mu\nu} - 2il_l \lambda_l \epsilon^{\mu\nu\sigma\lambda} q_\sigma k_{l,\lambda}, \\ L_{\gamma Z,\lambda_l}^{\mu\nu} &= (\bar{g}_{V_l} - l_l \lambda_l \bar{g}_{A_l}) L_{\gamma\gamma,\lambda_l}^{\mu\nu}, \\ L_{ZZ,\lambda_l}^{\mu\nu} &= (\bar{g}_{V_l}^2 + \bar{g}_{A_l}^2 - 2l_l \lambda_l \bar{g}_{V_l} \bar{g}_{A_l}) L_{\gamma\gamma,\lambda_l}^{\mu\nu}, \\ L_{W^\pm,\lambda_l}^{\mu\nu} &= 2(1 - l_l \lambda_l) L_{\gamma\gamma,\lambda_l}^{\mu\nu}. \end{aligned} \quad (2.16)$$

Here $l_l, \lambda_l = \pm 1$ represents lepton number, helicity of the incoming lepton respectively, used $e_l^2 = 1$ for charged lepton. Note, the mass of the lepton is dropped

throughout. Here, $\bar{g}_{V_i}, \bar{g}_{A_i}$ are related to vector and axial-vector couplings of the lepton to the electroweak gauge bosons see Eq. (2.13). The Levi-Civita tensor $\epsilon^{\mu\nu\sigma\lambda}$ is fully anti-symmetric tensor with $\epsilon_{0123} = -\epsilon^{0123} = 1$.

The hadronic tensor contains all information about the strong-interaction dynamics of the SIDIS process. It is defined through matrix elements of the electroweak current between hadronic states,

$$\begin{aligned}
W_{\mu\nu, \lambda_H}^j &= \frac{1}{4\pi M_H} \sum_X \int \frac{d^3 P_H}{(2\pi)^3 (2P_H^0)} \int \prod_{i=0}^X \frac{d^3 P_i}{(2\pi)^3 (2P_i^0)} \\
&\times (2\pi)^4 \delta(P + q - P_H - P_X) \delta\left(z - \frac{P \cdot P_H}{P \cdot q}\right) \\
&\times \left(\left\langle H(P, \lambda_H) \left| J_\mu^\dagger(0) \right| H'(P_H), X \right\rangle \left\langle H'(P_H), X \left| J_\nu(0) \right| H(P, \lambda_H) \right\rangle \right)^j, \quad (2.17)
\end{aligned}$$

where, J_μ denotes the electroweak current responsible for the interaction. The superscript j labels the ordered pair of electroweak currents entering the two current matrix elements, $j = \gamma\gamma, \gamma Z, ZZ, W^+, W^-$, where the first (second) entry refers to the current in the left (right) matrix element. The sum over X is performed inclusively over all hadronic states accompanying the observed hadron H' , and the delta functions enforce momentum conservation and fix the observed hadron energy fraction z .

Owing to the composite nature of hadrons, the hadronic tensor cannot be calculated directly in perturbation theory. Being a second-rank Lorentz tensor, the hadronic tensor can, subject to electromagnetic current conservation, parity, and time-reversal invariance, be parametrized in terms of the $g_{\mu\nu}, \epsilon_{\mu\nu\sigma\rho}$ and the vectors q, P and S , multiplied by Lorentz invariant structure functions (SFs). These structure functions encode the non-perturbative information of the process and depend on the kinematic variables x, z and Q^2 . The momentum of the observed hadron P_H enters through the scaling variable z and after integrated over hadron phase space subject to the constraint $\delta\left(z - \frac{P \cdot P_H}{P \cdot q}\right)$, the dependence on the observed hadron is entirely encoded

in the structure functions. The most general decomposition of the hadronic tensor is given by (considering only initial state hadron to be polarized),

$$\begin{aligned}
W_{\mu\nu,\lambda_H}^j = & \frac{1}{M_H} \left\{ \underbrace{\left(-g_{\mu\nu} + \frac{q_\mu q_\nu}{q^2} \right)}_{T_{1,\mu\nu}} F_1^j + \underbrace{\left(\frac{1}{P \cdot q} \hat{P}_\mu \hat{P}_\nu \right)}_{T_{2,\mu\nu}} F_2^j - i\epsilon_{\mu\nu\sigma\lambda} \frac{q^\sigma P^\lambda}{2P \cdot q} F_3^j \right. \\
& + i\epsilon_{\mu\nu\sigma\lambda} \frac{q^\sigma S^\lambda}{P \cdot q} g_1^j + i\epsilon_{\mu\nu\sigma\lambda} \frac{q^\sigma}{P \cdot q} \left(S^\lambda - \frac{S \cdot q}{P \cdot q} P^\lambda \right) g_2^j \\
& + \frac{1}{P \cdot q} \left[\frac{1}{2} \left(\hat{P}_\mu \hat{S}_\nu + \hat{S}_\mu \hat{P}_\nu \right) - \frac{S \cdot q}{P \cdot q} \hat{P}_\mu \hat{P}_\nu \right] g_3^j \\
& \left. + \frac{S \cdot q}{P \cdot q} \left[\left(\frac{1}{P \cdot q} \hat{P}_\mu \hat{P}_\nu \right) g_4^j + \left(-g_{\mu\nu} + \frac{q_\mu q_\nu}{q^2} \right) g_5^j \right] \right\}, \tag{2.18}
\end{aligned}$$

with $\hat{P}_\mu = \left(P_\mu - \frac{P \cdot q}{q^2} q_\mu \right)$ and $\hat{S}_\mu = \left(S_\mu - \frac{S \cdot q}{q^2} q_\mu \right)$. Here, $F_{1,2,3}^j = F_{1,2,3}^j(x, z, Q^2)$ denote the unpolarized SFs, while $g_{1,\dots,5}^j = g_{1,\dots,5}^j(x, z, Q^2)$ correspond to the polarized ones and S is the spin of incoming hadron aligned in longitudinal direction of lepton l , such that in $S = \lambda_H(0, 0, 0, M_H)$, in rest frame of incoming hadron and $S \cdot P = 0$ and $S^2 = -M_H^2$. Substituting Eqs. (2.16) and (2.18) in Eq. (2.7), we find differential cross section,

$$\begin{aligned}
\frac{d^3\sigma_{l_{\lambda_l} H_{\lambda_H} \rightarrow l' H' X}^{\text{NC/CC}}}{dx dy dz} = & \frac{4\pi\alpha_e^2}{Q^2} \left[y F_1^{\text{NC/CC}} + \left(\frac{1-y}{xy} - xy \frac{M_H^2}{Q^2} \right) F_2^{\text{NC/CC}} + \frac{2-y}{2} F_3^{\text{NC/CC}} \right. \\
& + \lambda_H \left\{ \left(2-y-2x^2y^2 \frac{M_H^2}{Q^2} \right) g_1^{\text{NC/CC}} \right. \\
& + 4x^2y \frac{M_H^2}{Q^2} g_2^{\text{NC/CC}} + 2x \frac{M_H^2}{Q^2} \left(1-y-x^2y^2 \frac{M_H^2}{Q^2} \right) g_3^{\text{NC/CC}} \\
& \left. \left. + \left(1+2x^2y \frac{M_H^2}{Q^2} \right) \left[\left(\frac{1-y}{xy} - xy \frac{M_H^2}{Q^2} \right) g_4^{\text{NC/CC}} + y g_5^{\text{NC/CC}} \right] \right\} \right], \tag{2.19}
\end{aligned}$$

From now on we'll consider $Q^2 \gg M_H^2$, such that all the hadron mass dependent terms in Eq. (2.19) and the SFs $g_2^{\text{NC/CC}}$ and $g_3^{\text{NC/CC}}$ can be dropped. The NC SFs can be decomposed into the $\gamma\gamma$, ZZ , and γZ contributions and CC SFs into W^+ or

W^- as,

$$\begin{aligned} F_{1,2}^{\text{NC}} &= \eta_{\gamma\gamma} F_{1,2}^{\gamma\gamma} + \eta_{ZZ} (g_{V_l}^2 + g_{A_l}^2 - 2l_l \lambda_l g_{V_l} g_{A_l}) F_{1,2}^{ZZ} + \eta_{\gamma Z} (g_{V_l} - l_l \lambda_l g_{A_l}) F_{1,2}^{\gamma Z}, \\ F_3^{\text{NC}} &= -l_l \lambda_l F_1^{\text{NC}} \Big|_{F_1^j \rightarrow F_3^j}, \quad F_{1,2,3}^{\text{CC}} = 2\eta_{W^\pm} (1 - l_l \lambda_l) F_{1,2,3}^{W^\pm}. \end{aligned} \quad (2.20)$$

For the polarized case, the decomposition is identical to that of unpolarized ones i.e.,

$$g_1^{\text{NC/CC}} = -l_l \lambda_l \times F_1^{\text{NC/CC}} \Big|_{F_1^j \rightarrow g_1^j}, \quad g_{4,5}^{\text{NC/CC}} = l_l \lambda_l \times F_3^{\text{NC/CC}} \Big|_{F_3^j \rightarrow g_{4,5}^j}. \quad (2.21)$$

Here, g_{V_l}, g_{A_l} corresponds to vector and axial-vector couplings of the lepton to the electroweak gauge bosons. The constants η_j encode the electroweak factors associated with the exchanged boson and are given by, (G_F is the Fermi constant)

$$\begin{aligned} \eta_{\gamma\gamma} &= 1, & \eta_{\gamma Z} &= \sqrt{\frac{\sqrt{2}G_F M_Z^2}{4\pi\alpha_e}} \frac{Q^2(Q^2 + M_Z^2)}{(Q^2 + M_Z^2)^2 + \Gamma_Z^2}, \\ \eta_{ZZ} &= \left(\frac{\sqrt{2}G_F M_Z^2}{4\pi\alpha_e} \right) \frac{(Q^2)^2}{(Q^2 + M_Z^2)^2 + \Gamma_Z^2}, & \eta_{W^\pm} &= \left(\frac{G_F M_W^2}{\sqrt{2}(4\pi\alpha_e)} \right) \frac{(Q^2)^2}{(Q^2 + M_W^2)^2 + \Gamma_W^2}. \end{aligned} \quad (2.22)$$

Since the tensors $T_{1,\mu\nu}$ and $T_{2,\mu\nu}$ Eq. (2.18) are symmetric in the indices μ and ν , the corresponding unpolarized SFs $F_{1,2}^{\text{NC}}$ receive contributions only from the vector-vector and axial-axial parts of the NC. If the incoming lepton is polarized, then the SFs $g_{4,5}^{\text{NC}}$ will receive contribution from interference of vector-axial vector parts. In contrast, due to anti-symmetric nature of Levi-Civita tensor, the SF F_3^{NC} arises from the interference of vector and axial-vector components of the NC for the unpolarized incoming lepton. When the incoming lepton is polarized, then the vector-vector and axial vector-axial vector parts will also contribute in g_1^{NC} .

The structure functions F_i^j and g_i^j encode all the non-perturbative information contained in the hadronic tensor and therefore constitute the fundamental observables

of SIDIS. They can be extracted experimentally through suitable combinations of polarized and unpolarized cross sections. From the theoretical perspective, the calculation of these structure functions relies on the QCD factorization theorem, which separates the short-distance dynamics associated with the hard scattering from the long-distance dynamics governing the structure and hadronization of partons.

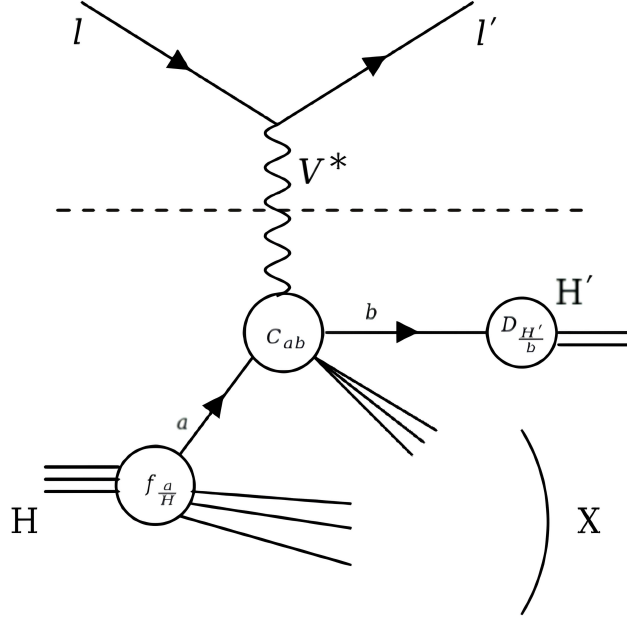


Figure 2.6: SIDIS process $l + H \rightarrow l' + H' + X$ mediated by a virtual vector boson V , illustrating the QCD factorization into PDFs ($f_{\frac{a}{H}}$), hard coefficient functions ($\mathcal{C}_{ab}$), and fragmentation functions ($D_{\frac{H'}{b}}$). The dashed line indicates the separation between leptonic and hadronic parts of the process.

In this thesis, we work within the framework of collinear (longitudinal) factorization, where the transverse momenta of both the incoming and fragmenting partons are integrated over. The QCD factorization allows the SFs to be expressed in terms of perturbatively calculable CFs $(\Delta)\mathcal{C}_{i,ab}^j$, the PDF $(\Delta)f_{\frac{a}{H}}$ of a parton a inside the incoming hadron H , and the FF $D_{\frac{H'}{b}}$ describing the fragmentation of parton b into the outgoing hadron H' , where the symbol (Δ) unifies the notation for unpolarized and polarized quantities,

$$(\Delta)\mathcal{F}_i^j(x, z, Q^2) = \sum_{a,b} \int_x^1 \frac{dx_1}{x_1} (\Delta)f_{\frac{a}{H}}(x_1, \mu_F^2) \int_z^1 \frac{dz_1}{z_1} D_{\frac{H'}{b}}(z_1, \mu_F^2)$$

$$\times (\Delta) \mathcal{C}_{i,ab}^j \left(\frac{x}{x_1}, \frac{z}{z_1}, \mu_F^2, Q^2 \right). \quad (2.23)$$

Note, the unpolarized SFs take indices $i = 1, 2, 3$ and polarized ones $i = 1, 4, 5$,

$$\mathcal{F}_{1,2,3}^j = \left\{ 2F_1^j, \frac{F_2^j}{x}, F_3^j \right\}, \quad \Delta \mathcal{F}_{1,4,5}^j = \left\{ g_1^j, \frac{g_4^j}{2x}, g_5^j \right\}. \quad (2.24)$$

In Eq. (2.23) the sum is over all possible incoming and outgoing partons $a, b = q, \bar{q}', g$ and μ_F is the factorization scale and $f_{\frac{a}{H}}$ denotes the spin averaged PDF and $\Delta f_{\frac{a}{H}} = f_{\frac{a(\uparrow)}{H(\uparrow)}} - f_{\frac{a(\downarrow)}{H(\uparrow)}}$. Here $j = \gamma\gamma, \gamma Z, ZZ, W^\pm$. The scaling variable x_1 is the momentum fraction carried away by the parton a of the hadron H such that $p_a = x_1 P$, and z_1 is the momentum fraction carried away by the final hadron H' from parton b , i.e. $P_{H'} = z_1 p_b$. Here, p_a and p_b are momenta of incident parton and fragmenting parton respectively. Further defining scaling variables $x' = x/x_1$ and $z' = z/z_1$.

The PDFs and FFs satisfy a number of important sum rules reflecting charge and momentum conservation. For example, the momentum carried by all partons inside a hadron must add up to the hadron momentum,

$$\sum_a \int_0^1 dx \, x f_{\frac{a}{H}}(x, \mu_F^2) = 1, \quad (2.25)$$

while the fragmentation functions obey the corresponding momentum sum rule

$$\sum_{H'} \int_0^1 dz \, z D_{\frac{H'}{b}}(z, \mu_F^2) = 1. \quad (2.26)$$

The above relation means that each parton b will fragment with a 100% probability into some hadron. These relations provide important constraints in global analyses of PDFs and FFs. These functions are extracted from experimental data and are process-independent i.e. once determined, can be used to a wide range of other experiments.

The CFs, $(\Delta)\mathcal{C}_{i,ab}^j$, describe the hard parton-level interactions and are process-dependent quantities that can be systematically calculated order by order in the strong coupling within perturbative QCD. The expansion in powers of the strong coupling constant $a_s(\mu_R^2)$ is given as

$$(\Delta)\mathcal{C}_{i,ab}^j\left(\frac{x}{x_1}, \frac{z}{z_1}, \mu_F^2, Q^2\right) = \sum_{k=0}^{\infty} a_s^k(\mu_R^2) (\Delta)\mathcal{C}_{i,ab}^{j,(k)}\left(\frac{x}{x_1}, \frac{z}{z_1}, \mu_F^2, \mu_R^2, Q^2\right), \quad (2.27)$$

where $a_s(\mu_R^2) = g_s^2(\mu_R^2)/(16\pi^2)$ in terms of the strong coupling g_s , defined in $\overline{\text{MS}}$ scheme at the renormalization scale μ_R . The CFs $(\Delta)\mathcal{C}_{i,ab}^j$ are obtained from the partonic subprocess cross sections denoted by $d(\Delta)\hat{\sigma}_{i,ab}^j$ by applying the corresponding projectors $(\Delta)\mathcal{P}_i^{\mu\nu}$.

$$d(\Delta)\hat{\sigma}_{i,ab}^j = \frac{(\Delta)\mathcal{P}_i^{\mu\nu}}{4\pi} \int d\text{PS}_{X+b} (\Delta)\bar{\Sigma} |M_{ab}|_{j,\mu\nu}^2 \delta\left(\frac{z}{z_1} - \frac{p_a \cdot p_b}{p_a \cdot q}\right), \quad (2.28)$$

where $(\Delta)M_{ab} = M_{a(\uparrow)b} + (-)M_{a(\downarrow)b}$ is the spin-independent (dependent) amplitude for the process, $a(p_a, s_a) + V^*(q) \rightarrow b(p_b) + X$, where the parton b fragments into the hadron H' and $V = \gamma, Z, W^\pm$. The spin label s_a appears only for polarized subprocesses, while in the unpolarized case the spin is averaged over and the dependence on s_a is suppressed. The superscript j labels the type of intermediate bosons: $j = \gamma\gamma, ZZ$, or γZ for NC, and $j = W^\pm$ for CC processes. The quantity $(\Delta)\bar{\Sigma}$ represents the sum (or difference, for polarized cases) over initial-state polarizations, and the average over final-state polarizations and color quantum numbers. Here, $d\text{PS}_{X+b}$ denotes the phase space for the final state particles, consisting of b and the unobserved hadronic remnant X . Note, the Dirac delta function arises from tagging the parton b , thereby constraining its phase space. In d space-time dimensions, the projectors $(\Delta)\mathcal{P}_i^{\mu\nu}$ are written in terms of partonic tensors defined as $t_1^{\mu\nu} = T_1^{\mu\nu}$, $t_2^{\mu\nu} = x_1 T_2^{\mu\nu}$, see Eq. (2.18), and are given by

$$\mathcal{P}_1^{\mu\nu} = -\Delta\mathcal{P}_5^{\mu\nu} = \frac{1}{d-2} \left(t_1^{\mu\nu} + \frac{Q^2}{p_a \cdot q} t_2^{\mu\nu} \right),$$

$$\begin{aligned}\Delta\mathcal{P}_1^{\mu\nu} &= \frac{1}{2}\mathcal{P}_3^{\mu\nu} = \frac{i}{(d-2)(d-3)}\epsilon^{\mu\nu\sigma\lambda}\frac{q_\sigma p_{a,\lambda}}{p_a \cdot q}, \\ \mathcal{P}_2^{\mu\nu} &= -\Delta\mathcal{P}_4^{\mu\nu} = \frac{Q^2}{(d-2)p_a \cdot q} \left(t_1^{\mu\nu} + \frac{(d-1)Q^2}{p_a \cdot q} t_2^{\mu\nu} \right).\end{aligned}\tag{2.29}$$

The perturbative coefficient functions, $(\Delta)\mathcal{C}_{i,ab}^j$ are computed as a power series in the strong coupling constant a_s see Eq. (2.27), where the successive terms correspond to the leading order (LO), next-to leading order (NLO), next-to-next-to leading order (NNLO), and higher-order contributions. The inclusion of higher-order corrections is essential for achieving precise theoretical predictions. While the LO calculation captures the basic dynamics of the process, it suffers from a dependence on the unphysical scales like renormalization and factorization scales, which are systematically reduced by including higher-order contributions, thereby improving the reliability of theoretical predictions and provide a more reliable description of experimental data. In addition, new partonic channels that open up at higher orders can give sizeable contributions to the CFs and therefore cannot be neglected in precision phenomenology.

Beyond improving perturbative stability, higher-order calculations are essential for the precise extraction of non-perturbative quantities, such as parton distribution functions (PDFs) and fragmentation functions (FFs), from experimental measurements enabling a more precise determination of the flavor and spin decomposition of PDFs and FFs [39–43, 62, 65, 68, 69, 139–143].

The increasing precision of SIDIS measurements, together with the physics programme of the forthcoming Electron-Ion Collider (EIC) [123, 125, 144, 145], demands theoretical predictions beyond NLO accuracy. The expected percent-level precision over a wide kinematic range will provide new opportunities to study flavour decomposition, quark helicity distributions, and parity-violating asymmetries, and will provide additional constraints on PDFs and FFs in a flavor-sensitive way. Achieving this precision requires higher-order QCD corrections, with electroweak effects

becoming relevant for future analyses.

The coefficient functions for SIDIS were first computed in perturbative QCD at next-to leading order (NLO) corrections long ago [97, 109], see also [74, 110, 129, 146, 147]. Beyond NLO, however, only partial results were available for a long time, see [148–151]. In the soft and collinear limit, the dominant threshold logarithms have been obtained up to N³LO accuracy in QCD [152, 153] and resummed to all orders in perturbation theory to next-to-next-to-next-to leading logarithmic (N³LL) accuracy, extending earlier SIDIS resummations studies that had achieved only to next-to-leading logarithm (NLL) accuracy [150, 154–156]. At the same time, measurements from SIDIS experiments [157–159] have played an increasingly important role in global QCD analyses. They have been used [140, 141, 160–164] to directly constrain FFs, and also in combined fits of FFs and spin-dependent PDFs [71, 77, 165–170].

Recently, we computed for the first time complete next-to-next-to leading order QCD corrections to the SIDIS coefficient functions, for both polarized and unpolarized initial lepton and hadron beams with photon exchange [171–174]. An independent calculation by another group has also been performed [175–177], see also [178]. The results obtained by both the groups are in full agreement. More recently, threshold resummation for the SIDIS CFs has been extended towards N⁴LL accuracy and approximate N⁴LO QCD corrections, including both soft-virtual (SV) and next-to-soft-virtual (NSV) contributions, have been derived within a systematic framework [179], see also [180]. Furthermore, QCD⊗QED corrections up to NNLO level for photon exchange SIDIS have also become available [181], see also [182]. A comprehensive study of both unpolarized and polarized SFs in QCD up to NNLO level for neutral as well as charged current reactions has been accomplished in [183–186]. These theoretical developments have enabled the first global analysis of SIDIS data at full NNLO accuracy, leading to improved determinations of parton distribution functions (PDFs) and fragmentation functions (FFs) [75, 79, 187–193]. The growing

interest in SIDIS is also reflected in extensive studies of observables differential in the transverse momentum of the detected hadron, see [194–198].

This thesis fills the long-standing gap in precision SIDIS phenomenology by providing the first complete next-to-next-to-leading-order (NNLO) QCD calculation of the SIDIS coefficient functions. In particular, we present NNLO QCD corrections to polarized SIDIS via photon exchange [172]. Building on the same framework, we extend the study to unpolarized and polarized SIDIS processes involving both neutral-current (NC) and charged-current (CC) electroweak interactions [186]. Furthermore, this thesis develops the theoretical framework for the resummation of large threshold logarithms arising in relevant kinematic regions of SIDIS up to N⁴LO accuracy, providing reliable phenomenological predictions [179].

2.5 Summary

This chapter has introduced the theoretical foundations of deep-inelastic scattering and its semi-inclusive extension, which serve as essential probes of the partonic structure of hadrons. The relevant kinematic variables, the leptonic and hadronic tensors, and the parametrization of the hadronic tensor in terms of Lorentz-invariant structure functions were presented. The QCD factorization theorem was then introduced, allowing these structure functions to be expressed as convolutions of universal parton distribution functions, fragmentation functions, and perturbatively calculable coefficient functions. The computation of these coefficient functions from partonic cross sections using suitable projection operators was outlined, together with their perturbative expansion in the strong coupling. Finally, the motivation for higher-order calculations was discussed, highlighting their importance for reducing theoretical uncertainties and achieving the precision required by current and future SIDIS experiments.

The theoretical framework developed in this chapter forms the basis for the higher-order calculations presented in the remainder of this thesis. Building upon this framework, the next chapter presents the complete next-to-next-to leading-order QCD calculation of polarized Semi-Inclusive Deep-Inelastic Scattering with a photon exchange, together with the corresponding computational framework and phenomenological analysis.

Chapter 3

Next-to-Next-to Leading order in QCD

This chapter presents the computation of the next-to-next-to leading-order (NNLO) QCD corrections to polarized Semi-Inclusive Deep-Inelastic Scattering (SIDIS) in the single virtual-photon exchange approximation. After introducing the polarized SIDIS cross section and its factorization framework, we discuss the partonic subprocesses contributing through NNLO and outline the computational methodology employed in the calculation. The treatment of infrared singularities using plus distributions and the implementation of mass factorization are then presented, leading to finite coefficient functions in the $\overline{\text{MS}}$ scheme. Finally, we investigate the phenomenological impact of the NNLO corrections through numerical predictions for the polarized SIDIS structure functions. The work presented here is based on the publication [\[172\]](#).

3.1 Introduction

Polarized DIS plays a central role in understanding the spin structure of the nucleon [199, 200]. While unpolarized DIS provides information on the momentum distributions of quarks and gluons inside the nucleon, polarized DIS probes how the nucleon spin is shared among its constituent quarks and gluons. It gives access to the longitudinal spin structure of hadrons [201], parameterised by helicity (spin-dependent) PDFs [77, 78, 170, 202], which describe the difference between the number densities of partons with spins aligned and anti-aligned with the parent nucleon spin. The proton spin can be determined from a sum-rule for those helicity PDFs and therefore provide essential information towards resolving the long-standing proton spin puzzle. In contrast to inclusive DIS, which mainly constrains flavor combinations of quark distributions, polarized SIDIS enables the separate extraction of quark and antiquark helicity PDFs from data and significantly improves our knowledge of the flavor decomposition of the nucleon spin. This makes it a prominent observable to be measured at the upcoming Electron-Ion collider (EIC) at the Brookhaven National Laboratory [145]. The unique opportunities to study it at the EIC challenge the accuracy of available QCD theory predictions and provide motivation for their improvements.

The unprecedented precision anticipated from future polarized SIDIS measurements demands equally precise theoretical predictions. In particular, the extraction of helicity PDFs and fragmentation functions requires accurate perturbative calculations of the hard-scattering coefficient functions entering the QCD factorization theorem.

The description of polarized SIDIS in QCD has only been available at NLO accuracy [74]. To match the anticipated experimental accuracy and to reduce theoretical uncertainties arising from renormalization and factorization scale dependence, it is necessary to extend these calculations to next-to-next-to-leading order (NNLO) in perturbative QCD.

This chapter presents the complete NNLO QCD calculation for polarized Semi-Inclusive Deep-Inelastic Scattering (SIDIS) in the single virtual-photon exchange approximation. We discuss all contributing partonic channels, the extraction of the finite coefficient functions in the $\overline{\text{MS}}$ factorization scheme, and their phenomenological implications. The NNLO results presented here, which have also been obtained independently by another group with full agreement [172, 176], close a long-standing gap in the theoretical description of polarized SIDIS and provide the level of precision required for reliable phenomenological studies.

The SIDIS process is given by

$$e^-(k_l, \lambda_l) + H(P, \lambda_P) \rightarrow e^-(k'_l) + H'(P_H) + X, \quad (3.1)$$

where, we consider the production of a hadron H' along with the scattered lepton e^- and other inclusive final state particles collectively denoted by X (summed over), when a lepton e^- scatters off a hadron H . Here, $k_l, k'_l(P, P_H)$ are momenta of incoming and outgoing leptons (hadrons), respectively. λ_l and λ_P are the helicity of incoming lepton and hadron respectively.

Consider the case in which both the incoming lepton and the hadronic target are longitudinally polarized. Polarized SIDIS is defined by the asymmetry,

$$\frac{d^3\Delta\sigma}{dxdydz} = \frac{1}{2} \left(\frac{d^3\sigma_{e^+_{\uparrow} H_{\uparrow} \rightarrow e^- H' X}}{dxdydz} - \frac{d^3\sigma_{e^+_{\uparrow} H_{\downarrow} \rightarrow e^- H' X}}{dxdydz} \right),$$

where $e^+_{\uparrow}, H_{\uparrow(\downarrow)}$ denote the (anti-)parallel spin-orientations of the colliding electron and hadron. Here $x = \frac{Q^2}{2P \cdot q}$ is the Bjorken variable, $y = \frac{P \cdot q}{P \cdot k_l}$ the inelasticity, and $z = \frac{P \cdot P_H}{P \cdot q}$ the scaling variable of the identified hadron.

We consider semi-inclusive deep-inelastic scattering in the electromagnetic interaction, where the interaction between the incoming lepton and hadron is through the exchange of a virtual photon. In this case, the polarized SIDIS cross section can be

expressed in terms of spin-dependent structure functions. In particular, for longitudinal polarization, the dominant contribution arises from the structure function g_1 , which encodes information about the helicity distributions of quarks and gluons inside the nucleon. The structure function g_1 therefore plays a central role in probing the spin-dependent partonic structure of the proton i.e. in understanding the spin contribution from different partons to the proton spin.

The longitudinal polarized hadronic differential cross section is given by,

$$\frac{d^3\Delta\sigma}{dxdydz} = \frac{4\pi\alpha_e^2}{Q^2}(2-y)g_1(x, z, Q^2), \quad (3.2)$$

where α_e is the fine structure constant. The QCD factorization at scale μ_F^2 for polarized SIDIS takes the form:

$$g_1 = \sum_{a,b} \int_x^1 \frac{dx_1}{x_1} \int_z^1 \frac{dz_1}{z_1} \Delta f_{\frac{a}{H}}(x_1, \mu_F^2) D_{\frac{H'}{b}}(z_1, \mu_F^2) \mathcal{G}_{1,ab} \left(\frac{x}{x_1}, \frac{z}{z_1}, Q^2, \mu_F^2 \right) \quad (3.3)$$

Here $\Delta f_{\frac{a}{P}}$ denotes the spin dependent parton distribution function (PDFs) given as the difference between the distributions of parton a with spin aligned and anti-aligned relative to the proton spin i.e. $\Delta f_{\frac{a}{H}} = f_{\frac{a(\uparrow)}{H(\uparrow)}} - f_{\frac{a(\downarrow)}{H(\uparrow)}}$ and $D_{\frac{H'}{b}}$ denote the spin-averaged fragmentation functions (FFs). Here x_1 represents the momentum fraction carried by the initial parton a of incident hadron H , i.e. $p_a = x_1 P$ and z_1 denotes the momentum fraction carried by the observed hadron H' with respect to the final state parton ' b ', such that $P_{H'} = z_1 p_b$. We define the scaling variables $x' = x/x_1$ and $z' = z/z_1$. These non perturbative quantities PDF and FF are process independent and therefore universal and are extracted for experiments [39–83].

The coefficient function (CF) $\mathcal{G}_{1,ab}$ is computable in perturbative QCD in powers of

the strong coupling, $a_s(\mu_R^2) = \alpha_s(\mu_R^2)/(4\pi)$, at the renormalization scale μ_R ,

$$\mathcal{G}_{1,ab}(\mu_F^2) = \sum_{i=0}^{\infty} a_s^i(\mu_R^2) \mathcal{G}_{1,ab}^{(i)}(\mu_F^2, \mu_R^2), \quad (3.4)$$

where we have suppressed the scaling variables. $\mathcal{G}_{1,ab}$ is related to the parton level scattering cross sections $d\Delta\hat{\sigma}_{1,ab}(=\hat{\mathcal{G}}_{1,ab})$ through projection with $\Delta\mathcal{P}_1^{\mu\nu}$,

$$d\Delta\hat{\sigma}_{1,ab} = \hat{\mathcal{G}}_{1,ab} = \frac{\Delta\mathcal{P}_1^{\mu\nu}}{4\pi} \int d\text{PS}_{X+b} \Sigma |\Delta M_{ab}|_{\mu\nu}^2 \delta\left(\frac{z}{z_1} - \frac{p_a \cdot p_b}{p_a \cdot q}\right) \quad (3.5)$$

where the projector in d space-time dimensions reads,

$$\Delta\mathcal{P}_1^{\mu\nu} = \frac{i}{(d-2)(d-3)} \epsilon^{\mu\nu\sigma\lambda} \frac{q_\sigma p_{a,\lambda}}{p_a \cdot q}. \quad (3.6)$$

Here, $\Delta M_{ab} = M_{a(\uparrow)b} - M_{a(\downarrow)b}$ denotes the spin-dependent amplitude for the process $a(p_a, \lambda_a) + \gamma^*(q) \rightarrow b(p_b) + X$, where the parton b fragments into the observed hadron H' . Also, λ_a is the helicity of the parton a , and $d\text{PS}_{X+b}$ represents the phase-space for the final-state system consisting of b and the unobserved hadronic remnant X . The symbol Σ denotes the sum over the spin (or polarization) and color quantum numbers of the final-state particles, together with the average over the color degrees of freedom of the incoming parton a .

To obtain the coefficient function $\mathcal{G}_{1,ab}$, we compute the corresponding partonic cross sections up to second order in the strong coupling constant, a_s . This requires the evaluation of the relevant Feynman diagrams contributing to the various partonic channels. At NNLO, the contributions are classified into double-virtual (VV), real-virtual (RV), and double-real (RR) corrections. Beyond leading order, the calculation involves loop and phase-space integrals, which are evaluated in dimensional regularization with $d = 4 + \epsilon$ space-time dimensions. The resulting partonic cross sections contain ultraviolet and infrared singularities. After UV renormalization and mass factorization, finite coefficient functions are obtained.

In the following sections, we describe the computation of the various contributions up to NNLO, discuss the techniques employed in their evaluation, and highlight the main theoretical subtleties. We conclude with a phenomenological study of the resulting NNLO corrections.

3.2 Partonic Subprocesses

In this section, we identify the partonic subprocesses contributing to SIDIS up to NNLO in perturbative QCD. Unlike inclusive DIS, SIDIS involves the observation of a final-state hadron originating from the fragmentation of a parton. Consequently, in addition to the incoming parton participating in the hard scattering, one must also identify the fragmenting parton in the final state. This additional constraint gives rise to new partonic channels, which are absent in the inclusive case.

The relevant Feynman diagrams are generated using **QGRAF** [203]. All Feynman diagrams presented here are visualized using **axodraw2** [204]. The symbolic output produced by **QGRAF** is subsequently converted into a **FORM** [205–207] format, where the Dirac and Lorentz algebra, polarization sums, and color algebra are performed.

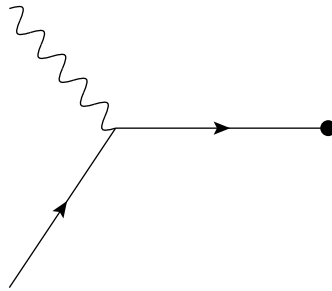


Figure 3.1: Feynman diagram for the LO process.

At leading order (LO), only single partonic subprocess contributes to polarized SIDIS, namely the quark (or anti-quark) scattering process i.e. $q(\bar{q})\gamma^* \rightarrow q(\bar{q})$, where the outgoing quark (anti-quark) subsequently fragments into the observed

hadron as shown in Fig. 3.1. The dot indicates the tagged fragmenting parton.

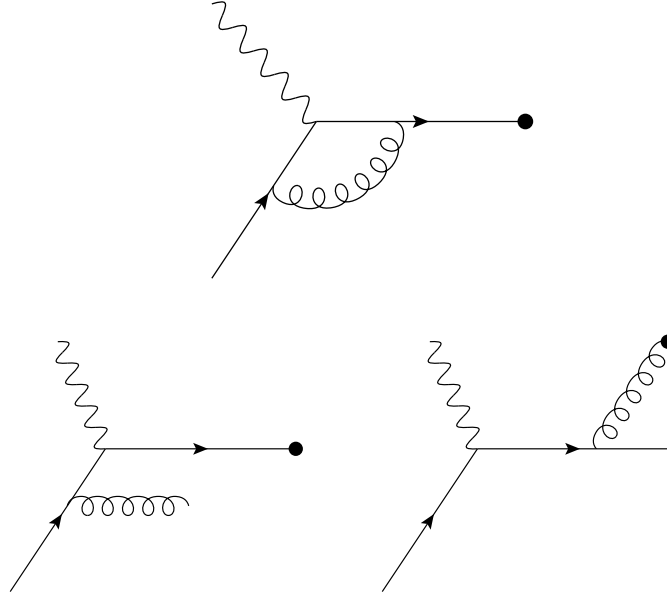


Figure 3.2: Quark initiated partonic subprocesses at NLO. Upper: virtual corrections. Bottom: real-emission corrections.

At next-to-leading order (NLO), both virtual corrections to the LO channel and real-emission subprocesses contribute. The quark (anti-quark) initiated subprocesses are (in Fig. 3.2),

$$q(\bar{q}) + \gamma^* \rightarrow q(\bar{q}) + \text{one-loop} , \quad (3.7)$$

$$q(\bar{q}) + \gamma^* \rightarrow q(\bar{q}) + g . \quad (3.8)$$

For the real-emission subprocess, either the final-state quark (antiquark) or the gluon can fragment into the observed hadron H' .

In addition, a gluon-initiated subprocess opens up at this order (Fig 3.3).

At next-to-next-to-leading order (NNLO), receives contribution from three distinct classes of subprocesses: two-loop virtual (VV) corrections, one-loop real virtual (RV) corrections, and double real-emission (RR) processes.

The VV contribution corresponds to the interference of the two-loop amplitude with

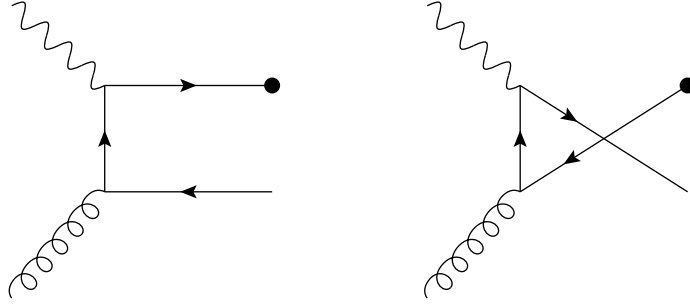


Figure 3.3: Gluon initiated partonic subprocesses at NLO

the Born amplitude together with the square of the one-loop amplitude. Representative VV diagrams are shown in Fig. 3.4.

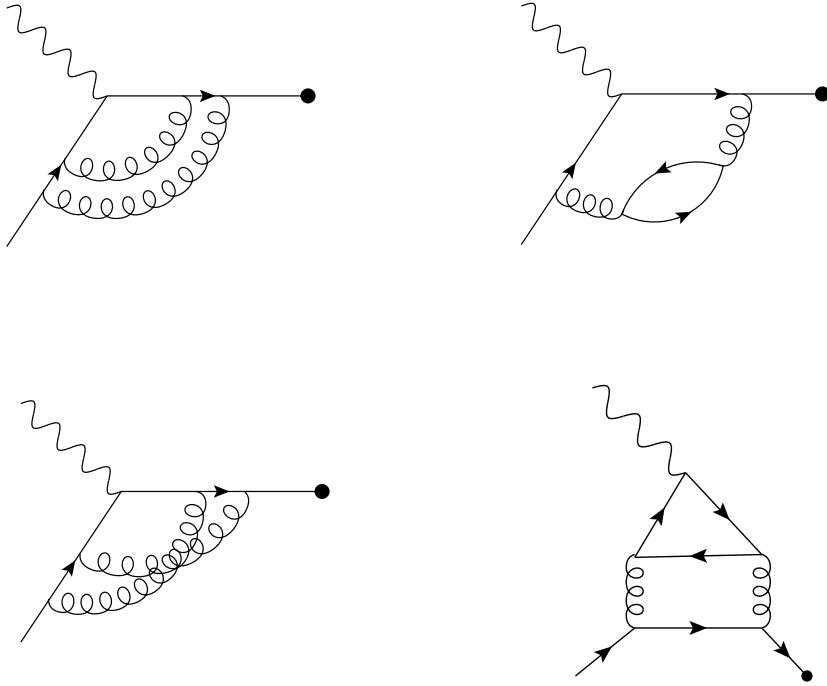


Figure 3.4: Representative Feynman diagrams contributing to the two-loop virtual corrections.

The RV contribution arises from one-loop corrections to the single real-emission amplitudes. For quark and gluon initiated channels, the corresponding subprocesses are

$$q(\bar{q}) + \gamma^* \rightarrow q(\bar{q}) + g + \text{one loop} , \quad (3.9)$$

$$g + \gamma^* \rightarrow q + \bar{q} + \text{one loop} . \quad (3.10)$$

The representative Feynman diagrams for this case are shown in Fig. 3.5. The corresponding RV contribution to the CF is obtained from the interference of one loop-one real emission amplitudes, Fig. 3.5 with the corresponding tree-level real-emission amplitudes shown in Fig. 3.2 and Fig. 3.3.

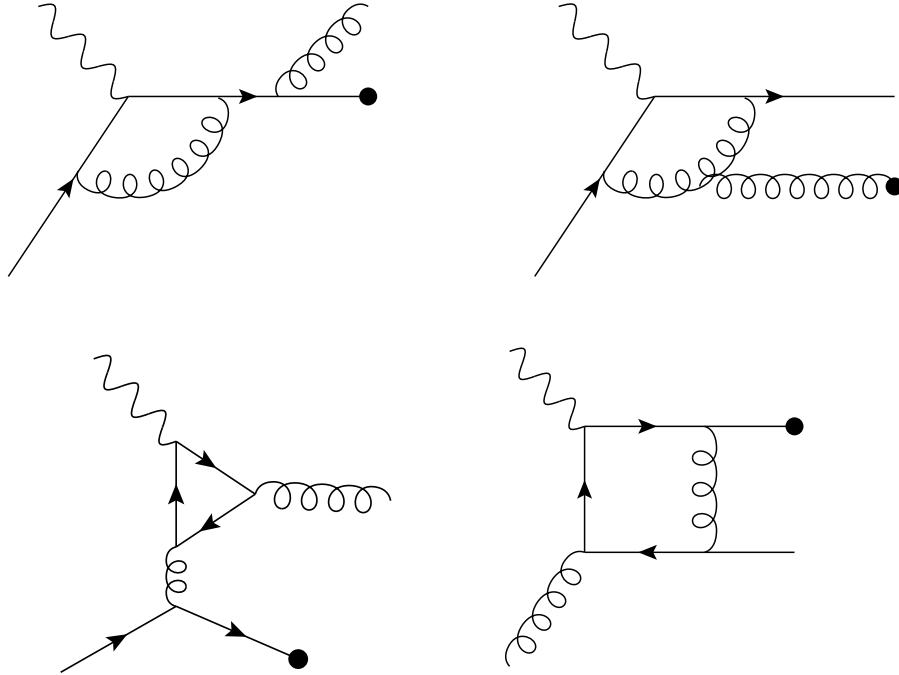


Figure 3.5: Real Virtual diagrams i.e. one-loop with one real emission at NNLO.

The two-parton real emissions (RR) contribution consists of tree-level subprocesses with two additional partons in the final state. The list of double real-emission subprocesses is given by

$$q(\bar{q}) + \gamma^* \rightarrow q(\bar{q}) + g + g , \quad (3.11)$$

$$q(\bar{q}) + \gamma^* \rightarrow q(\bar{q}) + q' + \bar{q}' , \quad (3.12)$$

$$q(\bar{q}) + \gamma^* \rightarrow q(\bar{q}) + q + \bar{q} \quad (3.13)$$

$$g + \gamma^* \rightarrow g + q + \bar{q}. \quad (3.14)$$

Here, q' denotes a quark of flavor different from the incoming quark. As in the NLO real-emission case, any of the parton in the final-state in above subprocesses can fragment into the observed hadron H' . The RR subprocesses may be grouped into three distinct classes: those with a pair of gluons in the final-state, those containing one gluon together with a quark anti-quark pair, and those involving an additional quark anti-quark pair in the final state.

The first class, corresponding to subprocesses with two gluons in the final state, is illustrated in Fig. 3.6.

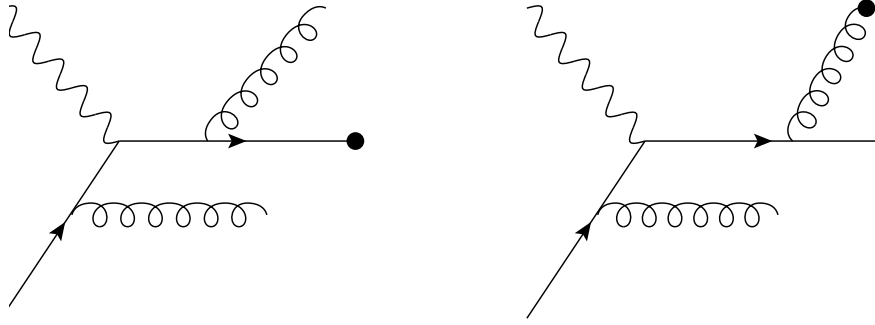


Figure 3.6: Sample Feynman diagrams for the RR subprocesses with two gluons in the final state. The dot indicates the tagged fragmenting parton.

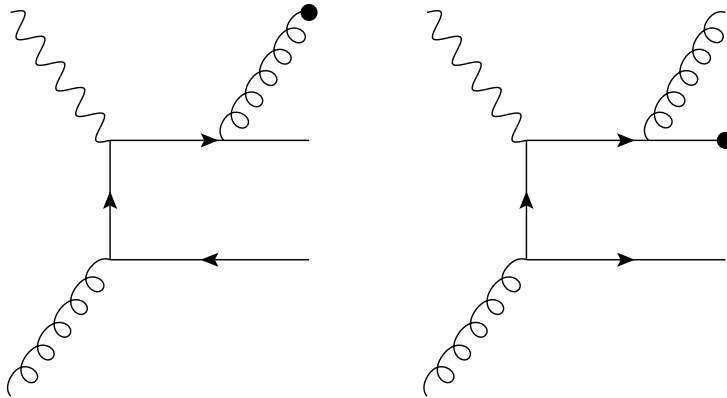


Figure 3.7: Representative gluon-initiated RR subprocesses.

The second class consists of gluon-initiated subprocesses containing one gluon together with a quark anti-quark pair in the final state, sample diagrams are shown in Fig. 3.7.

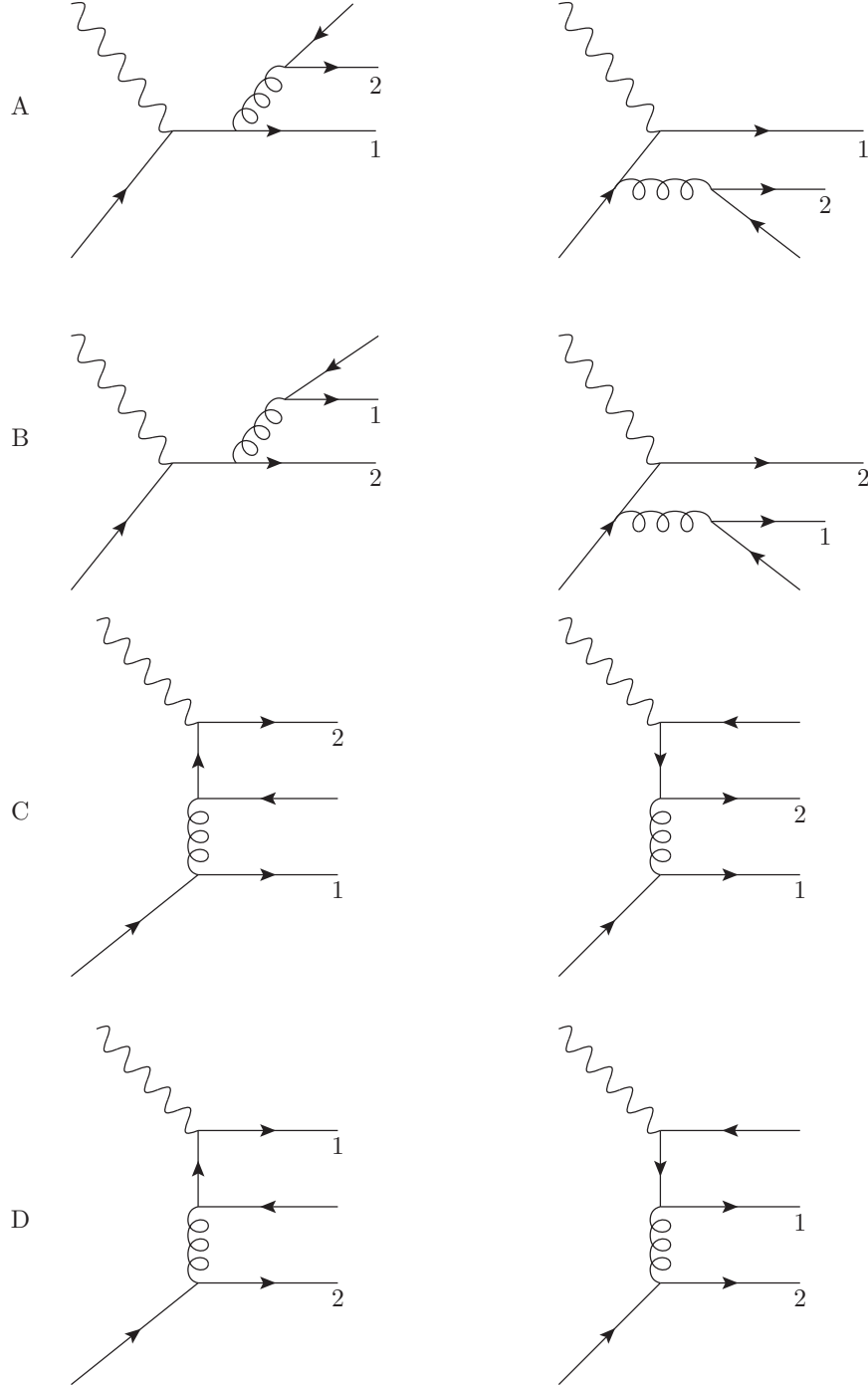


Figure 3.8: Feynman diagrams contributing to the subprocesses $q + \gamma^* \rightarrow q(1) + q(2) + \bar{q}$, labeled A, B, C, D.

The third class comprises the quark-initiated subprocess, $q + \gamma^* \rightarrow q(1) + q(2) + \bar{q}$, with an additional quark anti-quark pair in the final state. These are further classified into four distinct diagrams, depending on whether the produced quark pair is identical or non-identical to the incoming quark. The corresponding Feynman diagrams are shown in Fig. 3.8. For a non-identical quark pair, i.e. $q(1) \neq q(2)$, only the diagrams A and C contribute. When the produced quark has the same flavor as the incoming quark i.e. $q(1) = q(2)$, two additional diagrams, B and D, also contribute due to the presence of identical quarks in the final state.

After generating the diagrams, the Feynman rules are applied using a set of in-house routines. The resulting amplitudes are then manipulated symbolically using FORM to perform the Dirac algebra, Lorentz contractions, and simplification of the color factors using in-house codes. In the matrix element squared $|\Delta M_{ab}|_{\mu\nu}^2$, see Eq. (3.5), the Dirac matrix γ_5 arises due to spin dependent (anti-)quark states. In addition, we encounter Levi-Civita tensor from polarization of gluons and also from the projectors, see e.g. [208]. Since both the γ_5 matrix and the Levi-Civita tensor are intrinsically four-dimensional objects, a prescription is required to define them in $d = 4 + \epsilon$ dimensions [23, 209–221], see also [222–231]. Although several prescriptions have been proposed, none preserves the chiral Ward identity. A given prescription then requires an additional renormalization constant or an evanescent counter-term to preserve this identity. We employed Larin’s prescription [211] to define γ_5 in $d = 4 + \epsilon$,

$$\gamma_\mu \gamma_5 = \frac{i}{6} \epsilon_{\mu\nu\sigma\lambda} \gamma^\nu \gamma^\sigma \gamma^\lambda. \quad (3.15)$$

The Levi-Civita tensors contraction is expressed in terms of a determinant containing

metric tensors defined in $d = 4 + \epsilon$ dimensions.

$$\epsilon_{\mu_1\nu_1\lambda_1\sigma_1}\epsilon_{\mu_2\nu_2\lambda_2\sigma_2} = - \begin{vmatrix} g_{\mu_1\mu_2} & g_{\mu_1\nu_2} & g_{\mu_1\lambda_2} & g_{\mu_1\sigma_2} \\ g_{\nu_1\mu_2} & g_{\nu_1\nu_2} & g_{\nu_1\lambda_2} & g_{\nu_1\sigma_2} \\ g_{\lambda_1\mu_2} & g_{\lambda_1\nu_2} & g_{\lambda_1\lambda_2} & g_{\lambda_1\sigma_2} \\ g_{\sigma_1\mu_2} & g_{\sigma_1\nu_2} & g_{\sigma_1\lambda_2} & g_{\sigma_1\sigma_2} \end{vmatrix}, \quad (3.16)$$

such that in $d = 4$, $\epsilon_{\mu\nu\lambda\sigma}\epsilon^{\mu\nu\lambda\sigma} = -24$. The results obtained in Larin's scheme are transformed to the $\overline{\text{MS}}$ scheme through a finite renormalization scheme transformation. The associated renormalization constants [220, 232, 233] used for this scheme transformation restore the Ward identity and define the CFs in $\overline{\text{MS}}$ scheme. We discuss this procedure in detail in a subsequent section.

The contribution of each subprocess to the partonic cross section is accompanied by the appropriate symmetry and interference factors. In particular, subprocess containing two identical gluons in the final state where quark is fragmenting, i.e. $q(\bar{q}) + \gamma^* \rightarrow q(\bar{q}) + g + g$, is multiplied by a symmetry factor of $1/2$ to account for the indistinguishability of the final-state gluons. A similar factor arises for channels with identical quarks in the final state, for example for quark initiated and anti-quark fragmenting, $q + \gamma^* \rightarrow \bar{q} + q + q$, which also requires a symmetry factor of $1/2$.

Having discussed the various classes of subprocesses contributing through NNLO, the complete set of partonic channels is summarize in Table 3.1. For convenience, the corresponding representative Feynman diagrams and the perturbative order of each contribution are also listed.

With all partonic subprocesses specified, including the relevant symmetry and interference factors, the computation of the partonic cross sections reduces to the evaluation of the corresponding matrix elements. The structure function g_1 is then extracted by applying the projector given in Eq. (3.6). The resulting expressions

Figure	Partonic subprocess		
	Channel		
Fig. 3.1	LO	$q + \gamma^* \rightarrow q$	Born
Fig. 3.2	NLO	$q + \gamma^* \rightarrow q$	1-loop correction
Fig. 3.2		$q + \gamma^* \rightarrow q + g$	
Fig. 3.3		$g + \gamma^* \rightarrow q + \bar{q}$	
Fig. 3.4		$q + \gamma^* \rightarrow q$	2-loop correction
Fig. 3.5	NNLO	$q + \gamma^* \rightarrow q + g$	1-loop correction
Fig. 3.6		$q + \gamma^* \rightarrow q + g + g$	
Fig. 3.8		$q + \gamma^* \rightarrow q + q_i + \bar{q}_i$	
Fig. 3.5		$g + \gamma^* \rightarrow q + \bar{q}$	1-loop correction
Fig. 3.7		$g + \gamma^* \rightarrow q + \bar{q} + g$	

Table 3.1: Partonic subprocesses contributing up to NNLO. Here, q_i may be of the same or a different flavor than q .

involve loop integrals arising from virtual corrections as well as phase-space integrals associated with real-emission contributions.

3.3 Loop and Phase-space Integrals

Having constructed the squared amplitude in the Larin scheme, we proceed to the evaluation of the loop and phase-space integrals arising in the various partonic subprocesses. The partonic cross sections contain both ultraviolet (UV) and infrared (IR) divergences. The UV divergences originate from loop corrections, whereas the IR divergences arise from soft and collinear configurations present in both virtual and real-emission contributions. We have used dimensional regularization with $d = 4 + \epsilon$ space-time dimensions to regulate both UV and IR divergences.

The VV contributions involve one-loop and two-loop QCD corrections to the Born subprocess, together with the one-loop squared contribution at NNLO. These contributions can be obtained using the vector form factor which is known to fourth order in a_s [234]. The RV and RR contributions contain real parton emissions, with the RV terms corresponding to one-loop corrections to single-real emission processes, while the RR terms involve single-real emissions at NLO and double-real emissions at NNLO.

The loop integrals are first mapped onto predefined integral families. This is achieved using the package **REDUZE2** [235, 236], which identifies the loop momentum shifts and rewrites propagator belonging to different diagrams in terms of a common family of propagators. Because of presence of delta functions in the phase space integrals, arising from momentum conservation, on-shell conditions and the extra constraint in SIDIS, we cannot make momentum shift to real-emission. Following the identification of the integral families, all the scalar products appearing in the numerators are rewritten in terms of the propagators and thereby mapping the amplitudes onto integral families.

In the RV and RR contributions, due to the presence of the SIDIS constraint $\delta\left(\frac{z}{z_1} - \frac{p_a \cdot p_b}{p_a \cdot q}\right)$, the corresponding phase space integrals are more involved compared to fully inclusive DIS. With reverse unitarity [237–239], we have mapped, the two-body phase-space over one-loop Feynman integrals that appear in RV and three-body phase space integrals in RR to loop integrals. The constraint delta function $\delta\left(z' - \frac{p_a \cdot p_b}{p_a \cdot q}\right)$, recall $z' = z/z_1$, is replaced by a propagator-like term $-\frac{1}{\pi} \text{Im}(1/(z' - \frac{p_a \cdot p_b}{p_a \cdot q} + i\epsilon))$. This allows us to apply loop-integration techniques, namely integration-by-parts identities (IBP) [240, 241], to reduce them to a smaller number of integrals called master integrals (MIs). We have used the **Mathematica** package **LiteRed** [242–244] to generate the IBP rules for all VV, RV and RR contributions. Several other publicly available packages and computational frameworks

for IBP reduction have also been developed, see for e.g. [236, 245–253]. At NNLO, IBP reduction yields 4 MIs for VV, 7 MIs for RV, and 20 MIs for RR subprocesses. The results for VV MIs can be found in [254–256], the MIs of RV are given in [173, 254, 257], and the MIs of RR can be found in [174, 177].

The calculation of the MIs poses one of the primary challenges in this computation. More details regarding the integral families, and computation of master integrals will be explained in details in the next chapter.

3.4 Pole structure

After substituting the master integrals into the squared amplitudes, the UV and IR singularities manifested as poles in the dimensional regularization parameter ϵ . While the ultraviolet singularities are removed through renormalization, the infrared singularities must be isolated in a form suitable for subsequent factorization.

The infrared singularities originate from soft and collinear configurations of massless partons are of the form $(1 - x')^{-1}$ and/or $(1 - z')^{-1}$, which are divergent at threshold regions $x' \rightarrow 1$ and $z' \rightarrow 1$. In dimensional regularization, these singularities are regulated by factors of the form $(1 - x')^{a\epsilon}$ and $(1 - z')^{b\epsilon}$ arising from the phase-space measure.

To systematically extract the poles structure in ϵ , these singular terms are expanded in terms of ‘+’-distributions and regular functions using the following identity

$$(1 - \xi)^{-1+a\epsilon} = \frac{1}{a\epsilon} \delta(1 - \xi) + \sum_{k=0}^{\infty} \frac{(a\epsilon)^k}{k!} \mathcal{D}_{\xi}^k, \quad (3.17)$$

where $\xi = x', z'$ and $\mathcal{D}_{\xi}^k = \left[\frac{\log^k(1-\xi)}{(1-\xi)} \right]_+$ denote the usual ‘+’-distributions, as defined

by (see also Appendix-B)

$$\int_0^1 dw g_+(w) f(w) = \int_0^1 dw g(w) (f(w) - f(1)). \quad (3.18)$$

Since the singularities may occur simultaneously in both variables, the expansion is performed sequentially, first in one variable and subsequently in the other. The details of the plus-distribution procedure employed in this work are summarized in Appendix-B. As a result, all infrared singularities are expressed in terms of poles in ϵ , accompanied by delta functions, plus-distributions, and regular functions.

The structure of the singular terms depends on the perturbative order and the type of contribution under consideration. For the purely virtual contribution, the kinematics are fixed to the Born configuration and the result is proportional to $\delta(1-x'), \delta(1-z')$,

At NLO, the real-emission subprocesses generate endpoint singularities in both scaling variables. These singularities appear in the form $\frac{(1-x')^{\epsilon/2}}{1-x'}$ and $\frac{(1-z')^{\epsilon/2}}{1-z'}$, which upon expansion i.e. using Eq. (3.17), produce poles in ϵ .

At NNLO, the RV contributions involve more kinematics factors and IR singular terms of the form

$$\frac{(1-x')^{a\epsilon}(1-z')^{b\epsilon}|z'-x'|^{c\epsilon}|1-z'-x'|^{d\epsilon}}{(1-x')(1-z')(z'-x')(1-z'-x')} f_1(x', z'), \quad (3.19)$$

Similarly, in RR case the IR structure is of the form,

$$\frac{(1-x')^\epsilon(1-z')^\epsilon}{(1-x')(1-z')(z'-x')[(1+x')^2-4x'z']} f_2(x', z'), \quad (3.20)$$

where f_1 and f_2 are regular function of x' and z' .

After partial fractioning, intermediate expressions may contain, in addition to the

endpoint singularities at $x' = 1$ and $z' = 1$, apparent singularities at $x' = z'$ and $x' + z' = 1$. These singularities require special care during the distributional expansion. Furthermore, the resulting expressions involve multi-valued functions and we need to define them in different kinematic regions appropriately. We encounter different regions depending on whether $x' > z'$ with $x' + z' > 1$ and/or $x' + z' < 1$ or $x' < z'$ with $x' + z' > 1$ and/or $x' + z' < 1$. The corresponding expressions are related through analytic continuation, which is implemented using Feynman's $i0$ prescription to ensure a smooth continuation across one region to other.

Once the appropriate analytic continuation has been performed, the sequential plus-distribution procedure can be applied to systematically isolate the endpoint singularities. The singular contributions are thereby expressed in terms of poles in ϵ , plus-distributions, and regular functions, thereby exposing the infrared structure of the coefficient functions in a form suitable for mass factorization.

A few remarks regarding the singularity structure are in order. At NLO, the partonic cross sections contain poles up to $1/\epsilon^2$, while at NNLO highest pole is $1/\epsilon^4$. According to the Kinoshita-Lee-Nauenberg (KLN) theorem, the IR singularities cancel after summing over all degenerate real and virtual contributions. Consequently, the $1/\epsilon^2$ poles at NLO and the $1/\epsilon^4$ and $1/\epsilon^3$ poles at NNLO cancel after summing over the relevant subprocesses. In addition, the ultraviolet singularities arising from loop corrections are removed through coupling-constant renormalization.

Since we are not summing over initial and final state partons there are left over collinear singularities, originating from configurations in which massless partons become collinear to either the incoming or outgoing partons. These singularities are universal and are factored out, see [258–261]. These collinear singularities are systematically absorbed into the parton distribution functions and fragmentation functions through the procedure of mass factorization, yielding finite coefficient functions.

3.5 Mass factorization

We now discuss the implementation of mass factorization. According to the QCD factorization theorem, the remaining collinear singularities can be systematically absorbed into the renormalized parton distribution functions and fragmentation functions, leaving behind finite short-distance coefficient functions. The factorization theorem implies that the partonic cross sections, after combining the degenerate real and virtual subprocesses, can be expressed as convolutions of universal Altarelli–Parisi (AP) kernels and coefficient functions. The initial state collinear divergences are factored out in terms of spin-dependent space-like AP kernel $\Delta\Gamma^L$, defined in Larin scheme, while the final state collinear divergences are factored out as time-like AP kernels ($\tilde{\Gamma}$), defined in $\overline{\text{MS}}$ scheme. Since the spins of the observed final-state partons are summed over, the time-like kernels are unpolarized.

The partonic cross sections in Eq. (3.5) factorise into the AP kernels $\Delta\Gamma_{c\leftarrow a}^L$ of PDFs and $\tilde{\Gamma}_{b\leftarrow d}$ of FFs, appropriately convoluted with the finite CF ($\mathcal{G}_{1,cd}$) at factorization scale μ_F (suppressed here for brevity),

$$d\Delta\hat{\sigma}_{1,ab}(\epsilon) = \hat{\mathcal{G}}_{1,cd}^L = \Delta\Gamma_{c\leftarrow a}^L(\mu_F^2, \epsilon) \otimes \mathcal{G}_{1,cd}^L(\mu_F^2, \epsilon) \tilde{\otimes} \tilde{\Gamma}_{b\leftarrow d}(\mu_F^2, \epsilon), \quad (3.21)$$

where L denotes the Larin scheme. The summation over c, d is implied and $\otimes$ ($\tilde{\otimes}$) denotes a convolution over the scaling variable $x' = x/x_1$ ($z' = z/z_1$), defined as

$$A(x) \otimes \mathcal{C}(x, z) \tilde{\otimes} B(z) = \int_x^1 \frac{dx_1}{x_1} \int_z^1 \frac{dz_1}{z_1} A(x_1) \mathcal{C}\left(\frac{x}{x_1}, \frac{z}{z_1}\right) B(z_1). \quad (3.22)$$

The spin dependent space-like AP kernels ($\Delta\Gamma_{c\leftarrow a}$) in $\overline{\text{MS}}$ scheme are known at the order required [233, 262–269]. Since the partonic cross sections in Eq. (3.21) are derived in Larin’s scheme, these spin-dependent AP kernels need to be taken in the same scheme, see [233]. On the other hand, the spin-averaged time-like AP kernels

($\tilde{\Gamma}_{b \leftarrow d}$) are taken in the standard $\overline{\text{MS}}$ scheme [120, 270]. The AP kernels can be expanded in power of strong coupling constant of a_s as,

$$\Gamma_{c \leftarrow d}(\xi, \mu_F^2, \epsilon) = \delta_{cd} \delta(1 - \xi) + \sum_{l=1}^{\infty} a_s^l(\mu_F^2) \Gamma_{c \leftarrow d}^{(l)}(\xi, \epsilon), \quad (3.23)$$

where Γ denotes either the space-like kernels $\Delta\Gamma^L$ in Larin scheme or $\Delta\Gamma$ in $\overline{\text{MS}}$ scheme or the time-like kernels $\tilde{\Gamma}$. They subject to a renormalization group evolution equation,

$$\mu_F^2 \frac{d}{d\mu_F^2} \Gamma_{c \leftarrow d} = \frac{1}{2} \mathbb{P}_{ce}(a_s(\mu_F^2)) \otimes \Gamma_{e \leftarrow d}, \quad (3.24)$$

where we collectively denote the corresponding splitting functions by the set $\mathbb{P}$. Their perturbative expansion is given by $\mathbb{P}_{ce} = \sum_{l=1}^{\infty} a_s^l(\mu_F^2) \mathbb{P}_{ce}^{(l-1)}$. The splitting functions required for the present analysis are available in the literature to the relevant perturbative order and beyond. For the space-like polarized splitting functions ΔP in the $\overline{\text{MS}}$ scheme, see [233, 262–264, 267–269]. For the time-like unpolarized splitting functions $\tilde{P}$, see [120, 270] and also [271].

Similarly, the partonic cross section can be expanded in the strong coupling constant $a_s(\mu_R^2)$ as, (with the explicit Q^2 dependence is factored out)

$$\begin{aligned} \hat{\mathcal{G}}_{1,ab}(x', z', Q^2, \epsilon) &= \hat{\mathcal{G}}_{1,ab}^{(0)}(x', z') + a_s(\mu_R^2) \left(\frac{Q^2}{\mu_R^2} \right)^{\frac{\epsilon}{2}} \hat{\mathcal{G}}_{1,ab}^{(1)}(x', z', \epsilon) \\ &+ a_s^2(\mu_R^2) \left(\frac{2\beta_0}{\epsilon} \right) \left(\frac{Q^2}{\mu_R^2} \right)^{\frac{\epsilon}{2}} \hat{\mathcal{G}}_{1,ab}^{(1)}(x', z', \epsilon) \\ &+ a_s^2(\mu_R^2) \left(\frac{Q^2}{\mu_R^2} \right)^{\epsilon} \hat{\mathcal{G}}_{1,ab}^{(2)}(x', z', \epsilon) + O(a_s^3(\mu_R^2)). \end{aligned} \quad (3.25)$$

Upon substituting the perturbative expansions of the AP kernels $\Delta\Gamma_{c \leftarrow a}^{L,(l)}$ and $\tilde{\Gamma}_{b \leftarrow d}^{(l)}$ into Eq. (3.21), the finite coefficient functions $\mathcal{G}_{1,ab}$ entering Eq. (3.3) can be ex-

tracted order by order in a_s as

$$\begin{aligned}\mathcal{G}_{1,ab}(x', z', Q^2, \mu_F^2) = & \mathcal{G}_{1,ab}^{(0)}(x', z', Q^2, \mu_F^2, \mu_R^2) + a_s(\mu_R^2) \mathcal{G}_{1,ab}^{(1)}(x', z', Q^2, \mu_F^2, \mu_R^2) \\ & + a_s^2(\mu_R^2) \mathcal{G}_{1,ab}^{(2)}(x', z', Q^2, \mu_F^2, \mu_R^2) + O(a_s^3(\mu_R^2)).\end{aligned}\quad (3.26)$$

For equal scales, setting $\mu_R = \mu_F$, the CFs $\mathcal{G}_{1,ab}^{L,(l)}$ for $l = 0, 1, 2$ are given below, with Q^2 and μ_F^2 dependence suppressed in $\mathcal{G}_{1,ab}^{L,(l)}$.

At LO ($l = 0$):

$$\begin{aligned}q(\bar{q}) &\rightarrow q(\bar{q}) \\ \mathcal{G}_{1,qq}^{L,(0)}(x', z') &= \hat{\mathcal{G}}_{1,qq}^{L,(0)}(x', z') = e_q^2 \delta(1-x') \delta(1-z'),\end{aligned}\quad (3.27)$$

at NLO ($l = 1$):

$$\begin{aligned}q(\bar{q}) &\rightarrow q(\bar{q}) \\ \mathcal{G}_{1,qq}^{L,(1)}(x', z') &= \left(\frac{Q^2}{\mu_F^2}\right)^{\frac{\epsilon}{2}} \hat{\mathcal{G}}_{1,qq}^{L,(1)}(x', z') - e_q^2 \delta(1-x') \tilde{\Gamma}_{q \leftarrow q}^{(1)}(z') - e_q^2 \Delta \Gamma_{q \leftarrow q}^{L,(1)}(x') \delta(1-z'), \\ q(\bar{q}) &\rightarrow g \\ \mathcal{G}_{1,qg}^{L,(1)}(x', z') &= \left(\frac{Q^2}{\mu_F^2}\right)^{\frac{\epsilon}{2}} \hat{\mathcal{G}}_{1,qg}^{L,(1)}(x', z') - e_q^2 \delta(1-x') \tilde{\Gamma}_{g \leftarrow q}^{(1)}(z'), \\ g &\rightarrow q(\bar{q}) \\ \mathcal{G}_{1,gq}^{L,(1)}(x', z') &= \left(\frac{Q^2}{\mu_F^2}\right)^{\frac{\epsilon}{2}} \hat{\mathcal{G}}_{1,gq}^{L,(1)}(x', z') - e_q^2 \Delta \Gamma_{q \leftarrow g}^{L,(1)}(x') \delta(1-z'),\end{aligned}\quad (3.28)$$

at NNLO ($l = 2$):

$$\begin{aligned}q(\bar{q}) &\rightarrow q(\bar{q}) \\ \mathcal{G}_{1,qq}^{L,(2)}(x', z') &= \left(\frac{Q^2}{\mu_F^2}\right)^{\epsilon} \hat{\mathcal{G}}_{1,qq}^{L,(2)}(x', z') + \frac{2\beta_0}{\epsilon} \left(\frac{Q^2}{\mu_F^2}\right)^{\frac{\epsilon}{2}} \hat{\mathcal{G}}_{1,qq}^{L,(1)}(x', z') \\ &\quad - \mathcal{G}_{1,qq}^{L,(1)}(x', z') \tilde{\otimes} \tilde{\Gamma}_{q \leftarrow q}^{(1)}(z') - \mathcal{G}_{1,qg}^{L,(1)}(x', z') \tilde{\otimes} \tilde{\Gamma}_{q \leftarrow g}^{(1)}(z')\end{aligned}$$

$$\begin{aligned}
& -e_q^2 \delta(1-x') \tilde{\Gamma}_{q \leftarrow q}^{(2)}(z') - e_q^2 \Delta \Gamma_{q \leftarrow q}^{L,(2)}(x') \delta(1-z') \\
& -e_q^2 \Delta \Gamma_{q \leftarrow q}^{L,(1)}(x') \tilde{\Gamma}_{q \leftarrow q}^{(1)}(z') - \Delta \Gamma_{q \leftarrow q}^{L,(1)}(x') \otimes \mathcal{G}_{1,qq}^{L,(1)}(x', z') \\
& - \Delta \Gamma_{g \leftarrow q}^{L,(1)}(x') \otimes \mathcal{G}_{1,gq}^{L,(1)}(x', z'),
\end{aligned}$$

$$q(\bar{q}) \rightarrow g$$

$$\begin{aligned}
\mathcal{G}_{1,qg}^{L,(2)}(x', z') &= \left(\frac{Q^2}{\mu_F^2} \right)^\epsilon \hat{\mathcal{G}}_{1,qg}^{L,(2)}(x', z') + \frac{2\beta_0}{\epsilon} \left(\frac{Q^2}{\mu_F^2} \right)^{\frac{\epsilon}{2}} \hat{\mathcal{G}}_{1,qg}^{L,(1)}(x', z') \\
& - \mathcal{G}_{1,qg}^{L,(1)}(x', z') \tilde{\otimes} \tilde{\Gamma}_{g \leftarrow q}^{(1)}(z') - \mathcal{G}_{1,qg}^{L,(1)}(x', z') \tilde{\otimes} \tilde{\Gamma}_{g \leftarrow g}^{(1)}(z') \\
& - e_q^2 \delta(1-x') \tilde{\Gamma}_{g \leftarrow q}^{(2)}(z') - \Delta \Gamma_{q \leftarrow q}^{L,(1)}(x') \otimes \mathcal{G}_{1,qg}^{L,(1)}(x', z') \\
& - e_q^2 \Delta \Gamma_{q \leftarrow q}^{L,(1)}(x') \tilde{\Gamma}_{g \leftarrow q}^{(1)}(z'),
\end{aligned}$$

$$q(\bar{q}) \rightarrow \bar{q}(q)$$

$$\begin{aligned}
\mathcal{G}_{1,q\bar{q}}^{L,(2)}(x', z') &= \left(\frac{Q^2}{\mu_F^2} \right)^\epsilon \hat{\mathcal{G}}_{1,q\bar{q}}^{L,(2)}(x', z') - \mathcal{G}_{1,qg}^{L,(1)}(x', z') \tilde{\otimes} \tilde{\Gamma}_{\bar{q} \leftarrow g}^{(1)}(z') - e_q^2 \delta(1-x') \tilde{\Gamma}_{\bar{q} \leftarrow q}^{(2)}(z') \\
& - \Delta \Gamma_{g \leftarrow q}^{L,(1)}(x') \otimes \mathcal{G}_{1,g\bar{q}}^{L,(1)}(x', z') - e_q^2 \Delta \Gamma_{\bar{q} \leftarrow q}^{L,(2)}(x') \delta(1-z'),
\end{aligned}$$

$$q(\bar{q}) \rightarrow q'(\bar{q}'), \quad \text{for } \{q \neq q'\}$$

$$\begin{aligned}
\mathcal{G}_{1,qq'}^{L,(2)}(x', z') &= \left(\frac{Q^2}{\mu_F^2} \right)^\epsilon \hat{\mathcal{G}}_{1,qq'}^{L,(2)}(x', z') - \mathcal{G}_{1,qg}^{L,(1)}(x', z') \tilde{\otimes} \tilde{\Gamma}_{q \leftarrow g}^{(1)}(z') - e_q^2 \delta(1-x') \tilde{\Gamma}_{q' \leftarrow q}^{(2)}(z') \\
& - \Delta \Gamma_{g \leftarrow q}^{L,(1)}(x') \otimes \mathcal{G}_{1,qq'}^{L,(1)}(x', z') - e_{q'}^2 \Delta \Gamma_{q' \leftarrow q}^{L,(2)}(x') \delta(1-z'),
\end{aligned}$$

$$q(\bar{q}) \rightarrow \bar{q}'(q'), \quad \text{for } \{q \neq q'\}$$

$$\begin{aligned}
\mathcal{G}_{1,q\bar{q}'}^{L,(2)}(x', z') &= \left(\frac{Q^2}{\mu_F^2} \right)^\epsilon \hat{\mathcal{G}}_{1,q\bar{q}'}^{L,(2)}(x', z') - \mathcal{G}_{1,qg}^{L,(1)}(x', z') \tilde{\otimes} \tilde{\Gamma}_{\bar{q} \leftarrow g}^{(1)}(z') - e_q^2 \delta(1-x') \tilde{\Gamma}_{\bar{q}' \leftarrow q}^{(2)}(z') \\
& - \Delta \Gamma_{g \leftarrow q}^{L,(1)}(x') \otimes \mathcal{G}_{1,g\bar{q}'}^{L,(1)}(x', z') - e_{q'}^2 \Delta \Gamma_{\bar{q}' \leftarrow q}^{L,(2)}(x') \delta(1-z'),
\end{aligned}$$

$$g \rightarrow q(\bar{q})$$

$$\begin{aligned}
\mathcal{G}_{1,gq}^{L,(2)}(x', z') &= \left(\frac{Q^2}{\mu_F^2} \right)^\epsilon \hat{\mathcal{G}}_{1,gq}^{L,(2)}(x', z') + \frac{2\beta_0}{\epsilon} \left(\frac{Q^2}{\mu_F^2} \right)^{\frac{\epsilon}{2}} \hat{\mathcal{G}}_{1,gq}^{L,(1)}(x', z') \\
& - \mathcal{G}_{1,gq}^{L,(1)}(x', z') \tilde{\otimes} \tilde{\Gamma}_{q \leftarrow q}^{(1)}(z') - e_q^2 \Delta \Gamma_{q \leftarrow g}^{L,(1)}(x') \tilde{\Gamma}_{q \leftarrow q}^{(1)}(z') \\
& - \Delta \Gamma_{q \leftarrow g}^{L,(1)}(x') \otimes \mathcal{G}_{1,gq}^{L,(1)}(x', z') - \Delta \Gamma_{g \leftarrow g}^{L,(1)}(x') \otimes \mathcal{G}_{1,gq}^{L,(1)}(x', z') \\
& - e_q^2 \Delta \Gamma_{q \leftarrow g}^{L,(2)}(x') \delta(1-z'),
\end{aligned}$$

$$g \rightarrow g$$

$$\begin{aligned}
\mathcal{G}_{1,gg}^{L,(2)}(x', z') &= \left(\frac{Q^2}{\mu_F^2} \right)^\epsilon \hat{\mathcal{G}}_{1,gg}^{L,(2)}(x', z') - \sum_q \mathcal{G}_{1,gq}^{L,(1)}(x', z') \tilde{\otimes} \tilde{\Gamma}_{g \leftarrow q}^{(1)}(z') \\
&\quad - \sum_q \mathcal{G}_{1,g\bar{q}}^{L,(1)}(x', z') \tilde{\otimes} \tilde{\Gamma}_{g \leftarrow \bar{q}}^{(1)}(z') - \sum_q e_q^2 \Delta\Gamma_{q \leftarrow g}^{L,(1)}(x') \tilde{\Gamma}_{g \leftarrow q}^{(1)}(z') \\
&\quad - \sum_q e_q^2 \Delta\Gamma_{\bar{q} \leftarrow g}^{L,(1)}(x') \tilde{\Gamma}_{g \leftarrow \bar{q}}^{(1)}(z') - \sum_q \Delta\Gamma_{q \leftarrow g}^{L,(1)}(x') \otimes \mathcal{G}_{1,qg}^{L,(1)}(x', z') \\
&\quad - \sum_q \Delta\Gamma_{\bar{q} \leftarrow g}^{L,(1)}(x') \otimes \mathcal{G}_{1,\bar{q}g}^{L,(1)}(x', z'). \tag{3.29}
\end{aligned}$$

Note, in above e_q is the electric charge of quark q and e'_q is the electric charge of quark q' different flavor from q and summation in $g \rightarrow g$ channel is over the number of active flavor light quark.

Since the polarized hadronic SF g_1 is a physical observable, hence scheme independent, i.e. is independent of the prescription adopted for γ_5 , an additional finite renormalization is required to convert the Altarelli–Parisi kernels and the finite CFs from Larin to those in the conventional $\overline{\text{MS}}$ scheme. Denoting the PDFs and coefficient functions defined in Larin’s scheme by Δf_a^L and $\mathcal{G}_{1,ab}^L(\mu_F^2)$ respectively, the mass factorization for g_1 reads,

$$\begin{aligned}
g_1 &= \Delta f_c^L(\mu_F^2) \otimes \mathcal{G}_{1,cb}^L(\mu_F^2) \tilde{\otimes} D_b(\mu_F^2) \\
&= \Delta f_c^L(\mu_F^2) \otimes Z_{ca}(\mu_F^2) \otimes (Z^{-1}(\mu_F^2))_{ad} \otimes \mathcal{G}_{1,db}^L(\mu_F^2) \tilde{\otimes} D_b(\mu_F^2) \\
&= \Delta f_a(\mu_F^2) \otimes \mathcal{G}_{1,ab}(\mu_F^2) \tilde{\otimes} D_b(\mu_F^2). \tag{3.30}
\end{aligned}$$

where summation over a, b, c, d is implied. The CFs in the $\overline{\text{MS}}$ scheme are obtained by transforming Δf_c^L to $\overline{\text{MS}}$ PDFs through $\Delta f_a = Z_{ca}(\mu_F^2) \otimes f_c^L(\mu_F^2)$ and CFs to $\overline{\text{MS}}$ CFs, $\mathcal{G}_{1,ab} = (Z^{-1}(\mu_F^2))_{ad} \otimes \mathcal{G}_{1,db}^L(\mu_F^2)$. The CF $\mathcal{G}_{1,cb}^L$ in Eq. (3.30) requires the polarized AP kernels in Larin’s scheme, which can be derived from the polarized space-like AP kernels ($\Delta\Gamma_{c \leftarrow d}$) in the $\overline{\text{MS}}$ scheme through the relation Z_{ab} by $\Delta\Gamma^L = Z^{-1} \otimes \Delta\Gamma$. Using this along with Eq. (3.24), leads to the scheme transformation for

the splitting functions,

$$\Delta P_{ab} = Z_{ac} \otimes \Delta P_{cd}^L \otimes (Z^{-1})_{db} - 2\beta(a_s) Z_{ac} \otimes \frac{d}{da_s}(Z^{-1})_{cb}, \quad (3.31)$$

where $\beta(a_s) = -\sum_{l=0}^{\infty} a_s^{l+2}(\mu_F^2)\beta_l$.

The symmetric matrix valued Z -factor are dependent on x' and well known [220, 232, 233] and can be expanded perturbatively as,

$$Z_{ab}(x) = \delta(1-x) + \sum_{l=1}^{\infty} a_s^l z_{ab}^{(l)}(x), \quad (3.32)$$

and with $z_{qg}^{(l)} = z_{gq}^{(l)} = z_{gg}^{(l)} = 0$, we have $Z_{qg} = Z_{gq} = Z_{gg} = \delta(1-x)$. For the quark sector, the relevant elements of the Z -matrix are expanded as

$$\begin{aligned} Z_{q_i q_j} &= \delta(1-x) + a_s z_{q_i q_j}^{(1)} + a_s^2 z_{q_i q_j}^{(2)} + \mathcal{O}(a_s^3), \\ Z_{q_i \bar{q}_j} &= \delta(1-x) + a_s z_{q_i \bar{q}_j}^{(1)} + a_s^2 z_{q_i \bar{q}_j}^{(2)} + \mathcal{O}(a_s^3), \end{aligned} \quad (3.33)$$

The flavor structure of the finite renormalization coefficients is given by,

$$\begin{aligned} z_{q_i q_j}^{(l)} &= z_{\bar{q}_i \bar{q}_j}^{(l)} = \delta_{ij} z_{qq}^{(l),V} + z_{qq}^{(l),S}, \\ z_{q_i \bar{q}_j}^{(l)} &= z_{\bar{q}_i q_j}^{(l)} = \delta_{ij} z_{q\bar{q}}^{(l),V} + z_{q\bar{q}}^{(l),S}. \end{aligned} \quad (3.34)$$

Here i and j denote quark flavors, while the superscripts V and S correspond to the valence and pure-singlet contributions, respectively. At one loop, the pure-singlet terms vanish i.e. $z_{q\bar{q}}^{(1),S} = z_{q\bar{q}}^{(1),S} = 0$ and the remaining of $z_{ab}^{(k)}$ coefficients are given by:

$$\begin{aligned} z_{q_i q_j}^{(1)}(x) &= \delta_{ij} C_F \left\{ -8 + 8x \right\}, \quad z_{q_i \bar{q}_j}^{(1)}(x) = 0, \\ z_{q\bar{q}}^{(2),V}(x) &= C_F n_f T_F \left\{ \frac{16}{3} (1-x) \ln(x) + \frac{80}{9} (1-x) \right\} \end{aligned}$$

$$\begin{aligned}
& -C_A C_F \left\{ \left(\frac{80}{3} - \frac{8}{3}x \right) \ln(x) + 4(1-x) \ln^2(x) + \frac{592}{9}(1-x) - 8\zeta_2(1-x) \right\} \\
& + C_F^2 \left\{ 16(1-x) \ln(x) \ln(1-x) - 8(2+x) \ln(x) - 16(1-x) \right\}, \\
z_{q\bar{q}}^{(2),V}(x) = & - \left(C_F^2 - \frac{1}{2} C_A C_F \right) \left\{ 8(1+x) \left(4\text{Li}_2(-x) + 4\ln(x) \ln(1+x) - \ln^2(x) \right. \right. \\
& \left. \left. - 3\ln(x) + 2\zeta_2 \right) - 56(1-x) \right\}, \\
z_{qq}^{(2),S}(x) = & z_{q\bar{q}}^{(2),S}(x) = C_F T_F \left\{ 4(2+x) \ln^2(x) + 8(3-x) \ln(x) + 16(1-x) \right\}.
\end{aligned} \tag{3.35}$$

Using Eqs. (3.31) and (3.32), together with the perturbative expansion of the splitting functions, the spin dependent space-like splitting functions in Larin's scheme can be obtained as,

$$\begin{aligned}
\Delta P_{ab}^{L,(0)} &= \Delta P_{ab}^{(0)}, \\
\Delta P_{qq}^{L,(1)} &= \Delta P_{qq}^{(1)} + 2\beta_0 z_{qq}^{(1)}, \\
\Delta P_{qg}^{L,(1)} &= \Delta P_{qg}^{(1)} - \Delta P_{qg}^{(0)} \otimes z_{qq}^{(1)}, \\
\Delta P_{gq}^{L,(1)} &= \Delta P_{gq}^{(1)} + \Delta P_{gq}^{(0)} \otimes z_{qq}^{(1)}, \\
\Delta P_{q\bar{q}}^{L,(1)} &= \Delta P_{q\bar{q}}^{(1)}, \quad \Delta P_{qq'}^{L,(1)} = \Delta P_{qq'}^{(1)}, \\
\Delta P_{gg}^{L,(1)} &= \Delta P_{gg}^{(1)}.
\end{aligned} \tag{3.36}$$

Similarly, the coefficient functions in the $\overline{\text{MS}}$ scheme are given by:

$$\begin{aligned}
\mathcal{G}_{1,qq}^{(0)} &= \mathcal{G}_{1,qq}^{L,(0)} = e_q^2 \delta(1-x') \delta(1-z'), \\
\mathcal{G}_{1,qq}^{(1)} &= \mathcal{G}_{1,qq}^{L,(1)} + \left(-z_{qq}^{(1)} \right) \otimes \mathcal{G}_{1,qq}^{L,(0)}, \\
\mathcal{G}_{1,qg}^{(1)} &= \mathcal{G}_{1,qg}^{L,(1)}, \\
\mathcal{G}_{1,gq}^{(1)} &= \mathcal{G}_{1,gq}^{L,(1)}, \\
\mathcal{G}_{1,qq}^{(2)} &= \mathcal{G}_{1,qq}^{L,(2)} + \left(-z_{qq}^{(1)} \right) \otimes \mathcal{G}_{1,qq}^{L,(1)} \\
& + \left(z_{qq}^{(1)} \otimes z_{qq}^{(1)} - z_{qq}^{(2)} \right) \otimes \mathcal{G}_{1,qq}^{L,(0)},
\end{aligned}$$

$$\begin{aligned}
\mathcal{G}_{1,q\bar{q}}^{(2)} &= \mathcal{G}_{1,q\bar{q}}^{L,(2)} + \left(-z_{q\bar{q}}^{(2)} \right) \otimes \mathcal{G}_{1,q\bar{q}}^{L,(0)} , \\
\mathcal{G}_{1,qq'}^{(2)} &= \mathcal{G}_{1,qq'}^{L,(2)} + \left(-z_{qq'}^{(2)} \right) \otimes \mathcal{G}_{1,q'q'}^{L,(0)} , \\
\mathcal{G}_{1,q\bar{q}'}^{(2)} &= \mathcal{G}_{1,q\bar{q}'}^{L,(2)} + \left(-z_{q\bar{q}'}^{(2)} \right) \otimes \mathcal{G}_{1,\bar{q}'q'}^{L,(0)} , \\
\mathcal{G}_{1,qg}^{(2)} &= \mathcal{G}_{1,qg}^{L,(2)} + \left(-z_{qq}^{(1)} \right) \otimes \mathcal{G}_{1,qg}^{L,(1)} , \\
\mathcal{G}_{1,gq}^{(2)} &= \mathcal{G}_{1,gq}^{L,(2)} , \quad \mathcal{G}_{1,gg}^{(2)} = \mathcal{G}_{1,gg}^{L,(2)} .
\end{aligned} \tag{3.37}$$

The final $\overline{\text{MS}}$ scheme CFs thus obtained (after transformation from the Larin scheme) can be written as,

$$\begin{aligned}
\mathcal{G}_{1,ab} &= \sum_r \Delta C_{ab}^r h_r(x', z') + \sum_\beta \left(\Delta C_{ab,x'}^\beta(x') Z_\beta(z') + \Delta C_{ab,z'}^\beta(z') X_\beta(x') \right) \\
&\quad + \Delta R_{ab}(x', z') .
\end{aligned} \tag{3.38}$$

The soft plus virtual (SV) terms h_r contain the double distributions $h_{\delta_{x'}\delta_{z'}} = \delta(1-x')\delta(1-z')$, $h_{\delta_{x'}j} = \delta(1-x')\mathcal{D}_{z'}^j$, $h_{j\delta_{z'}} = \mathcal{D}_{x'}^j\delta(1-z')$, $h_{jk} = \mathcal{D}_{x'}^j\mathcal{D}_{z'}^k$. It gets contribution from only the diagonal channel i.e. $a = b = q$ or $\bar{q}$. Terms with single distributions, namely $Z_{\delta_{z'}}(z') = \delta(1-z')$, $Z_j(z') = \mathcal{D}_{z'}^j$, $X_{\delta_{x'}}(x') = \delta(1-x')$, $X_j(x') = \mathcal{D}_{x'}^j$ are called partial-SV (pSV) terms and regular terms are denoted by ΔR_{ab} . Our NLO results are in complete agreement with [74]. ΔC_{ab}^r are in complete agreement with those of unpolarized SFs $F_{1,2}$ [152, 171, 173, 175], see also [272, 273] and if we expand $\Delta C_{ab,x'}^\beta(x')$ and $\Delta C_{ab,z'}^\beta(z')$ around $x', z' \rightarrow 1$, the results are in complete agreement with the corresponding terms in the unpolarized case up to order $(1-x')^0$ and $(1-z')^0$ respectively, [173, 175, 274]. The remaining contributions in Eq. (3.38), i.e., single distributions X_β , Z_β and regular terms ΔR_{ab} are new.

For convenience, we extract the quark electric charge factors from the CF $\mathcal{G}_{1,ab}$ and define the reduced coefficient functions $G_{1,ab}$ as,

$$\mathcal{G}_{1,qq}^{(0)} = \mathcal{G}_{1,q\bar{q}}^{(0)} = e_q^2 \delta(1-x')\delta(1-z') ,$$

$$\begin{aligned}
\mathcal{G}_{1,q\bar{q}}^{(1)} &= \mathcal{G}_{1,\bar{q}\bar{q}}^{(1)} = e_q^2 G_{1,q\bar{q}}^{(1)}, \\
\mathcal{G}_{1,qg}^{(1)} &= \mathcal{G}_{1,\bar{q}g}^{(1)} = e_q^2 G_{1,qg}^{(1)}, \\
\mathcal{G}_{1,g\bar{q}}^{(1)} &= \mathcal{G}_{1,g\bar{q}}^{(1)} = e_q^2 G_{1,g\bar{q}}^{(1)}, \\
\mathcal{G}_{1,q\bar{q}}^{(2)} &= \mathcal{G}_{1,\bar{q}\bar{q}}^{(2)} = e_q^2 G_{1,q\bar{q}}^{(2),\text{NS}} + \left(\sum_{q_k} e_{q_k}^2 \right) G_{1,q\bar{q}}^{(2),\text{PS}}, \\
\mathcal{G}_{1,q\bar{q}}^{(2)} &= \mathcal{G}_{1,\bar{q}\bar{q}}^{(2)} = e_q^2 G_{1,q\bar{q}}^{(2)}, \\
\mathcal{G}_{1,q\bar{q}'}^{(2)} &= \mathcal{G}_{1,\bar{q}\bar{q}'}^{(2)} = e_q^2 G_{1,q\bar{q}'}^{(2),[1]} + e_{q'}^2 G_{1,q\bar{q}'}^{(2),[2]} + e_q e_{q'} G_{1,q\bar{q}'}^{(2),[3]}, \\
\mathcal{G}_{1,q\bar{q}'}^{(2)} &= \mathcal{G}_{1,\bar{q}\bar{q}'}^{(2)} = e_q^2 G_{1,q\bar{q}'}^{(2),[1]} + e_{q'}^2 G_{1,\bar{q}\bar{q}'}^{(2),[2]} - e_q e_{q'} G_{1,q\bar{q}'}^{(2),[3]}, \\
\mathcal{G}_{1,qg}^{(2)} &= \mathcal{G}_{1,\bar{q}g}^{(2)} = e_q^2 G_{1,qg}^{(2)}, \\
\mathcal{G}_{1,g\bar{q}}^{(2)} &= \mathcal{G}_{1,g\bar{q}}^{(2)} = e_q^2 G_{1,g\bar{q}}^{(2)}, \\
\mathcal{G}_{1,gg}^{(2)} &= \left(\sum_{q_k} e_{q_k}^2 \right) G_{1,gg}^{(2)}. \tag{3.39}
\end{aligned}$$

At NNLO, the quark coefficient function $\mathcal{G}_{1,q\bar{q}}^{(2)}$ or $\mathcal{G}_{1,\bar{q}\bar{q}}^{(2)}$ naturally decompose into flavor non-singlet (NS) and pure singlet (PS) contributions. The (PS) contribution originates from diagrams in which the virtual photon couples to a closed quark loop that is disconnected from the external quark line connecting the incoming parton to the fragmenting parton and is therefore proportional to the sum of the squared electric charges of all active quark flavors. It gets contribution only from the squared C type real-emission diagrams, denoted by C^2 in Fig. 3.8. The remaining contributions, in which the photon couples directly to the quark line connecting the initial state quark or the fragmenting quark, constitute the (NS) part and are proportional to the electric charge squared of the external quark. These receive contributions from the virtual-loop diagrams shown in Figs. 3.2 and 3.4, from the real-virtual (RV) diagrams shown in Fig. 3.5, and the double real-emission (RR) subprocesses. The latter include the two-gluon emission diagrams shown in Fig. 3.6 as well as the squared A, B and D type diagrams, as well as their mutual interference terms and their interference with the C type diagrams, cf. Fig. 3.8.

For subprocesses involving two distinct quark flavors namely, $\mathcal{G}_{1,q\bar{q}'}^{(2)}$ and $\mathcal{G}_{1,qq'}^{(2)}$, additional charge structures proportional to e_q^2 , $e_{q'}^2$, and $e_q e_{q'}$ appear, corresponding to the different ways in which the virtual photon couples to the quark lines. The contributions proportional to e_q^2 and $e_{q'}^2$, denoted by $G_{1,q\bar{q}'}^{(2),[1]}$ and $G_{1,qq'}^{(2),[2]}$, originate from the squared A² and C² type diagrams respectively. The mixed charge contribution proportional to $e_q e_{q'}$, denoted by $G_{1,q\bar{q}'}^{(2),[3]}$, arises from the interference between the A and C type diagrams, cf. Fig. 3.8.

It is worth noting that the flavor non-singlet coefficient function for polarized SIDIS coincide with those of the structure function F_3 , provided that the additional renormalization associated with the axial-vector current and the kinematics-independent transformation from Larin's scheme to the conventional $\overline{\text{MS}}$ scheme are taken into account [211, 275, 276]. This correspondence will be revisited in Chapter 6, where we extend our analysis to neutral-current and charged-current electroweak interactions.

Finally, the complete set of partonic coefficient functions obtained above is combined according to the factorization formula, Eq. (3.3), to construct the SIDIS structure functions. The following section presents a phenomenological analysis of the higher-order QCD corrections and assesses their impact on precision predictions for polarized SIDIS.

3.6 Phenemonology

In this section, we investigate the numerical impact of the newly computed coefficient functions on the polarized SIDIS structure function g_1 for various centre-of-mass energies $\sqrt{s}$ for the considered range of Bjorken scaling variable x and fragmentation variable z . The convolution of the CFs with PDFs and FFs provides $g_1 = \sum_{l=0} a_s^l g_1^{(l)}$, such that at LO $g_1^{(0)} = \sum_q e_q^2 H_{qq}$ (e_q being the electric charge of

quark q) and

$$g_1^{(1)} = \sum_q e_q^2 \left(H_{qq} \hat{\otimes} G_{1,qq}^{(1)} + H_{qg} \hat{\otimes} G_{1,qg}^{(1)} + H_{gq} \hat{\otimes} G_{1,gq}^{(1)} \right), \quad (3.40)$$

$$\begin{aligned} g_1^{(2)} = & \sum_q e_q^2 \left(H_{qq} \hat{\otimes} G_{1,qq,\text{NS}}^{(2)} + H_{q\bar{q}} \hat{\otimes} G_{1,q\bar{q}}^{(2)} + H_{qg} \hat{\otimes} G_{1,qg}^{(2)} + H_{gq} \hat{\otimes} G_{1,gq}^{(2)} \right) \\ & + \left(\sum_{q_i} e_{q_i}^2 \right) \left(H_{qq} \hat{\otimes} G_{1,qq,\text{PS}}^{(2)} + H_{gg} \hat{\otimes} G_{1,gg}^{(2)} \right) \\ & + \sum_q \sum_{q' \neq q} \left(e_q^2 H_{qq'}^+ \hat{\otimes} G_{1,qq',[1]}^{(2)} + e_{q'}^2 H_{qq'}^+ \hat{\otimes} G_{1,qq',[2]}^{(2)} + e_q e_{q'} H_{qq'}^- \hat{\otimes} G_{1,qq',[3]}^{(2)} \right). \end{aligned} \quad (3.41)$$

The symbol $\hat{\otimes}$ denotes convolution of $G_{1,ab}^{(l)}$ with H_{ab} in both variables x and z .

$$\begin{aligned} H_{qq} &= \Delta f_q(x) D_q(z) + \Delta f_{\bar{q}}(x) D_{\bar{q}}(z), \\ H_{q\bar{q}} &= \Delta f_q(x) D_{\bar{q}}(z) + \Delta f_{\bar{q}}(x) D_q(z), \\ H_{qg} &= \Delta f_q(x) D_g(z) + \Delta f_{\bar{q}}(x) D_g(z), \\ H_{gg} &= \Delta f_g(x) D_g(z), \\ H_{qq'}^\pm &= \Delta f_q(x) D_{q'}(z) \pm \Delta f_q(x) D_{\bar{q}'}(z) \pm \Delta f_{\bar{q}}(x) D_{q'}(z) + \Delta f_{\bar{q}}(x) D_{\bar{q}'}(z), \\ H_{gq} &= \Delta f_g(x) D_q(z) + \Delta f_{\bar{g}}(x) D_{\bar{q}}(z). \end{aligned} \quad (3.42)$$

We evaluate Eqs. (3.40) and (3.41) numerically for the $g_1^{\pi^+}$ SF (with an identified π^+ in the final state) as a function of x and Q^2 after integrating z over a range from 0.2 to 0.85. We use polarized PDFs from **MAPPDF10NLO** at LO and NLO and **MAPPDF10NNLO** at NNLO throughout [187]. The strong coupling constant α_s is taken from the PDF sets at the respective perturbative order and use $n_F = 3$ active flavors.

In Fig. 3.9, we show contributions to $g_1^{\pi^+}$ from all the partonic channels at various perturbative orders at $\sqrt{s} = 17.4$ GeV after setting the scales $\mu_R^2 = \mu_F^2 = Q^2$, and using FFs from **NNFF10** [64] at the respective perturbative orders. We observe at every order, that the partonic channel where incoming as well as fragmenting states

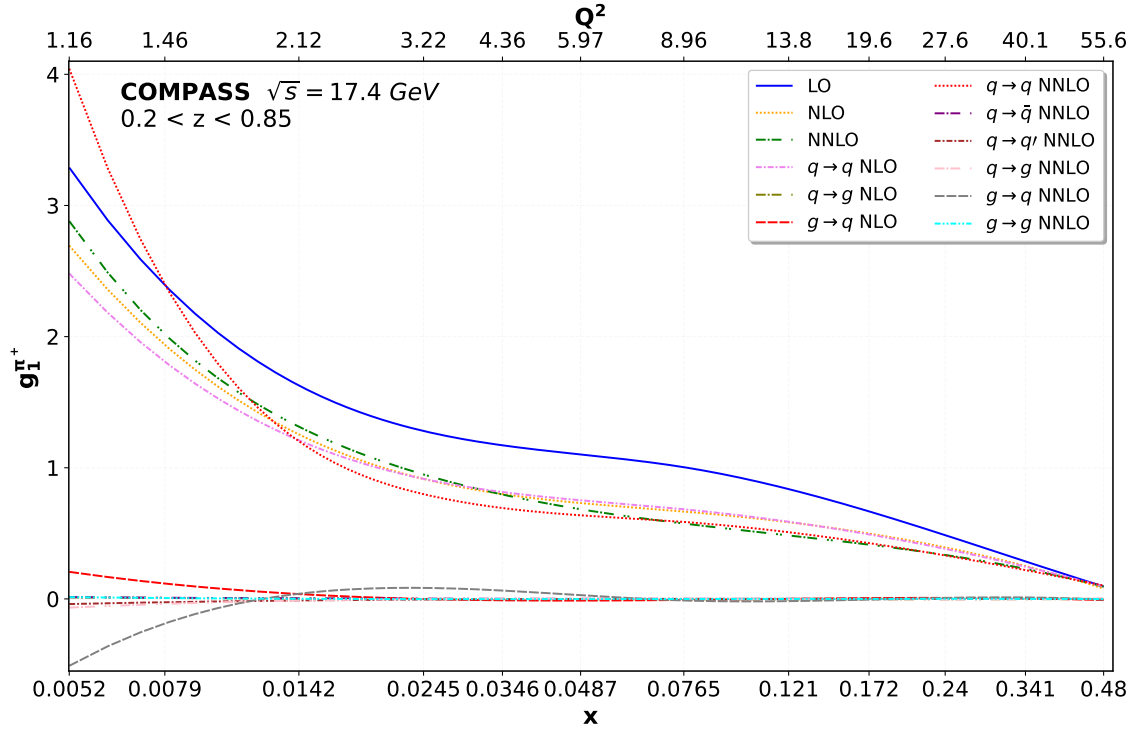


Figure 3.9: Contributions from all partonic channels to SF $g_1^{\pi^+}$ as a function of x for the COMPASS energy $\sqrt{s} = 17.4$ GeV.

are (anti-)quarks dominate over the rest of the partonic channels.

In the Fig. 3.10, we show how $g_1^{\pi^+}$ changes with respect to renormalization and factorization scales at various perturbative orders as a function of x at $\sqrt{s} = 45$ GeV. In each plot, the range of x is chosen by constraining $y = Q^2/(xs)$ to the range $0.5 \leq y \leq 0.9$. The bands at every order are the result of a 7-point scale variation around the central scale ($\mu_R^2 = \mu_F^2 = Q^2$) with $k_1\mu_R^2, k_2\mu_F^2$ where $(k_1, k_2) \in [1/2, 2]$ with a constraint $1/2 \leq k_1/k_2 \leq 2$. We have used FFs from MAPFF10NLO at LO and NLO, MAPFF10NNLO at NNLO [70]. It demonstrates clearly that the inclusion of NNLO corrections reduces the scale dependence when compared to the previous orders. We find at small Q^2 the sensitivity to these scales is larger compared to that at larger values of Q^2 . The reason for this is that at small Q^2 the strong coupling is large and the effect of scale variations is, therefore, amplified. We also observe that the bands from NLO and NNLO predictions are well separated at lower values

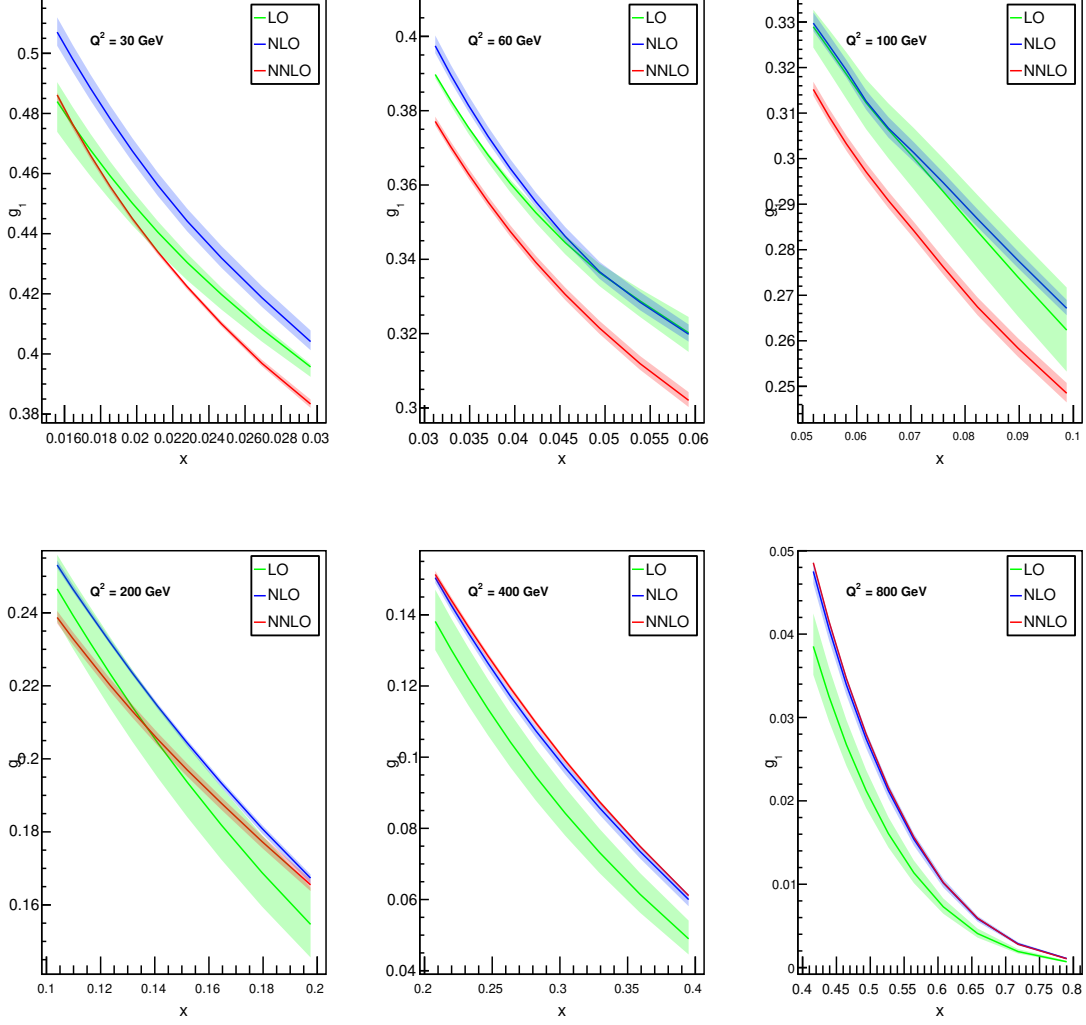


Figure 3.10: Dependence of $g_1^{\pi^+}$ on renormalization and factorization scales in 7-point variation of μ_R^2 and μ_F^2 , as a function of x at various values of Q^2 .

of Q^2 . The reason for this is that contributions from partonic channels at order α_s^2 (NNLO) are as large or even bigger than those at α_s (NLO).

In Fig. 3.11, we plot the ratio of the polarized SF $g_1^{\pi^+}$ to the unpolarized SF $F_1^{\pi^+}$ as a function of x for the COMPASS energy $\sqrt{s} = 17.4$ GeV, using NNPDF3.1 [277] for unpolarized PDFs and NNFF10 for FFs at the respective perturbative orders. The plot includes the 7-point scale variation at LO, NLO and NNLO and, for comparison, the experimental data taken from [122]. Given the accuracy of those data, Fig. 3.11 clearly indicates the need to reduce residual theory uncertainties in SIDIS predictions

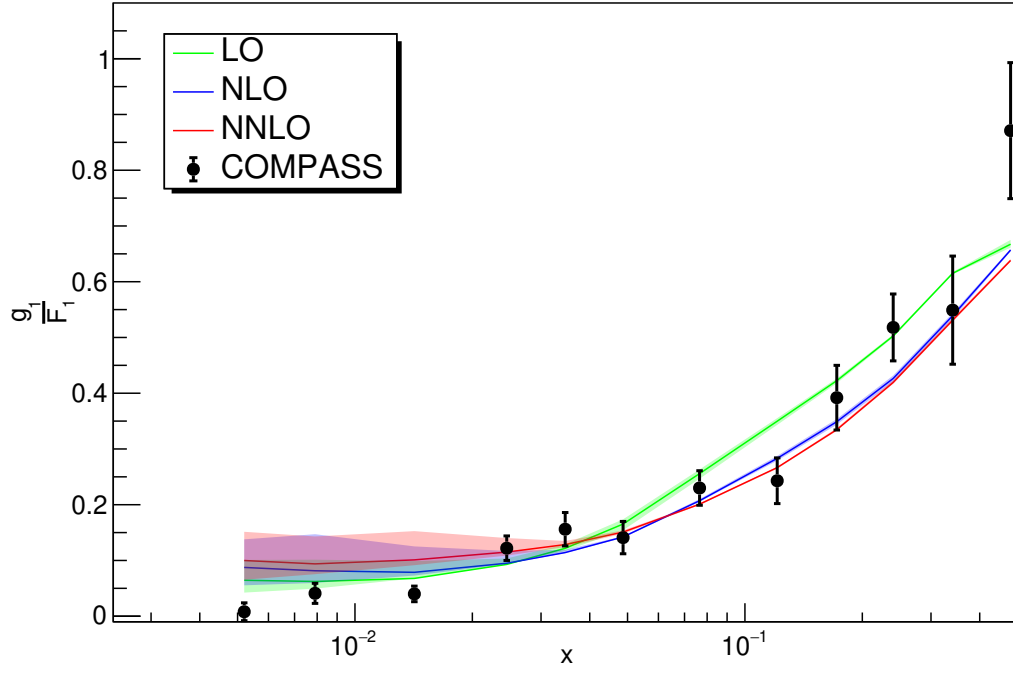


Figure 3.11: The ratio of SFs $g_1^{\pi^+}/F_1^{\pi^+}$ as a function of x for the COMPASS energy $\sqrt{s} = 17.4$ GeV. The bands correspond to the seven-point scale variation.

at NNLO accuracy.

Chapter 4

Master Integrals Evaluation

The evaluation of master integrals is one of the principal technical challenges in the NNLO computation of SIDIS coefficient functions. This chapter supplements the discussion of the previous chapter by presenting the methods used to evaluate the master integrals (MIs) appearing in the virtual-virtual (VV), real-virtual (RV), and double-real (RR) contributions. Particular emphasis is given to the analytic continuation of the RV master integrals and the evaluation of the new RR master integrals, which constitute the main bottleneck of the calculation. The latter are computed using two independent approaches: a direct phase-space parameterization in a suitable reference frame and the method of differential equations. Throughout this chapter, the master integrals are treated as functions of the dimensional regulator ϵ and the kinematic variables Q^2 , x' , and z' .

4.1 Introduction

The computation of the NNLO QCD corrections to semi-inclusive deep inelastic scattering (SIDIS) requires the evaluation of a large number of loop and phase-space integrals originating from the double virtual (VV), real-virtual (RV), and double-real (RR) subprocesses. Following the tensor decomposition and the application of Integration-by-Parts (IBP) identities [240,278], these integrals can be systematically reduced to a much smaller finite set of *master integrals* (MIs). The determination and solving these master integrals constitutes one of the central ingredients of the NNLO calculation. Throughout this chapter, all loop and phase-space integrals are evaluated in dimensional regularization with the space-time dimension $d = 4 + \epsilon$. A detailed discussion of the general concepts used here can be found in standard references, see for example [279–290]. Consequently, the problem of evaluating the complete NNLO contribution is reduced to determining these master integrals to the required order in the dimensional regularization parameter ϵ .

The VV contribution involves purely two-loop Feynman integrals evaluated at Born kinematics, whose analytical results are available in the literature. The real-virtual contribution contains one-loop amplitudes accompanied by the emission of an additional real parton and therefore requires the evaluation of loop integrals integrated over the two-body phase space. The RR contribution, involving two additional real emissions, requires the evaluation of three-body phase-space integrals. Compared to fully inclusive DIS, the SIDIS kinematics introduces an additional constraint due to identified hadron in the final state. At the partonic level, this introduces an additional kinematic constraint that fixes the momentum fraction carried by the fragmenting parton through the scaling variable z' , so the phase-space integrations are subject to an extra delta-function constraint. Employing the reverse unitarity method, the phase-space delta functions are written as cut propagators, thereby casting the phase-space integrals into loop integrals like form. This allows the ap-

plication of standard IBP reduction algorithms to identify the corresponding master integrals.

The Lorentz-invariant $(n + 1)$ -body phase-space corresponding to the scattering processes, $p_a + q \rightarrow p_b + \sum_{i=1}^n k_i$, subject to the constraint on the momentum of the fragmenting parton p_b , is given by

$$\begin{aligned} \int_{z'} [\text{dPS}]_{n+1} &= \prod_{i=1}^n \left(\int \frac{d^d k_i}{(2\pi)^{d-1}} \delta^+(k_i^2) \right) \int \frac{d^d p_b}{(2\pi)^{d-1}} \delta^+(p_b^2) \\ &\times (2\pi)^d \delta^d(p_b + K - p_a - q) \delta \left(z' - \frac{p_a \cdot p_b}{p_a \cdot q} \right), \end{aligned} \quad (4.1)$$

where the notation $\int_{z'}$ indicates that the phase-space integration is performed in the presence of the additional constraint, $\delta(z' - p_a \cdot p_b / p_a \cdot q)$. Here, $q = k_l - k'_l$ denotes the momentum transferred by the virtual photon, and $K = \sum_{i=1}^n k_i$ represents the total momentum of the remaining final-state partons. The last delta function imposes the extra constraint by fixing the scaling variable $z' = z/z_1$ associated with the fragmenting parton. For the processes considered in this work, it reduces to the two-body and three-body phase spaces corresponding to the RV and RR contributions, respectively. These special cases will be discussed in detail in the following sections.

The computation of the master integrals (MIs) constitutes one of the primary challenges in obtaining the NNLO coefficient functions. In the following sections, we present the evaluation of the complete set of MIs required for the present calculation. We first discuss the master integrals appearing in the double virtual contribution. We then introduce the reverse unitarity method, which provides a unified framework for the reduction of the phase-space integrals. The evaluation of the master integrals for the real-virtual contribution is subsequently presented using the two-body phase-space parametrization, together with the analytic continuation of the results to the physical SIDIS region. Finally, we discuss the master integrals arising from the double-real contribution, where the three-body phase-space parametrization and

the method of differential equations are employed to obtain their ϵ -expansion.

4.2 Double Virtual Integrals

The double-virtual (VV) contribution comprises the interference of the two-loop amplitude with the Born amplitude together with the square of the one-loop amplitude. Since no additional partons are emitted in the final state, the process is described by the Born kinematics,

$$a(p_a) + \gamma^*(q) \rightarrow b(p_b), \quad (4.2)$$

for which the phase-space integration reduces to the one-body phase-space. The virtual loop integrals are organized into integral families, which are subsequently reduced to a smaller set of master integrals using IBP identities.

The integral families are constructed from the two independent external momenta, p_a and q , together with the two loop momenta l_1 and l_2 . These four independent momenta give rise to 10 scalar products and 3 of which are fixed by the kinematic relations, (using $p_b^2 = (p_a + q)^2 = 0$),

$$p_a^2 = 0, \quad q^2 = -Q^2, \quad p_a \cdot q = \frac{Q^2}{2}. \quad (4.3)$$

Thus, 7 independent dot products remain. Accordingly, the integral family is defined by seven propagators, which form a complete basis for expressing all scalar products appearing in the integrals.

The two-loop integrals are organized into the following two integral families, specified by the ordered sets of propagators,

$$\begin{aligned}\mathcal{V}_1: & \{D_1^\mathcal{V}, D_2^\mathcal{V}, D_3^\mathcal{V}, D_4^\mathcal{V}, D_6^\mathcal{V}, D_7^\mathcal{V}, D_8^\mathcal{V}\} , \\ \mathcal{V}_2: & \{D_1^\mathcal{V}, D_2^\mathcal{V}, D_3^\mathcal{V}, D_5^\mathcal{V}, D_6^\mathcal{V}, D_7^\mathcal{V}, D_9^\mathcal{V}\} ,\end{aligned}$$

where the propagators $D_i^\mathcal{V}$ are defined as,

$$\begin{aligned}D_1^\mathcal{V} : & (l_1)^2 & D_2^\mathcal{V} : & (l_2)^2 & D_3^\mathcal{V} : & (l_1 - l_2)^2 \\ D_4^\mathcal{V} : & (l_1 + p_a)^2 & D_5^\mathcal{V} : & (l_1 - p_b)^2 & D_6^\mathcal{V} : & (l_1 + p_a - p_b)^2 \\ D_7^\mathcal{V} : & (l_2 + p_a)^2 & D_8^\mathcal{V} : & (l_2 + p_a - p_b)^2 & D_9^\mathcal{V} : & (l_1 - l_2 - p_b)^2\end{aligned}$$

Note, in the physical two-loop topologies contain at most 6 propagators. Therefore, one auxiliary propagator is introduced to complete each integral family. In particular, $D_7^\mathcal{V}$ and $D_5^\mathcal{V}$ serve as the auxiliary propagators for the families $\mathcal{V}_1$ and $\mathcal{V}_2$, respectively. The two-loop integrals $J(\mathcal{V}_n, n_1, \dots, n_7)$ for the family $\mathcal{V}_n$ are given by

$$J(\mathcal{V}_n, n_1, \dots, n_7) = \int \frac{d^d l_1}{(2\pi)^d} \frac{d^d l_2}{(2\pi)^d} \frac{1}{(D_{a_1}^\mathcal{V})^{n_1} \dots (D_{a_7}^\mathcal{V})^{n_7}}, \quad (4.4)$$

where the propagators are taken from the ordered set defining the family $\mathcal{V}_n$. The IBP identities for these families are generated using the *Mathematica* package *LiteRed* [242–244], all integrals belonging to these two families are then reduced to 4 master integrals,

$$\begin{aligned}J(\mathcal{V}_1; 0, 1, 1, 0, 1, 0, 0) & \quad J(\mathcal{V}_1; 1, 1, 0, 0, 1, 0, 1) \\ J(\mathcal{V}_1; 0, 1, 1, 1, 0, 0, 1) & \quad J(\mathcal{V}_2; 1, 1, 1, 0, 1, 1, 1) .\end{aligned}$$

Their analytical expressions are available in the literature [254–256], see also [291–293]. The planar topologies are described by the family $\mathcal{V}_1$, whereas the non-planar topology belongs to the family $\mathcal{V}_2$. For completeness, we quote the analytical expressions for the four master integrals below.

For convenience, we define

$$\tilde{S}_\epsilon = \frac{1}{(4\pi)^2} S_\epsilon = \frac{1}{(4\pi)^2} \exp\left(\frac{\epsilon}{2} (\gamma_E - \log(4\pi))\right) \quad (4.5)$$

where γ_E denotes the Euler-Mascheroni constant. The master integrals are given by,

$$\begin{aligned} J(\mathcal{V}_1; 0, 1, 1, 0, 1, 0, 0) &= \text{Diagram: a circle with an incoming arrow from the left labeled } q \text{ and an outgoing arrow to the right.} \\ &= \frac{Q^2}{2} (Q^2)^\epsilon \tilde{S}_\epsilon^2 \left\{ \frac{1}{\epsilon} - \frac{13}{4} + \epsilon \left(\frac{115}{16} - \frac{1}{4} \zeta_2 \right) \right. \\ &\quad \left. + \epsilon^2 \left(-\frac{865}{64} + \frac{13}{16} \zeta_2 + \frac{4}{3} \zeta_3 \right) \right. \\ &\quad \left. + \epsilon^3 \left(\frac{5971}{256} - \frac{115}{64} \zeta_2 - \frac{13}{3} \zeta_3 - \frac{57}{160} \zeta_2^2 \right) + \mathcal{O}(\epsilon^4) \right\} \quad (4.6) \end{aligned}$$

$$\begin{aligned} J(\mathcal{V}_1; 1, 1, 0, 0, 1, 0, 1) &= \text{Diagram: two circles connected by a horizontal line. The left circle has an incoming arrow from the left labeled } q \text{ and an outgoing arrow to the right. The right circle has an outgoing arrow to the right.} \\ &= (Q^2)^\epsilon \tilde{S}_\epsilon^2 \left\{ -\frac{4}{\epsilon^2} + \frac{8}{\epsilon} + (\zeta_2 - 12) + \epsilon \left(16 - 2\zeta_2 - \frac{7}{3} \zeta_3 \right) \right. \\ &\quad \left. + \epsilon^2 \left(-20 + 3\zeta_2 + \frac{14}{3} \zeta_3 + \frac{21}{40} \zeta_2^2 \right) \right. \\ &\quad \left. + \epsilon^3 \left(24 - 4\zeta_2 + \frac{7}{12} \zeta_2 \zeta_3 - 7\zeta_3 - \frac{31}{20} \zeta_5 - \frac{21}{20} \zeta_2^2 \right) + \mathcal{O}(\epsilon^4) \right\} \quad (4.7) \end{aligned}$$

$$\begin{aligned} J(\mathcal{V}_1; 0, 1, 1, 1, 0, 0, 1) &= \text{Diagram: a circle with a vertical line through its center. The left side of the circle has an incoming arrow from the left labeled } q. \text{ The top of the circle has an outgoing arrow labeled } p_a, \text{ and the bottom has an outgoing arrow labeled } p_b. \\ &= (Q^2)^\epsilon \tilde{S}_\epsilon^2 \left\{ -\frac{2}{\epsilon^2} + \frac{5}{\epsilon} - \left(\frac{19}{2} + \frac{\zeta_2}{2} \right) + \epsilon \left(\frac{65}{4} + \frac{5}{4} \zeta_2 - \frac{13}{6} \zeta_3 \right) \right. \\ &\quad \left. + \epsilon^2 \left(-\frac{211}{8} - \frac{19}{8} \zeta_2 + \frac{65}{12} \zeta_3 + \frac{41}{80} \zeta_2^2 \right) \right. \\ &\quad \left. + \epsilon^3 \left(\frac{133}{32} + \frac{65}{16} \zeta_2 - \frac{13}{12} \zeta_2 \zeta_3 - \frac{247}{24} \zeta_3 - \frac{121}{40} \zeta_5 - \frac{41}{32} \zeta_2^2 \right) \right\} \end{aligned}$$

$$+ \mathcal{O}(\epsilon^4) \Big\} \quad (4.8)$$

$$\begin{aligned}
J(\mathcal{V}_2; 1, 1, 1, 0, 1, 1, 1) &= \text{Diagram} \\
&= \left(\frac{2}{Q^2} \right)^2 (Q^2)^\epsilon \tilde{S}_\epsilon^2 \left\{ -\frac{4}{\epsilon^4} + \frac{6\zeta_2}{\epsilon^2} - \frac{83}{6} \frac{\zeta_3}{\epsilon} + \frac{177}{40} \zeta_2^2 \right. \\
&\quad + \epsilon \left(\frac{79}{8} \zeta_2 \zeta_3 - \frac{587}{40} \zeta_5 \right) + \epsilon^2 \left(-\frac{2567}{144} \zeta_3^2 - \frac{59}{112} \zeta_2^3 \right) \\
&\quad \left. + \epsilon^3 \left(\frac{3481}{320} \zeta_2^2 \zeta_3 + \frac{3594}{320} \zeta_2 \zeta_5 + \frac{5}{28} \zeta_7 \right) + \mathcal{O}(\epsilon^4) \right\} \quad (4.9)
\end{aligned}$$

4.3 Reverse Unitarity

Unlike the virtual contribution, the real-emission contributions involve integrations over the phase space of the emitted partons. As a result, the corresponding integrals contain Dirac delta functions enforcing the on-shell conditions of the final-state particles, together with the additional constraint associated with the observed fragmenting parton.

Employing the reverse unitarity method [238, 239], the phase-space delta functions are rewritten as cut propagators, thereby enabling the application of standard loop-integral techniques, including integration-by-parts (IBP) identities. In particular, the delta function is replaced by,

$$\delta(k_i^2) \rightarrow -\frac{1}{\pi} \text{Im} \left(\frac{1}{k_i^2 + i0} \right), \quad (4.10)$$

$$\text{Similarly,} \quad \delta \left(z' - \frac{p_a \cdot p_b}{p_a \cdot q} \right) \rightarrow -\frac{1}{\pi} \text{Im} \left(\frac{1}{z' - \frac{p_a \cdot p_b}{p_a \cdot q} + i0} \right) \quad (4.11)$$

In this representation, the Dirac delta functions are replaced by propagator-like objects. This allows the phase-space integrals to be interpreted as cut Feynman loop-integrals, where the cut propagators enforce the on-shell conditions of the final-

state particles as well as the kinematic constraint associated with the observed fragmenting parton. It should be noted that these on-shell constraints have important implications. In particular, any contribution containing factors proportional to a cut momentum vanishes due to $k_i^2 \delta(k_i^2) = 0$. Furthermore, unlike standard loop integrals, momentum shifts of the integration variables must be treated with care and are not permitted in phase-space integrals, since the on-shell delta functions fix the kinematics of the cut lines. Consequently, the reduction of phase-space integrals proceeds exactly as for ordinary loop integrals, allowing the systematic identification of master integrals (MIs).

4.4 Real-Virtual Integrals

The real-virtual contribution consists of one real emission together with a virtual loop correction and is evaluated over a two-body phase space. Using reverse unitarity, the corresponding phase-space integrations are expressed in terms of cut loop integrals. The underlying partonic process is

$$a(p_a) + \gamma^*(q) \rightarrow b(p_b) + k_1, \quad (4.12)$$

where k_1 denotes the emitted massless parton.

The Lorentz-invariant two-body phase space, together with the constraint associated with the observed fragmenting parton, is given by

$$\int_{z'} [\text{dPS}]_2 = \frac{1}{(2\pi)^{d-2}} \int d^d k_1 \int d^d p_b \delta^+(k_1^2) \delta^+(p_b^2) \delta^d(p_b + k_1 - p_a - q) \delta\left(z' - \frac{p_a \cdot p_b}{p_a \cdot q}\right). \quad (4.13)$$

Integrating over the momentum p_b using the momentum conserving delta function, leaves 3 cut propagators corresponding to the remaining delta functions. Because

of presence of extra constraint, the phase-space integration factorizes from the loop integration, so that the loop integral can be evaluated independently of the two-body phase-space measure.

The loop integrals depend on the three independent external momenta, p_a , q , and k_1 together with the loop momentum l_1 . These four independent momenta give rise to 10 scalar dot products, of which 3 are fixed i.e.,

$$p_a^2 = 0, \quad q^2 = -Q^2, \quad p_a \cdot q = \frac{Q^2}{2x'}, \quad (4.14)$$

leaving 7 independent scalar products. The phase-space constraints introduce three cut propagators, leaving the remaining four scalar products to be represented by standard propagators. To organize these integrals, suitable integral families must be constructed, which we describe as,

$$\begin{aligned} \mathcal{RV}_1: & \{D_1^{\mathcal{RV}}, D_2^{\mathcal{RV}}, D_3^{\mathcal{RV}}, D_6^{\mathcal{RV}}\} & \mathcal{RV}_2: & \{D_1^{\mathcal{RV}}, D_2^{\mathcal{RV}}, D_3^{\mathcal{RV}}, D_5^{\mathcal{RV}}\} \\ \mathcal{RV}_3: & \{D_1^{\mathcal{RV}}, D_2^{\mathcal{RV}}, D_4^{\mathcal{RV}}, D_5^{\mathcal{RV}}\} \end{aligned},$$

where the propagators $D_i^{\mathcal{RV}}$ are defined as,

$$\begin{aligned} D_1^{\mathcal{RV}} : & (l_1)^2 & D_2^{\mathcal{RV}} : & (l_1 - p_a)^2 & D_3^{\mathcal{RV}} : & (l_1 + q)^2 \\ D_4^{\mathcal{RV}} : & (l_1 - p_a - q + k_1)^2 & D_5^{\mathcal{RV}} : & (l_1 - p_a + k_1)^2 & D_6^{\mathcal{RV}} : & (l_1 + q - k_1)^2. \end{aligned}$$

We define an integral in the family $\mathcal{RV}_n$ as

$$J(\mathcal{RV}_n, n_1, \dots, n_4) = \int_{z'} [\text{dPS}]_2 \int \frac{d^d l_1}{(2\pi)^d} \frac{1}{(D_{a_1}^{\mathcal{RV}})^{n_1} \dots (D_{a_4}^{\mathcal{RV}})^{n_4}}, \quad (4.15)$$

for propagators $D_{a_1}^{\mathcal{RV}}, \dots, D_{a_4}^{\mathcal{RV}}$ taken from the ordered set of family $\mathcal{RV}_n$. Applying reverse unitarity, followed by the IBP reduction implemented in `LiteRed`, all integrals belonging to these families are reduced to the following 7 MIs,

$$\begin{array}{llll}
J(\mathcal{RV}_1; 0, 1, 1, 0) & J(\mathcal{RV}_1; 1, 0, 0, 1) & J(\mathcal{RV}_1; 1, 0, 1, 0) & J(\mathcal{RV}_2; 1, 0, 0, 1) \\
J(\mathcal{RV}_1; 1, 1, 1, 1) & J(\mathcal{RV}_2; 1, 1, 1, 1) & J(\mathcal{RV}_3; 1, 1, 1, 1) & .
\end{array}$$

The master integrals listed in the first row correspond to bubble integrals, whereas those in the second row correspond to box integrals.

A characteristic simplification of the RV contribution is that the two-body phase-space integration factorizes from the loop integration due to presence of the constraint $\delta\left(z' - \frac{p_a \cdot p_b}{p_a \cdot q}\right)$. The master integrals therefore factorize into a one-loop integral multiplied by the two-body phase-space factor,

$$\mathcal{PS}_2^{z'} = \int_{z'} [\text{dPS}]_2 = \frac{2\pi}{(4\pi)^{\frac{d}{2}} \Gamma_{\frac{d}{2}-1}} \left(\frac{Q^2(1-x')}{x'} \right)^{\frac{d}{2}-2} (z'(1-z'))^{\frac{d}{2}-2}, \quad (4.16)$$

Unlike the pure virtual case, the RV master integrals (MIs) require additional care when evaluated in the physical regions spanned by the scaling variables x' and z' . In the following, we first present the master integrals in their general form for arbitrary x' and z' and subsequently discuss their analytic continuation that can be used in different physical regions. The result of master integrals are given by (in $d = 4 + \epsilon$),

$$J(\mathcal{RV}_1; 0, 1, 1, 0) = \mathcal{PS}_2^{z'} \times \left\{ -i \frac{2}{\epsilon} \frac{C_\epsilon}{(1+\epsilon)} (-s)^{\epsilon/2} \right\}, \quad (4.17)$$

$$J(\mathcal{RV}_1; 1, 0, 0, 1) = \mathcal{PS}_2^{z'} \times \left\{ -i \frac{2}{\epsilon} \frac{C_\epsilon}{(1+\epsilon)} (-u)^{\epsilon/2} \right\}, \quad (4.18)$$

$$J(\mathcal{RV}_1; 1, 0, 1, 0) = \mathcal{PS}_2^{z'} \times \left\{ -i \frac{2}{\epsilon} \frac{C_\epsilon}{(1+\epsilon)} (Q^2)^{\epsilon/2} \right\}, \quad (4.19)$$

$$J(\mathcal{RV}_2; 1, 0, 0, 1) = \mathcal{PS}_2^{z'} \times \left\{ -i \frac{2}{\epsilon} \frac{C_\epsilon}{(1+\epsilon)} (-t)^{\epsilon/2} \right\}, \quad (4.20)$$

$$\begin{aligned}
J(\mathcal{RV}_1; 1, 1, 1, 1) = \mathcal{PS}_2^{z'} \times \left\{ -i \frac{8C_\epsilon}{\epsilon^2} \left[\frac{(Q^2)^{\epsilon/2}}{su} \text{F}_\epsilon \left(\frac{Q^2 t}{su} \right) - \frac{(-u)^{\epsilon/2}}{su} \text{F}_\epsilon \left(\frac{-t}{s} \right) \right. \right. \\
\left. \left. - \frac{(-s)^{\epsilon/2}}{su} \text{F}_\epsilon \left(\frac{-t}{u} \right) \right] \right\}, \quad (4.21)
\end{aligned}$$

$$J(\mathcal{RV}_2; 1, 1, 1, 1) = \mathcal{PS}_2^{z'} \times \left\{ -i \frac{8C_\epsilon}{\epsilon^2} \left[\frac{(Q^2)^{\epsilon/2}}{st} \text{F}_\epsilon \left(\frac{Q^2 u}{st} \right) - \frac{(-t)^{\epsilon/2}}{st} \text{F}_\epsilon \left(\frac{-u}{s} \right) \right. \right.$$

$$- \frac{(-s)^{\epsilon/2}}{st} F_{\epsilon} \left(\frac{-u}{t} \right) \Bigg] \Bigg\}, \quad (4.22)$$

$$J(\mathcal{RV}_3; 1, 1, 1, 1) = \mathcal{PS}_2^{z'} \times \left\{ -i \frac{8C_{\epsilon}}{\epsilon^2} \left[\frac{(Q^2)^{\epsilon/2}}{tu} F_{\epsilon} \left(\frac{Q^2 s}{tu} \right) - \frac{(-u)^{\epsilon/2}}{tu} F_{\epsilon} \left(\frac{-s}{t} \right) \right. \right. \\ \left. \left. - \frac{(-t)^{\epsilon/2}}{tu} F_{\epsilon} \left(\frac{-s}{u} \right) \right] \right\}, \quad (4.23)$$

where,

$$s = \frac{Q^2(1-x')}{x'}, \quad t = \frac{-Q^2(1-z')}{x'}, \quad u = \frac{-Q^2 z'}{x'}. \quad (4.24)$$

In the above expressions, C_{ϵ} is defined as,

$$C_{\epsilon} = \frac{1}{16\pi^2} \left(\frac{\Gamma(1 - \frac{\epsilon}{2}) \Gamma^2(1 + \frac{\epsilon}{2})}{(4\pi)^{\frac{\epsilon}{2}} \Gamma(1 + \epsilon)} \right), \quad (4.25)$$

while $F_{\epsilon}(\xi)$ denotes the hypergeometric function

$$F_{\epsilon}(\xi) = {}_2F_1 \left(1, \frac{\epsilon}{2}; 1 + \frac{\epsilon}{2}; \xi \right) = 1 - \sum_{n=1}^{\infty} \left(-\frac{\epsilon}{2} \right)^n \text{Li}_n(\xi). \quad (4.26)$$

Although the above expressions provide the complete analytical form of the RV master integrals, they are not yet suitable for direct use in the physical SIDIS region. Before performing the ϵ -expansion, the hypergeometric functions together with their accompanying kinematic prefactors must be analytically continued.

As a first step, the hypergeometric functions are rewritten using suitable transformation identities so that factors of the form $(1-x')^{\epsilon}$ and $(1-z')^{\epsilon}$ are made explicit. These factors are then extracted, thereby isolating the threshold behavior in the limits $x' \rightarrow 1$ and $z' \rightarrow 1$. The remaining hypergeometric functions, however, require further manipulation. Their arguments depend on the scaling variables x' and z' and may become equal to or larger than unity, particularly in the kinematic regions characterized by $x' \geq z'$ and/or $x' + z' \geq 1$. Since the hypergeometric function ${}_2F_1(a, b; c; \xi)$ is a multivalued function with a branch cut along $\xi \geq 1$, its direct

expansion in ϵ is not valid over the entire physical region. It is therefore necessary to analytically continue both the hypergeometric functions and their accompanying prefactors. In particular, the branch cuts at the kinematic endpoints $x' = 0, 1$ and $z' = 0, 1$ must be avoided, so that the arguments of the hypergeometric functions neither become unity nor $+\infty$. We discuss this procedure in the following subsection.

4.4.1 Analytical Continuation in RV case

The analytic continuation is carried out systematically in the following steps. First, we employ the well-known transformation identities of the hypergeometric function, such as the Euler and Pfaff transformations, see for e.g. [294–296], and Eq. (C.3) to extract the overall factors $(1 - x')^{a\epsilon}$ and $(1 - z')^{b\epsilon}$, thereby making the threshold behavior explicit. Next, Feynman’s $+i0$ prescription for the scaling variables i.e. $x' \equiv x' - i0$ and $z' \equiv z' - i0$, is implemented thereby retaining the $i0$ dependence explicitly in both the hypergeometric functions and their accompanying kinematic prefactors. Finally, identities involving Heaviside theta functions are used to decompose the physical phase space into the relevant kinematic regions, this allows the ϵ -expansion of the hypergeometric functions to be analytically continued onto the appropriate branch in each region.

Throughout we have used,

$$(-s)^{\epsilon/2} = (-1 - i0)^{\epsilon/2} \left(\frac{Q^2(1 - x')}{x'} \right)^{\epsilon/2}. \quad (4.27)$$

The prescription for selecting the appropriate branch of the hypergeometric functions along with the prefactors, is discussed in Appendix-A. Here, we state the branch to be chosen for each hypergeometric function appearing in the box master integrals. Since each MI contains three hypergeometric functions, we consider them separately. We begin with the first box master integral.

First box master integral: $J(\mathcal{RV}_1; 1, 1, 1, 1)$

$$\begin{aligned}
F_\epsilon \left(-\frac{t}{s} \right) &= \left(\frac{z' - x'}{1 - x'} \right)^{-\frac{\epsilon}{2}} \tilde{F}_\epsilon \left(\frac{1 - z'}{x' - z'} \right) \\
&= \left| \frac{z' - x'}{1 - x'} \right|^{-\frac{\epsilon}{2}} \left\{ \theta_{1a} \tilde{F}_\epsilon \left(\frac{1 - z'}{x' - z'} \right) + \theta_{1b} (-1 + i0)^{-\frac{\epsilon}{2}} \tilde{F}_\epsilon \left(\frac{1 - z'}{x' - z'} + i0 \right) \right\}, \\
F_\epsilon \left(-\frac{t}{u} \right) &= (z')^{\frac{\epsilon}{2}} \tilde{F}_\epsilon (1 - z'), \\
F_\epsilon \left(\frac{Q^2 t}{su} \right) &= \left(\frac{z' - x'}{z'(1 - x')} \right)^{-\frac{\epsilon}{2}} \tilde{F}_\epsilon \left(\frac{x'(1 - z')}{x' - z'} \right) \\
&= \left| \frac{z' - x'}{z'(1 - x')} \right|^{-\frac{\epsilon}{2}} \left\{ \theta_{1a} \tilde{F}_\epsilon \left(\frac{x'(1 - z')}{x' - z'} \right) \right. \\
&\quad + \theta_{1b} \theta_{2a} (-1 - i0)^{-\frac{\epsilon}{2}} \tilde{F}_\epsilon \left(\frac{x'(1 - z')}{x' - z'} - i0 \right) \\
&\quad \left. + \theta_{1b} \theta_{2b} (-1 + i0)^{-\frac{\epsilon}{2}} \tilde{F}_\epsilon \left(\frac{x'(1 - z')}{x' - z'} + i0 \right) \right\}. \tag{4.28}
\end{aligned}$$

Second box master integral: $J(\mathcal{RV}_2; 1, 1, 1, 1) = J(\mathcal{RV}_1; 1, 1, 1, 1) \big|_{z' \rightarrow 1 - z'}$

Third box master integral: $J(\mathcal{RV}_3; 1, 1, 1, 1)$

$$\begin{aligned}
F_\epsilon \left(-\frac{s}{u} \right) &= \left(\frac{z' + x' - 1}{z'} \right)^{-\frac{\epsilon}{2}} \tilde{F}_\epsilon \left(\frac{1 - x'}{1 - z' - x'} \right) \\
&= \left| \frac{1 - z' - x'}{z'} \right|^{-\frac{\epsilon}{2}} \left\{ \theta_{2b} \tilde{F}_\epsilon \left(\frac{1 - x'}{1 - z' - x'} \right) \right. \\
&\quad \left. + \theta_{2a} (-1 - i0)^{-\frac{\epsilon}{2}} \tilde{F}_\epsilon \left(\frac{1 - x'}{1 - z' - x'} - i0 \right) \right\}, \\
F_\epsilon \left(-\frac{s}{t} \right) &= \left(\frac{x' - z'}{1 - z'} \right)^{-\frac{\epsilon}{2}} \tilde{F}_\epsilon \left(\frac{1 - x'}{z' - x'} \right) \\
&= \left| \frac{x' - z'}{1 - z'} \right|^{-\frac{\epsilon}{2}} \left\{ \theta_{1b} \tilde{F}_\epsilon \left(\frac{1 - x'}{z' - x'} \right) + \theta_{1a} (-1 + i0)^{-\frac{\epsilon}{2}} \tilde{F}_\epsilon \left(\frac{1 - x'}{z' - x'} + i0 \right) \right\}, \\
F_\epsilon \left(\frac{Q^2 s}{tu} \right) &= \left(\frac{(z' - x')(1 - z' - x')}{z'(1 - z')} \right)^{-\frac{\epsilon}{2}} \tilde{F}_\epsilon \left(\frac{x'(1 - x')}{(x' - z')(1 - z' - x')} \right)
\end{aligned}$$

$$\begin{aligned}
&= \left| \frac{(z' - x')(1 - z' - x')}{z'(1 - z')} \right|^{-\frac{\epsilon}{2}} \left\{ \theta_{1a} \theta_{2a} \tilde{F}_\epsilon \left(\frac{x'(1 - x')}{(x' - z')(1 - z' - x')} + i0 \right) \right. \\
&\quad + \theta_{1a} \theta_{2b} (-1 + i0)^{-\frac{\epsilon}{2}} \tilde{F}_\epsilon \left(\frac{x'(1 - x')}{(x' - z')(1 - z' - x')} + i0 \right) \\
&\quad + \theta_{1b} \theta_{2b} \tilde{F}_\epsilon \left(\frac{x'(1 - x')}{(x' - z')(1 - z' - x')} - i0 \right) \\
&\quad \left. + \theta_{1b} \theta_{2a} (-1 - i0)^{-\frac{\epsilon}{2}} \tilde{F}_\epsilon \left(\frac{x'(1 - x')}{(x' - z')(1 - z' - x')} - i0 \right) \right\}. \quad (4.29)
\end{aligned}$$

In the above expressions, $(-1 \pm i0)^{\alpha\epsilon} = \exp(\pm i\pi\alpha\epsilon)$, and $\theta_{1a} = \theta(z' - x')$, $\theta_{1b} = \theta(x' - z')$, $\theta_{2a} = \theta(1 - z' - x')$, $\theta_{2b} = \theta(z' + x' - 1)$, with

$$\tilde{F}_\epsilon(\xi) = {}_2F_1\left(\frac{\epsilon}{2}, \frac{\epsilon}{2}; 1 + \frac{\epsilon}{2}; \xi\right) \quad (4.30)$$

and $|\xi|$ gives the absolute value of ξ . $\tilde{F}_\epsilon(\xi \pm i0)$ can be analytically continued to the appropriate region and expanded in a power series in ϵ , see [257, 297, 298]. After substituting these analytically continued expressions into the corresponding master integrals, the resulting expressions are continuous across all four kinematic boundaries. Furthermore, upon simplifying the ϵ -expanded MIs, all θ functions can be eliminated, removing the need to distinguish between the different regions of (x', z') kinematic plane.

For completeness, we present an alternative implementation of the analytic continuation that leads directly to a unified representation over the entire (x', z') plane, without introducing θ functions or making any explicit case distinction. Compared to the previous piecewise representation, this formulation is more compact. The continuation is carried out directly through a representation of the hypergeometric function that is valid over the entire physical region. We rewrite $F_\epsilon(\xi)$ in Eqs. (4.21)-(4.23) as,

$$F_\epsilon(\xi) = \frac{\epsilon^2(1 - \xi)}{4\xi^{1+\frac{\epsilon}{2}}} \mathcal{F}_\epsilon\left(1 - \frac{1}{\xi}\right) - \frac{\epsilon}{2\xi^{\frac{\epsilon}{2}}} \left[\psi\left(\frac{\epsilon}{2}\right) + \ln\left(\frac{1}{\xi} - 1\right) + \gamma_E \right], \quad (4.31)$$

where

$$\mathcal{F}_\epsilon(x) = {}_3F_2\left(1, 1, 1 + \frac{\epsilon}{2}; 2, 2; x\right), \quad (4.32)$$

and $\psi(x) = \Gamma'(x)/\Gamma(x)$. In this representation, the only function possessing a branch point at $\xi = 1$ is the logarithm term, $\ln\left(\frac{1}{\xi} - 1\right)$. Upon substituting Eq. (4.31) into Eqs. (4.21)–(4.23), these branching logarithms cancel among themselves, yielding expressions that are explicitly analytic throughout the whole physical region, see Eqs. (46)–(48) of [173].

4.5 Double-Real Integrals

We now turn to the double-real (RR) contribution, corresponding to the partonic process

$$p_a + q \rightarrow p_b + k_1 + k_2, \quad (4.33)$$

where p_b denotes the observed fragmenting parton, while k_1 and k_2 are the emitted massless partons. The corresponding three-body phase-space measure is,

$$\begin{aligned} \int_{z'} [\text{dPS}]_3 &= \frac{1}{(2\pi)^{2d-3}} \int d^d k_1 \int d^d k_2 \int d^d p_b \delta^+(k_1^2) \delta^+(k_2^2) \delta^+(p_b^2) \\ &\quad \times \delta^d(p_a + q - p_b - k_1 - k_2) \delta\left(z' - \frac{p_a \cdot p_b}{p_a \cdot q}\right). \end{aligned} \quad (4.34)$$

Compared to the fully inclusive-DIS case, the presence of the additional constraint on the scaling variable z' substantially complicates the evaluation of the phase-space integrals, see e.g. [299]. As in the RV contribution, we employ the reverse unitarity method to rewrite the phase-space delta functions as cut propagators, thereby converting the phase-space integrals into cut loop integrals. This enables

the application of standard loop-integral techniques, in particular IBP identities.

The significant number of RR partonic subprocesses gives rise to a correspondingly large set of phase-space integrals. Many of these integrals are related through IBP identities, enabling their systematic reduction to a much smaller set of master integrals. In the following, we construct the required integral families and perform the IBP reduction to obtain the complete set of RR master integrals.

The RR integrals depend on the four independent external momenta, p_a , q , k_1 , and k_2 . These give rise to 10 independent scalar products. Since 3 of them are fixed by the external kinematics Eq. (4.14), seven independent scalar products remain. The phase-space constraints introduce 4 cut propagators, leaving the remaining 3 scalar products to be represented by standard propagators. The integrals are represented by introducing a suitable set of propagators, from which the integral families are constructed.

The RR contribution is described by 13 integral families, denoted by $\mathcal{R}_i$ ($i = 1, \dots, 13$). Each family is specified by an ordered set of propagators,

$$\begin{aligned}
\mathcal{R}_1: & \{D_1^{\mathcal{R}}, D_5^{\mathcal{R}}, D_6^{\mathcal{R}}\} & \mathcal{R}_2: & \{D_1^{\mathcal{R}}, D_5^{\mathcal{R}}, D_7^{\mathcal{R}}\} & \mathcal{R}_3: & \{D_1^{\mathcal{R}}, D_5^{\mathcal{R}}, D_8^{\mathcal{R}}\} \\
\mathcal{R}_4: & \{D_1^{\mathcal{R}}, D_6^{\mathcal{R}}, D_8^{\mathcal{R}}\} & \mathcal{R}_5: & \{D_1^{\mathcal{R}}, D_2^{\mathcal{R}}, D_4^{\mathcal{R}}\} & \mathcal{R}_6: & \{D_1^{\mathcal{R}}, D_2^{\mathcal{R}}, D_8^{\mathcal{R}}\} \\
\mathcal{R}_7: & \{D_1^{\mathcal{R}}, D_4^{\mathcal{R}}, D_5^{\mathcal{R}}\} & \mathcal{R}_8: & \{D_1^{\mathcal{R}}, D_4^{\mathcal{R}}, D_7^{\mathcal{R}}\} & \mathcal{R}_9: & \{D_1^{\mathcal{R}}, D_4^{\mathcal{R}}, D_8^{\mathcal{R}}\} \\
\mathcal{R}_{10}: & \{D_2^{\mathcal{R}}, D_4^{\mathcal{R}}, D_5^{\mathcal{R}}\} & \mathcal{R}_{11}: & \{D_2^{\mathcal{R}}, D_5^{\mathcal{R}}, D_7^{\mathcal{R}}\} & \mathcal{R}_{12}: & \{D_2^{\mathcal{R}}, D_5^{\mathcal{R}}, D_8^{\mathcal{R}}\} \\
\mathcal{R}_{13}: & \{D_2^{\mathcal{R}}, D_5^{\mathcal{R}}, D_6^{\mathcal{R}}\},
\end{aligned}$$

where the propagators ($D_i^{\mathcal{R}}$) are

$$\begin{aligned}
D_1^{\mathcal{R}} : & (k_1 - p_a)^2 & D_2^{\mathcal{R}} : & (k_1 - q)^2 & D_3^{\mathcal{R}} : & (k_2 - p_a)^2 \\
D_4^{\mathcal{R}} : & (k_2 - q)^2 & D_5^{\mathcal{R}} : & (k_1 - p_a - q)^2 & D_6^{\mathcal{R}} : & (k_2 - p_a - q)^2 \\
D_7^{\mathcal{R}} : & (k_1 + k_2)^2 & D_8^{\mathcal{R}} : & (k_1 + k_2 - p_a)^2.
\end{aligned} \tag{4.35}$$

An integral belonging to the family $\mathcal{R}_n$ is defined as,

$$J(\mathcal{R}_n, n_1, n_2, n_3) = \int_{z'} [\text{dPS}]_3 \frac{1}{(D_{a_1}^{\mathcal{R}})^{n_1} (D_{a_2}^{\mathcal{R}})^{n_2} (D_{a_3}^{\mathcal{R}})^{n_3}}, \quad (4.36)$$

where $D_{a_1}^{\mathcal{R}}, \dots, D_{a_3}^{\mathcal{R}}$ denote the propagators belonging to the ordered set of the family $\mathcal{R}_n$. The IBP identities for these families are generated using **LiteRed**. After solving the resulting IBP system, all RR integrals are expressed in terms of the following 20 master integrals (MIs),

$$\begin{aligned} & J(\mathcal{R}_1; 0, 0, 0), \quad J(\mathcal{R}_1; 0, 0, 1), \quad J(\mathcal{R}_1; 1, 1, 1), \quad J(\mathcal{R}_2; 1, 1, 1), \quad J(\mathcal{R}_3; 0, 0, 1), \\ & J(\mathcal{R}_3; 1, 1, 1), \quad J(\mathcal{R}_4; 1, 1, 1), \quad J(\mathcal{R}_5; 0, 0, 1), \quad J(\mathcal{R}_5; 0, 0, 2), \quad J(\mathcal{R}_5; 0, 1, 1), \\ & J(\mathcal{R}_5; 1, 1, 1), \quad J(\mathcal{R}_6; 0, 1, 1), \quad J(\mathcal{R}_6; 1, 1, 1), \quad J(\mathcal{R}_7; 0, 1, 1), \quad J(\mathcal{R}_7; 1, 1, 1), \\ & J(\mathcal{R}_8; 1, 1, 1), \quad J(\mathcal{R}_{10}; 1, 1, 1), \quad J(\mathcal{R}_{11}; 1, 1, 1), \quad J(\mathcal{R}_{12}; 1, 1, 1), \quad J(\mathcal{R}_{13}; 1, 1, 1). \end{aligned} \quad (4.37)$$

The remaining task is to evaluate these 20 master integrals. In this work, we employ two independent methods for their computation, which also provide a valuable cross-check of the final results. In the following section, we briefly describe these methods.

4.6 Evaluation of the RR Master Integrals

The first approach is based on direct phase-space integration. We choose a suitable Lorentz frame in which the constraint on the scaling variable z' assumes a particularly simple form. In this frame, the three-body phase-space measure can be parameterized in terms of parametric integration together with the angular integrations (see Refs. [115, 254, 300, 301] for details). The master integrals are then evaluated by performing the angular integrations analytically, followed by the remaining parametric integration. The analytical evaluation yields the master integrals in terms

of Goncharov polylogarithms (GPLs) [302, 303], which are further simplified by expressing them in terms of classical and Nielsen polylogarithms.

The second approach is based on the method of differential equations (DEqs) [304, 305], see also, [282, 306]. We construct a coupled system of differential equations for the master integrals with respect to the kinematic variables Q^2 , x' , and z' using the **LiteRed** package. The resulting differential equations form a closed coupled system, which can be written compactly in matrix form with 20×20 coefficient matrices. We then transform this system into the canonical (ϵ -factorized) form [307] using algorithm of ref. [308] as implemented in the **Mathematica** package **Libra** [309]. In this form, the differential equations can be solved systematically order by order in the dimensional regulator ϵ , yielding the master integrals in terms of iterated integrals.

We have cross-checked the results obtained from both approaches and found perfect agreement, providing a strong check of the correctness of the final expressions.

4.6.1 Phase-Space Parameterization

In this approach, the RR master integrals are evaluated by direct integration over the three-body phase space in a suitably chosen Lorentz frame. The frame is chosen such that the kinematic constraint on the scaling variable z' takes a particularly simple form. We work in the center-of-mass (c.m.) frame of the two outgoing partons k_1 and k_2 , i.e. $\vec{k}_1 + \vec{k}_2 = 0$. Following Refs. [115, 254, 300, 301], the external momenta in the $k_1 - k_2$ c.m. frame are parameterized as follows,

$$\begin{aligned} p_a &= \frac{(s - t + Q^2)}{2\sqrt{s_{12}}}(1, \vec{0}, 0, 0, 1), \\ p_b &= \frac{(s - s_{12})}{2\sqrt{s_{12}}}(1, \vec{0}, 0, \sin \psi, \cos \psi), \\ k_1 &= \frac{\sqrt{s_{12}}}{2}(1, \vec{0}, \sin \phi \sin \theta, \cos \phi \sin \theta, \cos \theta), \end{aligned}$$

$$\begin{aligned}
k_2 &= \frac{\sqrt{s_{12}}}{2} (1, \vec{0}, -\sin \phi \sin \theta, -\cos \phi \sin \theta, -\cos \theta), \\
q &= p_b + k_1 + k_2 - p_a,
\end{aligned} \tag{4.38}$$

with

$$\begin{aligned}
s &= (p_a + q)^2, \quad t = 2p_a \cdot p_b, \quad u = 2p_b \cdot q, \quad s_{12} = (k_1 + k_2)^2 = s - t - u, \\
q^2 &= -Q^2, \quad \cos \psi = 1 - \frac{2s_{12}t}{(s - t + Q^2)(s - s_{12})}.
\end{aligned} \tag{4.39}$$

In this reference frame, the 3-body phase-space Eq. (4.34) can be written as,

$$\int_{z'} [\text{dPS}]_3 = \frac{1}{(4\pi)^d} \frac{(s + Q^2)^{3-d}}{\Gamma(d-3)} \int_0^\pi d\theta (\sin \theta)^{d-3} \int_0^\pi d\phi (\sin \phi)^{d-4} \tag{4.40}$$

$$\begin{aligned}
&\int_0^{s+Q^2} dt \int_{-Q^2 t/(s+Q^2)}^{s-t} du \left[t (su + Q^2(t+u)) \right]^{\frac{d-4}{2}} \\
&\times (s - t - u)^{\frac{d-4}{2}} \delta \left(z' - \frac{t}{s + Q^2} \right)
\end{aligned} \tag{4.41}$$

Further, changing the variable so that we map the integration limits to 0 to 1, i.e.

$$\int_0^{s+Q^2} dt \int_{-Q^2 t/(s+Q^2)}^{s-t} du = \int_0^1 dy \int_0^1 dz J(y, z) \tag{4.42}$$

Using the relations,

$$u = s(1-y)z - yQ^2 \quad \text{and} \quad t = (s + Q^2)y, \tag{4.43}$$

we get the Jacobian, $J(y, z) = s(s + Q^2)(1-y)$. So,

$$\begin{aligned}
u &= s \left(\frac{-x'y}{1-x'} + z - yz \right), & t &= \frac{sy}{1-x'}, \\
J &= \frac{s^2(1-y)}{1-x'}, & s &= \frac{Q^2(1-x')}{x'}.
\end{aligned} \tag{4.44}$$

The main advantage of this parameterization is that the constraint delta function $\delta\left(z' - \frac{p_a \cdot p_b}{p_a \cdot q}\right)$ reduces to $\delta(z' - y)$. So, the 3-body phase-space is rewritten as,

$$\int_{z'} [\text{dPS}]_3 = \frac{1}{(4\pi)^d \Gamma(d-3)} \left(\frac{Q^2(1-x')}{x'} \right)^{d-3} \int_0^\pi d\theta (\sin \theta)^{d-3} \int_0^\pi d\phi (\sin \phi)^{d-4} \int_0^1 dy \int_0^1 dz y^{\frac{d-4}{2}} (1-y)^{d-3} (z(1-z))^{\frac{d-4}{2}} \delta(y-z') \quad (4.45)$$

Note that the phase-space measure is symmetric under the transformation $z \rightarrow 1-z$. Finally, all propagators appearing in the master integrals, see Eq. (4.35), are expressed in terms of the variables x' , z' , z , θ , and ϕ , as,

$$\begin{aligned} D_1^{\mathcal{R}} &= -\frac{s(1-z')}{(1-x')} \frac{(1-\cos \theta)}{2}, \\ D_2^{\mathcal{R}} &= -\frac{s(x'(1-z(1-z')) + z'(1-z) + z)}{2(1-x')} \\ &\quad + \frac{s(z'-z(1+z') - x'(1-z(1+z')))}{2(1-x')} \cos \theta + s\sqrt{(1-z)zz'} \cos \phi \sin \theta, \\ D_3^{\mathcal{R}} &= -\frac{s(1-z')}{(1-x')} \frac{(1+\cos \theta)}{2}, \\ D_4^{\mathcal{R}} &= -\frac{s(x'(1-z(1-z')) + z'(1-z) + z)}{2(1-x')} \\ &\quad - \frac{s(z'-z(1+z') - x'(1-z(1+z')))}{2(1-x')} \cos \theta - s\sqrt{(1-z)zz'} \cos \phi \sin \theta, \\ D_5^{\mathcal{R}} &= \frac{s}{2} (1-z(1-z')) + \frac{s}{2} (1-z(1+z')) \cos \theta + s\sqrt{(1-z)zz'} \cos \phi \sin \theta, \\ D_6^{\mathcal{R}} &= \frac{s}{2} (1-z(1-z')) - \frac{s}{2} (1-z(1+z')) \cos \theta - s\sqrt{(1-z)zz'} \cos \phi \sin \theta, \\ D_7^{\mathcal{R}} &= sz(1-z'), \\ D_8^{\mathcal{R}} &= -\frac{s(1-z')(1-(1-x')z)}{(1-x')}, \\ D_5^{\mathcal{R}} + D_6^{\mathcal{R}} &= s(1-z(1-z')), \\ D_2^{\mathcal{R}} + D_4^{\mathcal{R}} &= -\frac{s(x'(1-z(1-z')) + z'(1-z) + z)}{(1-x')}. \end{aligned} \quad (4.46)$$

The phase space integral without any propagator is given by,

$$\mathcal{PS}_3^{z'} = \int_{z'} [\text{dPS}]_3 = \left(\frac{Q^2(1-x')}{x'} \right)^{1+\epsilon} \frac{2\pi}{(4\pi)^{4+\epsilon}} \left(\frac{\Gamma(1+\frac{\epsilon}{2})}{\Gamma(2+\epsilon)} \right)^2 z'^{\frac{\epsilon}{2}} (1-z')^{1+\epsilon}. \quad (4.47)$$

The parameterization introduced above allows all master integrals to be expressed as a product of angular and a parametric integration. The angular dependence arises solely through the propagators and can be integrated analytically. Thus, the evaluation of the master integrals reduces to a set of angular integrals of the form [293, 301, 310, 311],

$$\int_0^\pi d\theta \int_0^\pi d\phi \frac{(\sin \theta)^{1+\epsilon} (\sin \phi)^\epsilon}{(a + b \cos \theta)^i (A + B \cos \theta + C \sin \theta \cos \phi)^j}. \quad (4.48)$$

After appropriate partial-fraction decomposition of the propagator structures, all angular integrations encountered in the present calculation can be expressed in terms of the following four cases.

Case 1: $a^2 = b^2$ and $A^2 = B^2 + C^2$, [254, 293].

In this case, the angular integral can be evaluated in closed form as,

$$\int_0^\pi d\theta \int_0^\pi d\phi \frac{(\sin \theta)^{1+\epsilon} (\sin \phi)^\epsilon}{(1 - \cos \theta)^i (1 - \cos \chi \cos \theta - \sin \chi \sin \theta \cos \phi)^j} = 2^{1-i-j} \pi B \left(1 + \frac{\epsilon}{2} - i, 1 + \frac{\epsilon}{2} - j \right) \frac{\Gamma(1+\epsilon)}{\Gamma(1+\frac{\epsilon}{2})} {}_2F_1 \left(i, j; 1 + \frac{\epsilon}{2}; \cos^2 \frac{\chi}{2} \right) \quad (4.49)$$

Here $B(\alpha, \beta)$ denotes Euler Beta function.

Case 2: $a^2 \neq b^2$ and $A^2 = B^2 + C^2$, [254, 293].

In this case, the angular integral can be reduced to a one-dimensional integral in-

volving a hypergeometric function,

$$\begin{aligned}
& \int_0^\pi d\theta \int_0^\pi d\phi \frac{(\sin \theta)^{1+\epsilon} (\sin \phi)^\epsilon}{(a - \cos \theta) (1 - \cos \chi \cos \theta - \sin \chi \sin \theta \cos \phi)} \\
&= \pi \frac{\epsilon}{4} \frac{\Gamma(1+\epsilon)}{\Gamma^2(1+\frac{\epsilon}{2})} \int_0^1 dv \int_0^1 dw \frac{(1-v)^{-1+\frac{\epsilon}{2}} w^{-1+\frac{\epsilon}{2}} (1-w)^{\frac{\epsilon}{2}}}{\frac{1}{2}(a-1) + \frac{1}{2}v(1-\cos \chi)(1-w) + (1-v)(1-w)} \\
&= \frac{\pi}{a-1} \int_0^1 dv (1-v)^{-1+\frac{\epsilon}{2}} \left(1 + \frac{2}{a-1} \left(1 - v \cos^2 \frac{\chi}{2} \right) \right)^{-1+\frac{\epsilon}{2}} \\
&\quad \times {}_2F_1 \left(\epsilon, \frac{\epsilon}{2}; 1+\epsilon; \frac{-2}{a-1} \left(1 - v \cos^2 \frac{\chi}{2} \right) \right). \tag{4.50}
\end{aligned}$$

The above integral is symmetric under the transformation $v \rightarrow 1-v$ and can be evaluated order by order in ϵ .

Case 3: $a^2 = b^2$ and $A^2 \neq B^2 + C^2$.

This case is not independent. By performing a suitable angular rotation, the integral can be mapped onto the second case and can therefore be evaluated using the same procedure.

Case 4: $a^2 \neq b^2$ and $A^2 \neq B^2 + C^2$.

This is the most complicated case. The analytic expressions for these integrals for ϵ independent term were derived long ago [312–314], while their extension to higher orders in ϵ has been studied in [315–319], see also [174, 320–327].

After carrying out the angular integrations, the master integrals reduce to a single remaining parametric integration over the variable z . For the simpler MIs, this integration can be performed in closed form. In the more involved cases, the integrand is first expanded as a power series in ϵ [328–331], after which the resulting parametric integrals are evaluated analytically in terms of GPLs, which are subsequently

expressed in terms of classical and Nielsen polylogarithms.

4.6.2 Differential Equation Method

An elegant method for evaluating the master integrals is provided by the method of differential equations (DEqs) [282, 304, 305, 307, 332–339]. The basic idea is to exploit the dependence of the master integrals on the external kinematic variables by differentiating them with respect to these variables. The resulting derivatives can again be expressed as linear combinations of the same master integrals using IBP identities. Consequently, the master integrals satisfy a closed system of coupled first-order differential equations.

For the RR master integrals, we construct the differential equations with respect to the kinematic variables Q^2 , x' , and z' . The required derivatives and the subsequent IBP reductions are generated using the `LiteRed` package [242, 243]. Denoting the vector of master integrals by $\vec{I}$, the system takes the form

$$\frac{\partial \vec{I}}{\partial Q^2} = \hat{A}_Q(Q^2, x', z', \epsilon) \vec{I}, \quad \frac{\partial \vec{I}}{\partial x'} = \hat{A}_{x'}(Q^2, x', z', \epsilon) \vec{I}, \quad \frac{\partial \vec{I}}{\partial z'} = \hat{A}_{z'}(Q^2, x', z', \epsilon) \vec{I}. \quad (4.51)$$

where $\hat{A}_Q$, $\hat{A}_{x'}$, and $\hat{A}_{z'}$ are the corresponding 20×20 connection matrices. The matrix $\hat{A}_Q$ is diagonal, reflecting the fact that the dependence of the master integrals on the overall mass scale Q^2 factorizes trivially. Consequently, the Q^2 dependence can be extracted analytically, and in the following we set, $Q^2 = 1$ without loss of generality. Furthermore, by construction of the master integral basis, the matrices $\hat{A}_{x'}$ and $\hat{A}_{z'}$ possess a lower-triangular form. Since the master integrals depend simultaneously on the variables x' and z' , the coupled differential equations must satisfy the integrability condition, ensuring that the solution is independent of the

integration path. This requires

$$\frac{\partial^2 \vec{I}}{\partial z' \partial x'} = \frac{\partial^2 \vec{I}}{\partial x' \partial z'} \implies \frac{\partial \hat{A}_{x'}}{\partial z'} - \frac{\partial \hat{A}_{z'}}{\partial x'} + [\hat{A}_{x'}, \hat{A}_{z'}] = 0 \quad (4.52)$$

Several methods have been developed for solving systems of differential equations for Feynman integrals. Early approaches relied on series expansions around singular points [340–344] and on difference equation techniques based on Laplace (Mellin) transform, which have been successfully applied to a wide variety of multi-loop calculations [278, 306, 345–347]. More generally, one may solve the coupled system recursively by exploiting its triangular structure, using forward or backward substitution together with the method of variation of constants. Alternatively, the system may be decoupled into higher-order differential equations for individual master integrals, which can then be solved independently [304, 305, 333, 334, 348–351]. The system of differential equations is not unique, as it depends on the choice of the master-integral basis. A suitable change of basis can significantly simplify the system and in favorable cases, transform it into the canonical (ϵ -factorized) form. Numerous methods and computational tools have been developed for constructing such a basis, see for e.g. [285, 307–309, 352–370]. Several public packages are available for the numerical evaluation of Feynman integrals using differential equations, including `DiffExp`, `SeaSyde`, `LINE` and `AMFlow` [341–344, 371], see also [340, 360, 372–381].

In the present work, we adopt the canonical differential equation approach [307]. The central idea is to perform a change of basis i.e $\vec{I} \rightarrow \vec{J} = \hat{T}^{-1} \vec{I}$ (or gauge transformation), such that in the differential equation system the ϵ factors out,

$$\left\{ \begin{array}{l} \frac{\partial \vec{I}}{\partial x'} = \hat{A}_{x'}(x', z', \epsilon) \vec{I} \\ \frac{\partial \vec{I}}{\partial z'} = \hat{A}_{z'}(x', z', \epsilon) \vec{I} \end{array} \right\} \longrightarrow \left\{ \begin{array}{l} \frac{\partial \vec{J}}{\partial x'} = \epsilon \hat{\mathcal{A}}_{x'}(x', z') \vec{J} \\ \frac{\partial \vec{J}}{\partial z'} = \epsilon \hat{\mathcal{A}}_{z'}(x', z') \vec{J} \end{array} \right\}.$$

The matrices $\hat{\mathcal{A}}_{x'}$ and $\hat{\mathcal{A}}_{z'}$ are independent of ϵ and are related to $\hat{A}_{x'}$ and $\hat{A}_{z'}$ as,

$$\begin{aligned}\hat{\mathcal{A}}_{x'} &= \hat{T}^{-1} \hat{A}_{x'} \hat{T} - \hat{T}^{-1} \frac{\partial \hat{T}}{\partial x'}, \\ \hat{\mathcal{A}}_{z'} &= \hat{T}^{-1} \hat{A}_{z'} \hat{T} - \hat{T}^{-1} \frac{\partial \hat{T}}{\partial z'}.\end{aligned}\tag{4.53}$$

The solution of the canonical system can be written in terms of the path-ordered exponential,

$$\vec{J}(x', z', \epsilon) = \mathcal{P} \exp \left[\epsilon \int_{x'_0, z'_0}^{x', z'} \left(\hat{\mathcal{A}}_{x'} dx'_1 + \hat{\mathcal{A}}_{z'} dz'_1 \right) \right] \vec{J}(x'_0, z'_0, \epsilon) \tag{4.54}$$

where $\vec{J}(x'_0, z'_0, \epsilon) \equiv \vec{J}_0(\epsilon)$ denotes the vector of boundary constants and $\mathcal{P}$ represents path ordering. Expanding the path-ordered exponential order-by-order in ϵ gives,

$$\begin{aligned}\vec{J}(x', z', \epsilon) &= \vec{J}_0(\epsilon) + \epsilon \underbrace{\left[\int_0^{x'} dx'_1 \hat{\mathcal{A}}_{x'}(x'_1, 0) + \int_0^{z'} dz'_1 \hat{\mathcal{A}}_{z'}(x', z'_1) \right]}_{\hat{H}_1(x', z')} \vec{J}_0(\epsilon) \\ &\quad + \epsilon^2 \underbrace{\left[\int_0^{x'} dx'_2 \hat{\mathcal{A}}_{x'}(x'_2, 0) \hat{H}_1(x'_2, 0) + \int_0^{z'} dz'_2 \hat{\mathcal{A}}_{z'}(x', z'_2) \hat{H}_1(x', z'_2) \right]}_{\hat{H}_2(x', z')} \vec{J}_0(\epsilon) \\ &\quad + \mathcal{O}(\epsilon^3).\end{aligned}\tag{4.55}$$

The solution is therefore obtained iteratively order by order in ϵ , generating Chen iterated integrals, which can subsequently be expressed in terms of GPLs.

The integrability condition guarantees that the solution is independent of the integration path in the (x', z') plane. Consequently, the integration contour may be chosen for convenience when evaluating the path-ordered exponential. Throughout this work, we choose the integration path to start from the reference point

$$(x'_0, z'_0) = (0, 0),$$

and integrate first along the x' direction and subsequently along the z' direction, as illustrated in Fig. 4.1. To determine the integration constants, however, it is sufficient to know the master integrals at any convenient kinematic point, which need not coincide with the starting point of the integration. The boundary vector $\vec{J}_0(\epsilon)$ is determined from the behavior of the master integrals in the $k_1 - k_2$ center-of-mass frame in the limit $x' \rightarrow 1$ and $z' \rightarrow 1$, retaining the factors $(1 - x')^{a\epsilon+b}$ and $(1 - z')^{c\epsilon+d}$ explicitly, see Appendix-D.

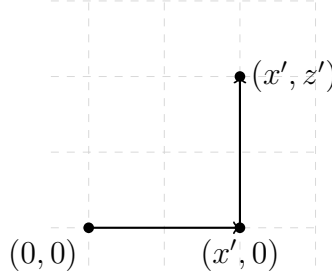


Figure 4.1: Integration path chosen for solving the canonical differential equations.

In the present calculation, the transformation matrix $\hat{T}$ is constructed using **Libra** [309] which is based on the algorithm described in [222, 308, 382], such that the transformed basis satisfies the canonical differential equations. In particular, it is constructed so that the boundary vector admits the following expansion in ϵ ,

$$\vec{J}_0(\epsilon) = \sum_{k=0}^{\infty} \epsilon^k \vec{J}_0^{(k)}, \quad (4.56)$$

while the original MIs are recovered through $\vec{I} = \hat{T} \vec{J}$. An important consequence of this choice of basis is that the canonical master integrals $\vec{J}$ are of uniform transcendental (UT) weight. Consequently, upon expanding them in ϵ ,

$$\vec{J}(x', z', \epsilon) = \sum_{k=0}^{\infty} \epsilon^k \vec{J}^{(k)}(x', z'), \quad (4.57)$$

each coefficient $\vec{J}^{(k)}$ is of uniform transcendental weight k . Thus, the transcendental weight increases uniformly by one at each successive order in the ϵ expansion.

The solution of canonical differential equations is naturally expressed in terms iterated integrals, whose integration kernels are constructed from the following set,

$$\begin{aligned} & x', z', (x' - 1), (x' + 1), (z' - 1), (z' - x'), (z' + x'), \\ & \left(z' + \frac{1}{x'}\right), (1 - z')^2 + 4x'z', (1 + x')^2 - 4x'z', \\ & \sqrt{x'}, \sqrt{z'}, \sqrt{(1 - z')^2 + 4x'z'}, \sqrt{(1 + x')^2 - 4x'z'}. \end{aligned} \quad (4.58)$$

Among these functions, four involve square roots. An important simplification is that the complicated square roots never appear simultaneously in the same iterated integral, hence they can be rationalized independently.

Following the procedure described in [383], the iterated integrals are first express in terms of symbolic G-functions. The algebraic kernels are then rationalized, allowing these iterated integrals to be rewritten in terms of GPLs. The square roots are rationalized using Euler substitutions, see also [384–389]. As a representative example, consider the square root,

$$\sqrt{(1 - z)^2 + 4x'z}. \quad (4.59)$$

Introducing the variable y through the Euler substitution,

$$\sqrt{(1 - z)^2 + 4x'z} = 2x'y + (1 - z), \quad (4.60)$$

one obtains

$$z = \frac{y(1 + x'y)}{1 + y}, \quad dz = \frac{1 + x'y(2 + y)}{(1 + y)^2} dy. \quad (4.61)$$

The integration limits transform according to

$$z = 0 \implies y = 0, \quad (4.62)$$

$$z = z' \implies y = \frac{\sqrt{(1-z')^2 + 4x'z'} - (1-z')}{2x'}. \quad (4.63)$$

After this transformation, the integration kernels become rational functions of y , and the resulting iterated integrals can be expressed directly in terms of GPLs. Similar Euler substitutions are employed for the remaining algebraic letters whenever required.

The procedure is illustrated below through two representative examples. Consider first,

$$\begin{aligned} G(r_1, r_2; z') &= \int_0^{z'} \frac{dz_1}{z_1 \sqrt{(1-z_1)^2 + 4x'z_1}} \int_0^{z_1} \frac{dz_2}{\sqrt{(1-z_2)^2 + 4x'z_2}} \\ &= \int_0^{\frac{\sqrt{(1-z')^2 + 4x'z'} - (1-z')}{2x'}} \frac{dy_1}{y_1(1+x'y_1)} \int_0^{y_1} \frac{dy_2}{(1+y_2)} \end{aligned} \quad (4.64)$$

Performing a partial-fraction decomposition,

$$\begin{aligned} G(r_1, r_2; z') &= \int_0^{\frac{\sqrt{(1-z')^2 + 4x'z'} - (1-z')}{2x'}} dy_1 \left(\frac{1}{y_1} - \frac{1}{y_1 + \frac{1}{x'}} \right) \int_0^{y_1} \frac{dy_2}{y_2 + 1} \\ &= G\left(0, -1; \frac{\sqrt{(1-z')^2 + 4x'z'} - (1-z')}{2x'}\right) \\ &\quad - G\left(-\frac{1}{x'}, -1; \frac{\sqrt{(1-z')^2 + 4x'z'} - (1-z')}{2x'}\right) \end{aligned} \quad (4.65)$$

As a second example,

$$G(0, r_2; z') = \int_0^{z'} \frac{dz_1}{z_1} \int_0^{z_1} \frac{dz_2}{\sqrt{(1-z_2)^2 + 4x'z_2}}. \quad (4.66)$$

Using the same Euler substitution throughout,

$$\begin{aligned} G(0, r_2; z') &= \int_0^{\frac{\sqrt{(1-z')^2 + 4x'z'} - (1-z')}{2x'}} dy_1 \frac{1+x'y_1(2+y_1)}{y_1(1+y_1)(1+x'y_1)} \int_0^{y_1} \frac{dy_2}{1+y_2} \\ &= \int_0^{\frac{\sqrt{(1-z')^2 + 4x'z'} - (1-z')}{2x'}} dy_1 \left(\frac{1}{y_1} - \frac{1}{y_1+1} + \frac{1}{y_1+\frac{1}{x'}} \right) \int_0^{y_1} dy_2 \frac{1}{y_2+1} \end{aligned}$$

$$\begin{aligned}
&= G \left(0, -1; \frac{\sqrt{(1-z')^2 + 4x'z'} - (1-z')}{2x'} \right) \\
&\quad - G \left(-1, -1; \frac{\sqrt{(1-z')^2 + 4x'z'} - (1-z')}{2x'} \right) \\
&\quad + G \left(-\frac{1}{x'}, -1; \frac{\sqrt{(1-z')^2 + 4x'z'} - (1-z')}{2x'} \right)
\end{aligned} \tag{4.67}$$

The remaining algebraic letters are treated analogously. Since the rationalization and subsequent partial-fraction decomposition follow a systematic procedure, the entire conversion to GPLs can be fully automated.

The resulting GPLs are evaluated numerically using packages such as `PolyLogTools` [390], `handyG` [391], see also [392–403]. In addition, the final analytic expressions for the master integrals have been independently validated against numerical solutions obtained with `AMFlow` and found perfect agreement.

4.7 Summary

In this chapter, we presented the computational framework used to evaluate the loop and phase-space integrals required for the NNLO QCD corrections to SIDIS. A central ingredient of the calculation is the reduction of the large number of Feynman and phase-space integrals to a minimal set of master integrals through integration-by-parts (IBP) identities. By employing the reverse-unitarity technique, the phase-space integrals associated with real-emission processes are mapped onto loop integrals, allowing the same IBP machinery to be applied to both virtual and real contributions.

The real-virtual (RV) and double-real (RR) contributions constitute the most challenging parts of the NNLO calculation. For the real-virtual contribution, we discussed the analytic continuation of the known master integrals to the SIDIS physical

region, ensuring the correct analytic structure of the coefficient functions. For the double-real contribution, we constructed the required integral families, performed the IBP reduction, and obtained a complete set of new RR master integrals.

The evaluation of these new RR master integrals, which represents one of the principal bottlenecks of the NNLO computation, was carried out using two independent approaches. The first approach is based on an explicit phase-space parameterization in a suitable center-of-mass frame, reducing the integrals to angular and parametric integrations that can be evaluated analytically. The second approach employs the method of differential equations, where the master integrals are transformed to a canonical basis and solved systematically in terms of Chen iterated integrals and Goncharov polylogarithms. The complete agreement between the two methods provides a strong validation of the final analytic expressions.

The techniques and results presented in this chapter provide the complete set of master integrals required for the NNLO coefficient functions. They overcome one of the major technical obstacles in the computation of NNLO corrections to SIDIS and form the foundation for the derivation of precise perturbative predictions presented in the thesis. Such precision calculations are essential for fully exploiting the physics potential of the future Electron-Ion Collider, where NNLO contributions will play a crucial role.

Chapter 5

Going beyond NNLO: Threshold resummation

In this chapter, we develop the threshold resummation formalism for semi-inclusive deep-inelastic scattering (SIDIS). Using factorization property of the SIDIS cross section and the renormalization group invariance of QCD, the threshold-enhanced logarithms contributions are systematically resummed to all orders in perturbation theory. We further derive higher-order soft-virtual contributions using recent advances in perturbative QCD and investigate the numerical impact of the resummed predictions, demonstrating improved perturbative stability and reduced scale dependence when matched to the exact NNLO results. The work presented here is based on the publication [\[179\]](#).

5.1 Introduction

In Chapter 2, we studied the fixed-order QCD corrections to polarized semi-inclusive deep-inelastic scattering (SIDIS) mediated by the exchange of a virtual photon. In the present chapter, we extend the discussion to both polarized and unpolarized SIDIS processes and investigate the effects of threshold-enhanced logarithmic contributions.

Within the framework of QCD factorization, the SIDIS cross section can be expressed as a convolution of perturbatively calculable coefficient functions (CFs) with non-perturbative parton distribution and fragmentation functions. The fixed order results for the CFs, parameterizing the hard scattering, often provide reliable theoretical predictions for wide range of kinematic variables. However, in the threshold region, corresponding to the limit $x' \rightarrow 1$ and $z' \rightarrow 1$, they fail because of the presence of large logarithms. In the case of SIDIS, these logarithms originate from the partonic configurations where partons are soft and/or collinear to each other. Although the CFs in SIDIS are infrared-safe, meaning that soft and collinear divergences cancel out, these cancellations lead to certain distributions in CFs represented by distributions such as $\delta(1 - \xi)$ and

$$\mathcal{D}_{\bar{\xi}}^j = \left[\frac{\ln^j(1 - \xi)}{1 - \xi} \right]_+, \quad j = 0, 1, \dots \quad (5.1)$$

where $\bar{\xi} = 1 - \xi$ and $\xi = x', z'$ are appropriate scaling variables. Here subscript $+$ means that $\mathcal{D}_{\bar{\xi}}^j$ is a plus distributions defined as,

$$\int_0^1 d\xi f(\xi) \mathcal{D}_{\bar{\xi}}^j = \int_0^1 d\xi \left(f(\xi) - f(1) \right) \frac{\ln^j(1 - \xi)}{1 - \xi} \quad (5.2)$$

where $f(\xi)$ is regular at $\xi = 1$. We call them soft plus virtual (SV) contributions, and their importance was recognized early on, leading to several improvements in QCD

perturbation theory, see [148–151]. Currently, approximations at next-to-next-to-next-to leading order (N^3LO) accuracy taking into account only threshold contributions, also called SV and threshold resummation to next-to-next-to-next-to leading logarithmic (N^3LL) accuracy are available [150, 152, 153], improving upon earlier results [154–156] at next-to-leading logarithmic (NLL) accuracy. These achievements were possible thanks to an intriguing connection between SIDIS and the rapidity distributions of pair of leptons in the Drell-Yan (DY) process, [150, 346, 404, 405]. Beyond the SV contributions, one encounters terms with logarithmic enhancement of the type $\ln^j(1 - \xi)$, with $\xi = x', z'$, for $j = 0, 1, \dots$, which are classified as next-to-leading power (NLP) corrections or next-to-SV (NSV) terms.

Threshold resummation provides a framework to systematically organize and resum these large logarithms, i.e. the SV terms in Eq. (5.1) and NSV terms, to all orders in perturbation theory. As a result, the perturbative predictions exhibit improved convergence and stability, leading to more reliable phenomenological predictions. In this work, we push threshold resummation for the SIDIS CFs to N^4LL except N independent terms coming from real emission processes and provide their approximations at N^4LO in QCD, accounting for both SV as well as NSV terms in a systematic procedure.

In this chapter, we develop the threshold resummation formalism for semi-inclusive deep inelastic scattering (SIDIS) by exploiting the factorization properties of the cross section together with the renormalization group invariance of QCD. This framework enables the all-order resummation of threshold-enhanced logarithms in Mellin space and allows us to predict higher-order soft-virtual and next-to-soft-virtual contributions beyond the currently available fixed-order calculations.

The chapter is organized as follows. In Sec. 5.2, we review the theoretical framework of SIDIS, recall the essential aspects of mass factorization in QCD. In Sec. 5.3, we present the master formula for the diagonal coefficient functions, where we discuss

in detail the individual building blocks entering the master formula and the differential equations that they satisfy. These ingredients are then combined in Sec. 5.4 to derive the all-order structure of the threshold-enhanced SV and NSV contributions. The predictive all-order structure obtained therein forms the basis of the threshold resummation framework. In Sec. 5.5, we derive the all-order resummed expression for the threshold logarithms in Mellin space, expressed in terms of the complex Mellin variables N_1 and N_2 , conjugate to the scaling variables x' and z' , respectively. An alternative approach based on the physical evolution kernel (PEK) is discussed in Sec. 5.6. The phenomenological implications of the resummed results are presented in Sec. 5.7. Finally, we conclude with a summary of our main findings. Additional formulae relevant to the threshold resummation formalism are collected in the Appendix-F.

5.2 Factorization and Threshold Structure

In perturbative QCD, the structure functions factorize as a convolution of the (spin-dependent) PDFs, $(\Delta)f_{a/P}(x_1, \mu_F^2)$, and FFs, $D_{H'/b}(z_1, \mu_F^2)$, with the corresponding (spin-dependent) CFs, $(\Delta)\mathcal{C}_{J,ab}(x/x_1, z/z_1, Q^2, \mu_F^2)$, the latter being calculable in perturbation theory. Here and throughout, the symbol (Δ) indicates the polarized case, while the absence of it corresponds to the unpolarized case.

$$\begin{aligned} (g_J)F_J(x, z, Q^2) = & \sum_{a,b=q,\bar{q},g} \int_x^1 \frac{dx_1}{x_1} (\Delta)f_{a/P}(x_1, \mu_F^2) \int_z^1 \frac{dz_1}{z_1} D_{H'/b}(z_1, \mu_F^2) \\ & \times (\Delta)\mathcal{C}_{J,ab}\left(\frac{x}{x_1}, \frac{z}{z_1}, Q^2, \mu_F^2\right). \end{aligned} \quad (5.3)$$

Using the same notation and conventions as in the previous chapters, (μ_F) denotes the factorization scale, (x_1) and (z_1) are the momentum fractions associated with the incoming and outgoing partons, respectively. Note also, $f_{a/P}$ denotes the spin

averaged PDF and $\Delta f_{a/P}$ denotes spin-dependent PDFs, $(\Delta)f_{a/P} = f_{a(\uparrow)/P(\uparrow)}(-) + f_{a(\downarrow)/P(\uparrow)}$, where arrows denote the polarisations of respective particles with respect to beam direction. Also, $\mathcal{C}_{J,ab} \equiv \mathcal{F}_{J,ab}$ for $J = 1, 2$ and $\Delta\mathcal{C}_{1,ab} \equiv \mathcal{G}_{1,ab}$.

The SIDIS CFs are obtained from the corresponding partonic subprocesses via mass factorization. In the massless quark approximation, these partonic quantities contain collinear divergences associated with collinear parton emissions from the initial and final states. In dimensional regularization ($d = 4 + \epsilon$), these divergences appear as poles in ϵ . Thanks to QCD factorization, these singularities factorize from the bare (spin-dependent) CFs $(\Delta)\hat{\mathcal{C}}_{J,ab}(x', z', \epsilon)$, through universal Altarelli-Parisi kernels at the scale μ_F ,

$$(\Delta)\hat{\mathcal{C}}_{J,ab}(x', z', \epsilon) = (\Delta)\Gamma_{c \leftarrow a}(x', \mu_F^2, \epsilon) \otimes (\Delta)\mathcal{C}_{J,cd}(x', z', \mu_F^2, \epsilon) \tilde{\otimes} \tilde{\Gamma}_{b \leftarrow d}(z', \mu_F^2, \epsilon) \quad (5.4)$$

The kernels $(\Delta)\Gamma_{c \leftarrow a}$ and $\tilde{\Gamma}_{b \leftarrow d}$ are given in terms of space- and time-like splitting functions and encode the collinear divergences through poles in ϵ , see, e.g. [173]. The partonic scaling variables are $x' = x/x_1$ and $z' = z/z_1$ and the convolutions $\otimes$ and $\tilde{\otimes}$ are defined in Eq. (3.22).

The collinear finite CFs $(\Delta)\mathcal{C}_{J,ab}$ in Eq. (5.4) are expanded in powers of strong coupling constant $a_s = \alpha_s/(4\pi)$ at the renormalisation scale μ_R as,

$$(\Delta)\mathcal{C}_{J,ab}(x', z', \mu_F^2) = \delta_{ab}\delta(1-x')\delta(1-z') + \sum_{i=1}^{\infty} a_s^i(\mu_R^2)(\Delta)\mathcal{C}_{J,ab}^{(i)}(x', z', \mu_F^2, \mu_R^2). \quad (5.5)$$

The CFs $(\Delta)\mathcal{C}_{J,ab}$ in general contain distributions $\delta(1-\xi)$ and $\mathcal{D}_{\xi}^j$, cf. Eq. (5.1), where $\xi = x', z'$ and regular functions of x', z' . We can write $(\Delta)\mathcal{C}_{J,ab}$ as,

$$\begin{aligned} (\Delta)\mathcal{C}_{J,ab} &= (\Delta)C_{J,ab}^{\delta_x \delta_z} \delta(1-x')\delta(1-z') \\ &+ \sum_j \left((\Delta)C_{J,ab}^{\delta_x j} \delta(1-x')\mathcal{D}_{z'}^j + (\Delta)C_{J,ab}^{j \delta_z} \delta(1-z')\mathcal{D}_{x'}^j \right) \end{aligned}$$

$$\begin{aligned}
& + \sum_{j,k} (\Delta) C_{J,ab}^{ij,k} \mathcal{D}_{\bar{x}'}^j \mathcal{D}_{\bar{z}'}^k + (\Delta) C_{J,ab,z'}^{\delta_x}(z') \delta(1-x') + (\Delta) C_{J,ab,x'}^{\delta_z}(x') \delta(1-z') \\
& + \sum_j ((\Delta) C_{J,ab,z'}^j(z') \mathcal{D}_{\bar{x}'}^j + (\Delta) C_{J,ab,x'}^j(x') \mathcal{D}_{\bar{z}'}^j) + (\Delta) R_{J,ab}(x', z'), \quad (5.6)
\end{aligned}$$

The functions $(\Delta)R_{J,ab}$ contain all remaining terms that are regular (no distributions). Furthermore, we expand the CFs $(\Delta)C_{J,ab,x'}$ and $(\Delta)C_{J,ab,z'}$ in Eq. (5.6) around $x' = 1$ and $z' = 1$, we obtain a series of the form: $(1-\xi)^i \ln^j(1-\xi)$, $\xi = x', z'$ for $i, j = 0, 1$ etc. The leading terms in this series ($i = 0$) are the so-called NSV terms, while the rest with powers $i > 0$ are denoted as beyond-NSV (BNSV) terms.

In this notation, the CFs in Eq. (5.6) read

$$(\Delta)\mathcal{C}_{J,ab} = \delta_{ab} \left((\Delta)\mathcal{C}_J^{\text{SV}} \right) + (\Delta)\mathcal{C}_{J,ab}^{\text{NSV}} + (\Delta)\mathcal{C}_{J,ab}^{\text{BNSV}}, \quad (5.7)$$

where the SV term does not receive any contributions if $a = b = g$. Each term in the above equation can be expanded in powers series of a_s as,

$$\begin{aligned}
(\Delta)\mathcal{C}_J^{\text{SV}} &= (\Delta)C_{J,cc}^{(0),\delta_x\delta_z} \delta(1-x')\delta(1-z') \\
&+ \sum_{n=1}^{\infty} a_s^n \left[(\Delta)C_{J,cc}^{(n),\delta_x\delta_z} \delta(1-x')\delta(1-z') + \sum_{j=0}^{2n-1} (\Delta)C_{J,cc}^{(n),\delta_x j} \delta(1-x') \mathcal{D}_{\bar{z}'}^j \right. \\
&+ \sum_{j=0}^{2n-1} (\Delta)C_{J,cc}^{(n),j\delta_z} \delta(1-z') \mathcal{D}_{\bar{x}'}^j + \left. \sum_{j=0}^{2n-2} \sum_{k=0}^{2n-2-j} (\Delta)C_{J,cc}^{(n),jk} \mathcal{D}_{\bar{x}'}^j \mathcal{D}_{\bar{z}'}^k \right], \\
(\Delta)\mathcal{C}_{J,ab}^{\text{NSV}} &= \sum_{n=1}^{\infty} a_s^n \left[\sum_{j=0}^{2n-1} \left((\Delta)C_{J,ab}^{(n),\delta_x j} \delta(1-x') L_j(z') + (\Delta)C_{J,ab}^{(n),j\delta_z} \delta(1-z') L_j(x') \right) \right. \\
&+ \left. \sum_{j=0}^{2n-2} \sum_{k=0}^{2n-2-j} \left((\Delta)C_{J,ab}^{(n),jk} \mathcal{D}_{\bar{x}'}^j L_k(z') + (\Delta)C_{J,ab}^{(n),jk} \mathcal{D}_{\bar{z}'}^j L_k(x') \right) \right], \quad (5.8)
\end{aligned}$$

where $L_j(\xi) = \ln^j(1-\xi)$, $\xi = x', z'$ and $c = q, \bar{q}$. Schematically, $(\Delta)\mathcal{C}_J^{\text{SV}}$ contains double distributions and $(\Delta)\mathcal{C}_{J,ab}^{\text{NSV}}$ contains single distribution in x' or z' each multiplied by powers of $\ln^j(1-z')$ or $\ln^j(1-x')$ respectively, where $j = 0, 1, 2$ etc. Any regular terms in x', z' which is proportional to $(1-x')$ or/and $(1-z')$ that

do not contain any distributions fall within the BNSV category. The NNLO results in [171–173, 175, 176, 184] for the CFs $(\Delta)\mathcal{C}_J^{\text{SV}}$ are in complete agreement with SV predictions for unpolarised structure functions $F_{1,2}$ [152], see also [272, 273]. The leading terms of the NSV contributions agree as well with ref. [152], where the dominant NLP terms have been presented.

The first principle’s derivation of the threshold enhanced logarithms in Eq. (5.8) exploits the renormalisation group equations and the factorization of soft and collinear singularities to all orders in QCD, building on well-known developments for inclusive cross sections such as DIS, DY and Higgs boson production (or, more generally, colorless n -particle production), see e.g. [272, 310, 311, 406–439]. For observables in differential kinematics, where the threshold limit is approached in terms of two different scaling variables, such as the rapidity distributions of lepton pairs in the DY process or Higgs boson production, threshold logarithms have also been systematically resummed to all orders in perturbation theory, see [272, 273, 405, 407, 424, 433, 440–453]. In addition, both single as well as double variable resummations were extended for flavor diagonal channels to include NSV contributions [274, 452, 454–475], also see [476]. The kinematics in these cases, is similar to the SIDIS process, where the limits $x' \rightarrow 1$ and $z' \rightarrow 1$ are considered.

In the following we develop the formalism to resum both SV as well as NSV logarithms of flavor diagonal contributions, namely $(\Delta)\mathcal{C}_{J,cc}$ with $(c = q, \bar{q})$, to all orders both in (x', z') space as well in their corresponding Mellin space (N_1, N_2) . The reason to consider only flavor diagonal channels is because of their simple collinear factorisation structure. The starting point is the mass factorised form of the bare CFs in Eq. (5.4) in $d = 4 + \epsilon$ dimensions, expanding the sum over the parton channels,

$$\begin{aligned} (\Delta)\hat{\mathcal{C}}_{J,qq}(x', z', \epsilon) &= (\Delta)\Gamma_{q \leftarrow q} \otimes (\Delta)\mathcal{C}_{J,qq} \tilde{\otimes} \tilde{\Gamma}_{q \leftarrow q} + (\Delta)\Gamma_{q \leftarrow q} \otimes (\Delta)\mathcal{C}_{J,q\bar{q}} \tilde{\otimes} \tilde{\Gamma}_{q \leftarrow \bar{q}} \\ &+ (\Delta)\Gamma_{q \leftarrow q} \otimes (\Delta)\mathcal{C}_{J,qg} \tilde{\otimes} \tilde{\Gamma}_{q \leftarrow g} + (\Delta)\Gamma_{\bar{q} \leftarrow q} \otimes (\Delta)\mathcal{C}_{J,\bar{q}q} \tilde{\otimes} \tilde{\Gamma}_{q \leftarrow q} \end{aligned}$$

$$\begin{aligned}
& + (\Delta)\Gamma_{\bar{q} \leftarrow q} \otimes (\Delta)\mathcal{C}_{J,\bar{q}\bar{q}} \tilde{\tilde{\Gamma}}_{q \leftarrow \bar{q}} + (\Delta)\Gamma_{\bar{q} \leftarrow q} \otimes (\Delta)\mathcal{C}_{J,\bar{q}g} \tilde{\tilde{\Gamma}}_{q \leftarrow g} \\
& + (\Delta)\Gamma_{g \leftarrow q} \otimes (\Delta)\mathcal{C}_{J,gq} \tilde{\tilde{\Gamma}}_{q \leftarrow q} + (\Delta)\Gamma_{g \leftarrow q} \otimes (\Delta)\mathcal{C}_{J,g\bar{q}} \tilde{\tilde{\Gamma}}_{q \leftarrow \bar{q}} \\
& + (\Delta)\Gamma_{g \leftarrow q} \otimes (\Delta)\mathcal{C}_{J,gg} \tilde{\tilde{\Gamma}}_{q \leftarrow g} .
\end{aligned} \tag{5.9}$$

The convolutions with the space- and time-like AP kernels $(\Delta)\Gamma_{a \leftarrow b}$ and $\tilde{\tilde{\Gamma}}_{a \leftarrow b}$ can be distinguished as follows:

- (i) Terms involving only diagonal combinations, such as $(\Delta)\Gamma_{q \leftarrow q} \otimes (\Delta)\mathcal{C}_{J,qq} \tilde{\tilde{\Gamma}}_{q \leftarrow q}$;
- (ii) Contributions involving a product of one diagonal with a pair of non-diagonal terms, for example $(\Delta)\Gamma_{q \leftarrow q} \otimes (\Delta)\mathcal{C}_{J,qg} \tilde{\tilde{\Gamma}}_{q \leftarrow g}$.

The terms in (i) contain SV plus NSV terms when the convolutions have been performed, while the latter ones in case (ii) will be composed beyond NSV terms only. The above observation follows from the schematic convolution relations,

$$\begin{aligned}
\text{SV} \otimes \text{SV} & \sim \text{SV} + \text{NSV} + \text{BNSV}, \quad \text{SV} \otimes \text{NSV} \sim \text{NSV} + \text{BNSV}, \\
\text{NSV} \otimes \text{NSV} & \sim \text{BNSV}.
\end{aligned} \tag{5.10}$$

To illustrate this, take for example,

$$\begin{aligned}
\mathcal{D}_\xi^0 \otimes \mathcal{D}_\xi^0 & = 2\mathcal{D}_\xi^1 - \zeta_2 \delta(1-\xi) - \frac{\ln \xi}{1-\xi}, \\
& = \underbrace{2\mathcal{D}_\xi^1 - \zeta_2 \delta(1-\xi)}_{\text{SV}} + \underbrace{1}_{\text{NSV}} + \mathcal{O}((1-\xi))
\end{aligned} \tag{5.11}$$

$$\begin{aligned}
D_\xi^1 \otimes \ln(1-\xi) & = \text{Li}_3(1-\xi) - 2\text{S}_{12}(1-\xi) + \zeta_3 - \ln(\xi(1-\xi))\text{Li}_2(1-\xi) \\
& \quad + \zeta_2 \ln\left(\frac{\xi}{1-\xi}\right) + \frac{1}{2} \ln^3(1-\xi) - \ln(\xi) \ln^2(1-\xi) \\
& = \underbrace{\frac{1}{2} \ln^3(1-\xi) - \zeta_2 \ln(1-\xi) + \zeta_3}_{\text{NSV}} + \mathcal{O}((1-\xi)),
\end{aligned} \tag{5.12}$$

$$1 \otimes \ln(1-\xi) = \text{Li}_2(\xi) - \zeta_2 = -(1-\xi)(1 - \ln(1-\xi)) + \mathcal{O}((1-\xi)^2), \tag{5.13}$$

here, Li_n and S_{12} are classical and Nielsen polylogarithms. Note, in all above equations the terms of $\mathcal{O}((1 - \xi))$ contributes at BNSV accuracy.

Note that the diagonal AP kernels $(\Delta)\Gamma_{q \leftarrow q}$ and $\tilde{\Gamma}_{q \leftarrow q}$ contain convolutions among diagonal splitting functions, $(\Delta)P_{qq}$ and $\tilde{P}_{qq}$ respectively, or one diagonal and a pair of off-diagonal ones, $(\Delta)P_{ab}, \tilde{P}_{ab}, a \neq b$. We drop those terms in $(\Delta)\Gamma_{q \leftarrow q}$ ($\tilde{\Gamma}_{q \leftarrow q}$), that contain a pair of off-diagonal splitting functions $(\Delta)P_{ab}$ ($\tilde{P}_{ab}$), as they contribute only beyond NSV accuracy. In addition, we drop all the BNSV terms in the diagonal splitting functions as well. This leads to

$$(\Delta)\hat{\mathcal{C}}_{J,qq}^{\text{SV+NSV}} = (\Delta)\Gamma_{q \leftarrow q}^{\text{SV+NSV}} \otimes (\Delta)\mathcal{C}_{J,qq}^{\text{SV+NSV}} \tilde{\otimes} \tilde{\Gamma}_{q \leftarrow q}^{\text{SV+NSV}}. \quad (5.14)$$

Here, the superscript on the AP kernels indicate their truncation to SV and NSV terms only. In this way we can write the bare CFs in Eq. (5.4) in terms of only diagonal quantities, i.e., $(\Delta)\hat{\mathcal{C}}_{J,qq}$, $(\Delta)\mathcal{C}_{J,qq}$ and AP kernels $(\Delta)\Gamma_{q \leftarrow q}$, $\tilde{\Gamma}_{q \leftarrow q}$, where BNSV terms and the sum ab over the parton channels are dropped.

The bare off-diagonal CFs instead contain both diagonal and off-diagonal terms from $(\Delta)\mathcal{C}_{J,ab}$ and AP kernels. For instance $(\Delta)\hat{\mathcal{C}}_{J,qg}$ reads

$$\begin{aligned} (\Delta)\hat{\mathcal{C}}_{J,qg}(x', z', \epsilon) = & (\Delta)\Gamma_{q \leftarrow q} \otimes (\Delta)\mathcal{C}_{J,qq} \tilde{\otimes} \tilde{\Gamma}_{g \leftarrow q} + (\Delta)\Gamma_{q \leftarrow q} \otimes (\Delta)\mathcal{C}_{J,q\bar{q}} \tilde{\otimes} \tilde{\Gamma}_{g \leftarrow \bar{q}} \\ & + (\Delta)\Gamma_{q \leftarrow q} \otimes (\Delta)\mathcal{C}_{J,qg} \tilde{\otimes} \tilde{\Gamma}_{g \leftarrow g} + (\Delta)\Gamma_{\bar{q} \leftarrow q} \otimes (\Delta)\mathcal{C}_{J,\bar{q}q} \tilde{\otimes} \tilde{\Gamma}_{g \leftarrow q} \\ & + (\Delta)\Gamma_{\bar{q} \leftarrow q} \otimes (\Delta)\mathcal{C}_{J,\bar{q}\bar{q}} \tilde{\otimes} \tilde{\Gamma}_{g \leftarrow \bar{q}} + (\Delta)\Gamma_{\bar{q} \leftarrow q} \otimes (\Delta)\mathcal{C}_{J,\bar{q}g} \tilde{\otimes} \tilde{\Gamma}_{g \leftarrow g} \\ & + (\Delta)\Gamma_{g \leftarrow q} \otimes (\Delta)\mathcal{C}_{J,gq} \tilde{\otimes} \tilde{\Gamma}_{g \leftarrow q} + (\Delta)\Gamma_{g \leftarrow q} \otimes (\Delta)\mathcal{C}_{J,g\bar{q}} \tilde{\otimes} \tilde{\Gamma}_{g \leftarrow \bar{q}} \\ & + (\Delta)\Gamma_{g \leftarrow q} \otimes (\Delta)\mathcal{C}_{J,gg} \tilde{\otimes} \tilde{\Gamma}_{g \leftarrow g}. \end{aligned} \quad (5.15)$$

Unlike the diagonal case in Eq. (5.9), no single term provides pure SV contributions in the threshold limit. Hence, the mass factorised result for the off-diagonal channel contains NSV terms only and those beyond, where the former ones come from

contributions that contain at least two diagonal quantities, either from $(\Delta)\mathcal{C}_{J,ab}$ or $(\Delta)\Gamma_{a\leftarrow b}, \tilde{\Gamma}_{a\leftarrow b}$. Dropping all terms that contain more than two off-diagonal quantities in the mass factorisation formula, we obtain

$$(\Delta)\hat{\mathcal{C}}_{J,qg}^{\text{NSV}} = (\Delta)\Gamma_{q\leftarrow q}^{\text{SV+NSV}} \otimes (\Delta)\mathcal{C}_{J,qg}^{\text{SV+NSV}} \tilde{\otimes} \tilde{\Gamma}_{g\leftarrow q}^{\text{NSV}} + (\Delta)\Gamma_{q\leftarrow q}^{\text{SV+NSV}} \otimes (\Delta)\mathcal{C}_{J,qg}^{\text{NSV}} \tilde{\otimes} \tilde{\Gamma}_{g\leftarrow g}^{\text{SV+NSV}}, \quad (5.16)$$

which receives contribution from both CFs, $(\Delta)\mathcal{C}_{J,qg}$ and $(\Delta)\mathcal{C}_{J,qq}$, unlike the diagonal channel in Eq. (5.14) which is directly proportional to $(\Delta)\hat{\mathcal{C}}_{J,qq}$.

The simple and remarkable structure in the diagonal channel (5.14) makes it easy for us to study its all order structure of SV and NSV logarithms. We achieve this by setting up a homogeneous differential equations for CFs in terms of the soft and collinear anomalous dimensions. In contrast, presence of inhomogeneous terms in corresponding differential equations for the off-diagonal channel poses technical challenges when solving them. For this reason, we restrict our analysis in this thesis to the flavor-diagonal partonic channels.

5.3 Master Formula

We begin by considering the mass-factorization relation Eq. (5.14) rewrite it as,

$$\begin{aligned} (\Delta)\mathcal{C}_{J,qq}^{\text{SV+NSV}} &= \left((\Delta)\Gamma \right)_{q\leftarrow q}^{-1} (x', \mu_F^2, \epsilon) \otimes (\Delta)\hat{\mathcal{C}}_{J,qq}(x', z', \mu_F^2, \epsilon) \tilde{\otimes} \left(\tilde{\Gamma} \right)_{q\leftarrow q}^{-1} (z', \mu_F^2, \epsilon) \\ &= \left| \hat{F}_q(Q^2, \epsilon) \right|^2 \\ &\quad \times \left((\Delta)\Gamma \right)_{q\leftarrow q}^{-1} (x', \mu_F^2, \epsilon) \otimes (\Delta)\hat{\mathcal{S}}_{J,q}(Q^2, x', z', \epsilon) \tilde{\otimes} \left(\tilde{\Gamma} \right)_{q\leftarrow q}^{-1} (z', \mu_F^2, \epsilon). \end{aligned} \quad (5.17)$$

The above equation is the master formula expressing the diagonal coefficient functions in terms of the quark form factor, the AP kernels, and the soft function.

Here, $\hat{F}_q(Q^2, \epsilon)$ is the massless quark form factor (FF) in dimensional regularization which captures pure virtual contributions and $(\Delta)\hat{\mathcal{S}}_{J,q}(Q^2, x', z', \epsilon)$, called soft function which gets contributions from real emissions, is defined by

$$(\Delta)\hat{\mathcal{S}}_{J,q}(Q^2, x', z', \epsilon) = \frac{(\Delta)\hat{\mathcal{C}}_{J,qq}(Q^2, x', z', \epsilon)}{\left|\hat{F}_q(Q^2, \epsilon)\right|^2} \quad (5.18)$$

Note that in the absence of any real radiation, the soft functions is constrained by kinematics and takes the simple form: $(\Delta)\hat{\mathcal{S}}_{J,q}|_{\text{no radiation}} = \delta(1-x')\delta(1-z')$.

The vector form factor $\hat{F}$ has been subject to extensive studies, see, e.g. [256, 421, 477–484], see also [276, 485–487]. In massless QCD and within dimensional regularization it exhibits IR and UV singularities as poles in ϵ . The UV divergences can be removed by renormalisation of the strong coupling, while the soft and collinear, i.e., IR singularities, factorise as

$$\hat{F}_q(Q^2, \epsilon) = Z_{\hat{F}_q}(Q^2, \mu_s^2, \epsilon) F_{q,fin}(Q^2, \mu_s^2, \epsilon), \quad (5.19)$$

where $Z_{\hat{F}_q}$ is IR singular and $F_{q,fin}$ is IR finite, the scale μ_s is IR factorisation scale. Renormalisation group invariance implies that

$$\mu_s^2 \frac{d}{d\mu_s^2} \ln Z_{\hat{F}_q}(\mu_s^2) = \gamma_{\hat{F}_q}(\mu_s^2), \quad (5.20)$$

where $\gamma_{\hat{F}_q}$ to all order in a_s takes the form

$$\gamma_{\hat{F}_q} = \frac{1}{2} \left(-A^q(\mu_s^2) \ln \left(\frac{Q^2}{\mu_s^2} \right) + 2B^q(\mu_s^2) + f^q(\mu_s^2) \right). \quad (5.21)$$

Here, A^q, B^q, f^q denote the cusp, the quark virtual and the eikonal anomalous dimensions respectively, they all have expansions in powers of the strong coupling as $A^q(\mu_s^2) = \sum_{i=1}^{\infty} a_s^i(\mu_s^2) A_i^q$ etc. They are currently known to four-loop accuracy in QCD [488–495]. Thus, the solution to Eq. (5.20) for $Z_{\hat{F}_q}$ in the $\overline{\text{MS}}$ scheme contains

only poles in ϵ whose coefficients are completely controlled by universal anomalous dimensions A^q, B^q and f^q and the coefficients of QCD β function, the latter being known even to five loops [26–29].

The bare form factor $\hat{F}_q$ is subject to a differential equation with respect to Q^2 ,

$$Q^2 \frac{d}{dQ^2} \ln \hat{F}_q(Q^2, \epsilon) = \Gamma_{\hat{F}_q}(Q^2, \epsilon), \quad (5.22)$$

where

$$\Gamma_{\hat{F}_q}(Q^2, \epsilon) = \frac{1}{2} \left(K_d^q(\mu_s^2, \epsilon) + G_d^q(Q^2, \mu_s^2, \epsilon) \right). \quad (5.23)$$

The kernel $K_d^q = 2d \ln Z_{\hat{F}_q} / d \ln(Q^2)$ contains entire IR singular terms while the function $G_d^q = 2d \ln F_{q,fin} / d \ln(Q^2)$ is IR finite by definition. Since, we have defined the form factor in dimensional regularisation, the solution to this $K + G$ equation takes the simple form

$$\hat{F}_q(Q^2, \epsilon) = \exp \left(\int_0^{Q^2} \frac{d\lambda^2}{\lambda^2} \Gamma_{\hat{F}_q}(\lambda^2, \epsilon) \right), \quad (5.24)$$

with $\hat{F}_q(Q^2 = 0, \epsilon) = 1$ as boundary condition. Since all IR poles in ϵ are contained in K_d^q only and G_d^q is finite, the solution reveals the remarkable structure for the form factor, namely, at given order a_s^i , all the poles except the single pole in ϵ can be predicted from knowledge of K_d^q and G_d^q at previous orders up to a_s^{i-1} . Explicit results for K_d^q and G_d^q are presented in [420, 421] and also in Appendix-F.1.

Next, we briefly review the structure of the AP kernels in Eq. (5.17) and the associated splitting functions, controlling their evolution as a function of the factorisation scale μ_F . We denote space-like (unpolarized and polarized) and time-like kernels collectively by $\Gamma_{c \leftarrow c}$ and their respective splitting functions by $\mathbb{P}_{c \leftarrow c}$. In the threshold

limit only the diagonal splitting functions $\mathbb{P}_{c \leftarrow c}$, $c = q, \bar{q}$ contribute,

$$\mu_F^2 \frac{d}{d\mu_F^2} \mathbb{F}_{c \leftarrow c}(\mu_F^2, \xi) = \frac{1}{2} \mathbb{P}_{c \leftarrow c}(\mu_F^2, \xi) \otimes \mathbb{F}_{c \leftarrow c}(\mu_F^2, \xi), \quad (5.25)$$

where $\xi = x', z'$. The splitting functions are expanded in powers of $a_s(\mu_F^2)$ as $\mathbb{P}_{c \leftarrow c}(\mu_F^2) = \sum_{i=1}^{\infty} a_s^i(\mu_F^2) \mathbb{P}_{i-1}^c$ and we have suppressed any dependence on ϵ in both $\mathbb{F}_{c \leftarrow c}$ and $\mathbb{P}_{c \leftarrow c}$. Due to its simple structure the all order solution of Eq. (5.25) takes the simple form

$$\mathbb{F}_{c \leftarrow c}(\mu_F^2, \xi, \epsilon) = \mathcal{C} \exp \left(\frac{1}{2} \int_0^{\mu_F^2} \frac{d\lambda^2}{\lambda^2} \mathbb{P}_{c \leftarrow c}(\lambda^2, \xi) \right), \quad (5.26)$$

where the symbol $\mathcal{C}$ denotes an ordered exponential, appropriately defined through iterated convolutions with respect to x' or z' , see [421], for brevity, we write

$$\mathcal{C} \exp(a_s f(x)) = \delta(1-x) + \frac{a_s}{1!} f(x) + \frac{a_s^2}{2!} f(x) \otimes f(x) + \frac{a_s^3}{3!} f(x) \otimes f(x) \otimes f(x) + \dots \quad (5.27)$$

The relevant splitting functions are known to third order in perturbative QCD [120, 233, 262–270] and their expansion in the soft and collinear limit reads

$$\mathbb{P}_{c \leftarrow c}(\mu_F^2, \xi) = 2 \left(\frac{A^c(\mu_F^2)}{(1-\xi)_+} + B^c(\mu_F^2) \delta(1-\xi) + \mathbb{C}^c(\mu_F^2) \ln(1-\xi) + \mathbb{D}^c(\mu_F^2) \right), \quad (5.28)$$

in terms of the cusp and the virtual anomalous dimensions A^c and B^c already encountered in the form factor above. The NSV terms, denoted as $\mathbb{C}^c$, and $\mathbb{D}^c$, are determined from A^c , B^c and coefficients of the QCD β -function at lower orders. There is distinction between space- and time-like kinematics, i.e. $\mathbb{C}^c = C^q$, $\mathbb{D}^c = D^q$ for space-like and $\mathbb{C}^c = \tilde{C}^q$, $\mathbb{D}^c = \tilde{D}^q$ for time-like splitting functions. Explicit results are listed in Appendix-F.4.

The final ingredient in the threshold factorization formulae in Eq. (5.17) is the soft function $(\Delta)\hat{S}_{J,q}$, hereafter denoted by $\hat{S}_q$. A differential equation for $\hat{S}_q$ in dimensional regularisation, organizing its all-order perturbative structure, can be obtained with Eq. (5.17) and the differential equation for the form factor, see Eq. (5.22).

$$Q^2 \frac{d}{dQ^2} \mathcal{C} \ln \hat{S}_q(Q^2, \epsilon) = \Gamma_{\hat{S}_q}(Q^2, \epsilon), \quad (5.29)$$

where we have suppressed the dependence on x', z' and

$$\begin{aligned} \Gamma_{\hat{S}_q}(Q^2, \epsilon) = & Q^2 \frac{d}{dQ^2} \left(\mathcal{C} \ln(\Delta) \mathcal{C}_{J,qq}(Q^2, \mu_R^2, \mu_F^2, x', z', \epsilon) \right. \\ & \left. - \ln |\hat{F}_q(Q^2, \epsilon)|^2 \delta(1-x') \delta(1-z') \right). \end{aligned} \quad (5.30)$$

The symbol $\mathcal{C}$ represents that each product of x' (z') dependent functions in the expansion of $\ln(\Delta) \mathcal{C}_{J,qq}$ in a_s is treated as convolution with respect to x' (z') see Eq. (5.27). The fact that $\hat{S}_q$ is renormalization group invariant with respect to μ_R and μ_F implies that the Q^2 derivative of $(\Delta) \mathcal{C}_{J,qq}$ in the first term in Eq. (5.30) has to be a function of only Q^2 and x', z' . This implies that $\Gamma_{\hat{S}_q}$ is independent of μ_R and μ_F . Observe that the first term is finite and the second term contains both singular and finite parts through K_d^q and G_d^q via $K + G$ equation of $\Gamma_{\hat{F}_q}$, see Eq. (5.22). This means that we can express the kernel $\Gamma_{\hat{S}_q}$ in Eq. (5.30) as a sum of singular term $\overline{K}_d^q$ and finite $\overline{G}_d^q$ pieces to all orders in perturbation theory, similar to the Q^2 evolution equation of the form factor, i.e., $\Gamma_{\hat{S}_q} = (\overline{K}_d^q(\mu_s^2, x', z') + \overline{G}_d^q(Q^2, \mu_s^2, x', z'))/2$. Since the singular part of the kernel comes from K_d^q of the form factor, the term $\overline{K}_d^q$ can depend only on μ_s and process independent anomalous dimension, A^q . The finite $\overline{G}_d^q(Q^2, \mu_s^2, z)$ will contain G_d^q from the form factor and the other process dependent terms from CF $(\Delta) \mathcal{C}_{J,qq}$.

The fact that the kernel admits the decomposition of singular and finite parts as it happens for the form factor, implies that the $\hat{S}_q$ is also factorisable, i.e., we can

write

$$\hat{\mathcal{S}}_q(Q^2, x', z') = Z_q(Q^2, \mu_s^2, x', z') \otimes \mathcal{S}_{q,\text{fin}}(Q^2, \mu_s^2, x', z'), \quad (5.31)$$

where $\mathcal{S}_{q,\text{fin}}$ is IR finite, Z_q is IR singular and identify the IR singular $\overline{K}_d^q = 2d \ln Z_q / d \ln(Q^2)$ and IR finite $\overline{G}_d^q = 2d \ln \mathcal{S}_{q,\text{fin}} / d \ln(Q^2)$. Since $\overline{K}_d^q(\mu_s^2)$ is independent of Q^2 , we can fix only the $\ln(Q^2)$ terms in Z_q . The factorisation of $\hat{\mathcal{S}}_q$ in terms of Z_q and $\mathcal{S}_{q,\text{fin}}$ at arbitrary scale μ_s leads to the renormalisation group equation,

$$\mu_s^2 \frac{dZ_q(Q^2, \mu_s^2)}{d\mu_s^2} = \gamma_{\hat{\mathcal{S}}_q}(Q^2, \mu_s^2) \otimes Z_q(Q^2, \mu_s^2),$$

where we have suppressed any dependence on x', z' in Z_q and $\gamma_{\hat{\mathcal{S}}_q}$. From our NNLO results we find that $\gamma_{\hat{\mathcal{S}}_q}$ takes the remarkable structure, namely $\gamma_{\hat{\mathcal{S}}_q}(Q^2, \mu_s^2) = \xi_1(\mu_s^2, x', z') \ln(Q^2/\mu_s^2) + \xi_2(\mu_s^2, x', z')$. This is expected to continue to all orders in perturbation theory because it results from the IR pole structure of $\hat{\mathcal{S}}_q$. In other words, the singular part of $\hat{\mathcal{S}}_q$, namely, Z_q has to contain precisely those IR poles to cancel against the ones from the form factor and AP kernels leaving $(\Delta)\mathcal{C}_{J,qq}$ finite and this pole structure determines the structure of $\gamma_{\hat{\mathcal{S}}_q}$. Since the poles of the form factor and AP kernels are controlled by the cusp, virtual and eikonal anomalous dimensions, $\gamma_{\hat{\mathcal{S}}_q}$ can be expressed as follows:

$$\gamma_{\hat{\mathcal{S}}_q} = \delta(\bar{x}') \delta(\bar{z}') A^q(\mu_s^2) \ln\left(\frac{Q^2}{\mu_s^2}\right) + P'_{q \leftarrow q}(\mu_s, \bar{x}', \bar{z}'), \quad (5.32)$$

where

$$\begin{aligned} P'_{q \leftarrow q} = & \left[-\frac{1}{2} \delta(\bar{x}') \delta(\bar{z}') f^q(\mu_s^2) + \delta(\bar{z}') \frac{A^q(\mu_s^2)}{(\bar{x}')_+} + \delta(\bar{z}') \left(C^q(\mu_s^2) \ln(\bar{x}') + D^q(\mu_s^2) \right) \right] \\ & + \left(\bar{x}' \leftrightarrow \bar{z}', C^q \leftrightarrow \tilde{C}^q, D^q \leftrightarrow \tilde{D}^q \right), \end{aligned} \quad (5.33)$$

and we use the shorthand notation $\bar{x}' = 1 - x'$, $\bar{z}' = 1 - z'$.

With the boundary $Q^2 = 0$, $\hat{\mathcal{S}}_q(Q^2 = 0, x', z', \epsilon) = \delta(1 - x')\delta(1 - z')$ to all orders in a_s we obtain the solution to Eq. (5.29) as

$$\begin{aligned}\hat{\mathcal{S}}_q(Q^2, x', z', \epsilon) &= \mathcal{C} \exp \left(\int_0^{Q^2} \frac{d\lambda^2}{\lambda^2} \Gamma_{\hat{\mathcal{S}}_q}(\lambda^2, x', z', \epsilon) \right) \\ &= \mathcal{C} \exp \left(2\Phi_{d,q}(Q^2, x', z', \epsilon) \right) .\end{aligned}\tag{5.34}$$

The exponent $\Phi_{d,q}$ can be decomposed into an IR singular part $\Phi_{d,q,s}$ and a finite part $\Phi_{d,q,f}$, i.e., $\Phi_{d,q} = \Phi_{d,q,s} + \Phi_{d,q,f}$. Using this decomposition, we obtain $Z_q = \mathcal{C} \exp(2\Phi_{d,q,s})$ and $\mathcal{S}_{q,fin} = \mathcal{C} \exp(2\Phi_{d,q,f})$. The singular part is controlled by $\gamma_{\hat{\mathcal{S}}_q}$ given in Eq. (5.32). A careful inspection of the one- and two-loop results for $\hat{\mathcal{S}}_q$, i.e., using the results presented in [171, 172], provides hints to its all order structure. However, before we proceed, we split $\Phi_{d,q}$ into the sum of two parts. The SV part denoted by $\Phi_{d,q}^{\text{SV}}$ contains only distributions such as $\delta(1 - \xi)$ and $\mathcal{D}_{\xi,i}$, while NSV part $\Phi_{d,q}^{\text{NSV}}$ summarizes all terms that are products of distributions and $\ln^i(1 - \xi)$ with $\xi = x', z'$. We find that $\Phi_{d,q}^{\text{SV}}$ is symmetric under the interchange of x' and z' while $\Phi_{d,q}^{\text{NSV}}$ is not. Our observations for $\Phi_{d,q}$ read as follows:

- For the SV terms, at order $\hat{a}_s$, the leading pole in ϵ starts at order two, at $\hat{a}_s^2$ it is three and it is expected to increase by one unit at every order in $\hat{a}_s$. Hence, at order $\hat{a}_s^i$, the leading pole in ϵ will be of order $i + 1$. As we had already mentioned, this pole structure is completely dictated by pole structure of $\ln |\hat{F}_q|^2$ and the AP kernels. For the NSV terms, we find that at order $\hat{a}_s$ the leading pole in ϵ is of order one and at two loops, it is two etc. This pattern indicates that the increment of one unit for the leading poles is expected to continue with the order of perturbation and hence at order $\hat{a}_s^i$, the leading pole will be of order i .
- At every order in $\hat{a}_s$, for a given color factor, the combination of ϵ and the

leading logarithm shows uniform transcendentality weight. If we assign n_ϵ weight for ϵ^{-n} and $n_{\mathcal{D}}$ for $\mathcal{D}_\xi^n$, n_L for $\ln^n(1-\xi)$ and n_ζ for ζ_n then the highest weight at every order in ϵ shows uniform transcendentality $\omega = n_\epsilon + n_{\mathcal{D}} + n_L + n_\zeta$. For example, in SV, at NLO, we find $\omega = 2$ at every order of ϵ and at NNLO it is three ($\omega = 3$) etc. For NSV, $\omega = 1$ at NLO and $\omega = 2$ at NNLO at every order in ϵ etc.

The above observations on the fixed order results and the resemblance of Eq. (5.22) with Eq. (5.29), the similarity in the pole structure of the respective kernels Eqs. (5.23) and (5.30) and the renormalization group invariance reveal an all order structure for $\Phi_{d,q}^{\text{SV}}$ of the form:

$$\Phi_{d,q}^{\text{SV}} = \sum_{i=1}^{\infty} \hat{a}_s^i \left(\frac{Q^2(1-x')(1-z')}{\mu^2} \right)^{i\frac{\epsilon}{2}} S_\epsilon^i \left[\frac{(i\epsilon)^2}{4(1-x')(1-z')} \hat{\phi}_{d,q}^{\text{SV},(i)}(\epsilon) \right], \quad (5.35)$$

where

$$\hat{\phi}_{d,q}^{\text{SV},(i)}(\epsilon) = \frac{1}{i\epsilon} \left[\overline{K}_d^{q(i)}(\epsilon) + \overline{G}_{d,\text{SV}}^{q(i)}(\epsilon) \right], \quad (5.36)$$

and for NSV part

$$\begin{aligned} \Phi_{d,q}^{\text{NSV}} &= \sum_{i=1}^{\infty} \hat{a}_s^i \left(\frac{Q^2(1-x')(1-z')}{\mu^2} \right)^{i\frac{\epsilon}{2}} S_\epsilon^i \\ &\times \left[\frac{i\epsilon}{4(1-x')} \hat{\phi}_{d,z',q}^{\text{NSV},(i)}(z', \epsilon) + \frac{i\epsilon}{4(1-z')} \hat{\phi}_{d,x',q}^{\text{NSV},(i)}(x', \epsilon) \right]. \end{aligned} \quad (5.37)$$

Here $S_\epsilon = \exp\left(\frac{\epsilon}{2} [\gamma_E - \ln 4\pi]\right)$ with γ_E being the Euler Mascheroni constant. For reader's convenience, we have listed the results of $\overline{K}_d^{q(i)}$ and $\overline{G}_{d,\text{SV}}^{q(i)}$ in the Appendix-F.2. After substituting them the constants $\hat{\phi}_{d,q}^{\text{SV},(i)}(\epsilon)$ are found to be

$$\hat{\phi}_{d,q}^{\text{SV},(1)}(\epsilon) = \frac{1}{\epsilon^2} \left(2A_1^q \right) + \frac{1}{\epsilon} \left(\overline{\mathcal{G}}_{d,1}^q(\epsilon) \right),$$

$$\begin{aligned}
\hat{\phi}_{d,q}^{\text{SV},(2)}(\epsilon) &= \frac{1}{\epsilon^3} \left(-\beta_0 A_1^q \right) + \frac{1}{\epsilon^2} \left(\frac{1}{2} A_2^q - \beta_0 \bar{\mathcal{G}}_{d,1}^q(\epsilon) \right) + \frac{1}{2\epsilon} \bar{\mathcal{G}}_{d,2}^q(\epsilon), \\
\hat{\phi}_{d,q}^{\text{SV},(3)}(\epsilon) &= \frac{1}{\epsilon^4} \left(\frac{8}{9} \beta_0^2 A_1^q \right) + \frac{1}{\epsilon^3} \left(-\frac{2}{9} \beta_1 A_1^q - \frac{8}{9} \beta_0 A_2^q - \frac{4}{3} \beta_0^2 \bar{\mathcal{G}}_{d,1}^q(\epsilon) \right) \\
&\quad + \frac{1}{\epsilon^2} \left(\frac{2}{9} A_3^q - \frac{1}{3} \beta_1 \bar{\mathcal{G}}_{d,1}^q(\epsilon) - \frac{4}{3} \beta_0 \bar{\mathcal{G}}_{d,2}^q(\epsilon) \right) + \frac{1}{\epsilon} \left(\frac{1}{3} \bar{\mathcal{G}}_{d,3}^q(\epsilon) \right), \\
\hat{\phi}_{d,q}^{\text{SV},(4)}(\epsilon) &= \frac{1}{\epsilon^5} \left(-\beta_0^3 A_1^q \right) + \frac{1}{\epsilon^4} \left(\frac{2}{3} \beta_0 \beta_1 A_1^q + \frac{3}{2} \beta_0^2 A_2^q - 2\beta_0^3 \bar{\mathcal{G}}_{d,1}^q(\epsilon) \right) \\
&\quad - \frac{1}{\epsilon^3} \left(\frac{1}{12} \beta_2 A_1^q - \frac{1}{4} \beta_1 A_2^q - \frac{3}{4} \beta_0 A_3^q + \frac{4}{3} \beta_0 \beta_1 \bar{\mathcal{G}}_{d,1}^q(\epsilon) + 3\beta_0^2 \bar{\mathcal{G}}_{d,2}^q(\epsilon) \right) \\
&\quad + \frac{1}{\epsilon^2} \left(\frac{1}{8} A_4^q - \frac{1}{6} \beta_2 \bar{\mathcal{G}}_{d,1}^q(\epsilon) - \frac{1}{2} \beta_1 \bar{\mathcal{G}}_{d,2}^q(\epsilon) - \frac{3}{2} \beta_0 \bar{\mathcal{G}}_{d,3}^q(\epsilon) \right) + \frac{1}{\epsilon} \left(\frac{1}{4} \bar{\mathcal{G}}_{d,4}^q(\epsilon) \right).
\end{aligned} \tag{5.38}$$

The cusp anomalous dimensions A_i^q in the above equations carry the right sign to cancel all the leading singularities against the form factor contributions in CFs. The ϵ dependent terms $\bar{\mathcal{G}}_{d,i}^q$ originate from $|\hat{F}_q|^2$ as well as the CFs $(\Delta)\mathcal{C}_{J,qq}$ in Eq. (5.30). Using renormalization group invariance and demanding the cancellation of single poles in Eq. (5.38) against the form factor and the AP kernels, we can parameterize $\bar{\mathcal{G}}_{d,i}^q$ as,

$$\bar{\mathcal{G}}_{d,i}^q(\epsilon) = -f_i^q + \bar{\chi}_{d,i}^q + \sum_{j=1}^{\infty} \epsilon^j \bar{\mathcal{G}}_{d,i}^{q,(j)}, \tag{5.39}$$

where

$$\begin{aligned}
\bar{\chi}_{d,1}^q &= 0, \bar{\chi}_{d,2}^q = -2\beta_0 \bar{\mathcal{G}}_{d,1}^{q,(1)}, \bar{\chi}_{d,3}^q = -2\beta_1 \bar{\mathcal{G}}_{d,1}^{q,(1)} - 2\beta_0 \left(\bar{\mathcal{G}}_{d,2}^{q,(1)} + 2\beta_0 \bar{\mathcal{G}}_{d,1}^{q,(2)} \right) \\
\bar{\chi}_{d,4}^q &= -2\beta_2 \bar{\mathcal{G}}_{d,1}^{q,(1)} - 2\beta_1 \left(\bar{\mathcal{G}}_{d,2}^{q,(1)} + 4\beta_0 \bar{\mathcal{G}}_{d,1}^{q,(2)} \right) - 2\beta_0 \left(\bar{\mathcal{G}}_{d,3}^{q,(1)} + 2\beta_0 \bar{\mathcal{G}}_{d,2}^{q,(2)} + 4\beta_0^2 \bar{\mathcal{G}}_{d,1}^{q,(3)} \right).
\end{aligned} \tag{5.40}$$

$$\begin{aligned}
\overline{\mathcal{G}}_{d,1}^{q,(1)} &= C_F \left\{ -\zeta_2 \right\}, & \overline{\mathcal{G}}_{d,1}^{q,(2)} &= C_F \left\{ \frac{1}{3}\zeta_3 \right\}, \\
\overline{\mathcal{G}}_{d,1}^{q,(3)} &= C_F \left\{ \frac{1}{80}\zeta_2^2 \right\}, & \overline{\mathcal{G}}_{d,1}^{q,(4)} &= C_F \left\{ \frac{1}{20}\zeta_5 - \frac{1}{24}\zeta_2\zeta_3 \right\}, \\
\overline{\mathcal{G}}_{d,1}^{q,(5)} &= C_F \left\{ \frac{1}{144}\zeta_3^2 - \frac{1}{896}\zeta_2^3 \right\}, \\
\overline{\mathcal{G}}_{d,2}^{q,(1)} &= C_F n_f \left\{ -\frac{328}{81} + \frac{8}{3}\zeta_3 + \frac{10}{3}\zeta_2 \right\} + C_F C_A \left\{ \frac{2428}{81} - \frac{44}{3}\zeta_3 - \frac{67}{3}\zeta_2 - 4\zeta_2^2 \right\}, \\
\overline{\mathcal{G}}_{d,2}^{q,(2)} &= C_F n_f \left\{ \frac{976}{243} - \frac{70}{27}\zeta_3 - \frac{28}{9}\zeta_2 + \frac{29}{60}\zeta_2^2 \right\} - C_F C_A \left\{ \frac{7288}{243} - 43\zeta_5 - \frac{469}{27}\zeta_3 \right. \\
&\quad \left. - \frac{202}{9}\zeta_2 + \frac{71}{3}\zeta_2\zeta_3 + \frac{319}{120}\zeta_2^2 \right\}, \\
\overline{\mathcal{G}}_{d,3}^{q,(1)} &= C_F n_f^2 \left\{ \frac{11584}{2187} - \frac{320}{81}\zeta_3 - \frac{316}{27}\zeta_2 + \frac{152}{45}\zeta_2^2 \right\} - C_F^2 n_f \left\{ \frac{42727}{324} - \frac{112}{3}\zeta_5 \right. \\
&\quad \left. - \frac{1672}{27}\zeta_3 - \frac{275}{6}\zeta_2 + 40\zeta_2\zeta_3 - \frac{152}{15}\zeta_2^2 \right\} + C_F C_A^2 \left\{ \frac{7135981}{8748} - \frac{1430}{3}\zeta_5 - 936\zeta_3 \right. \\
&\quad \left. + \frac{536}{3}\zeta_3^2 - \frac{379417}{486}\zeta_2 + \frac{4136}{9}\zeta_2\zeta_3 + \frac{1538}{45}\zeta_2^2 + \frac{17392}{315}\zeta_2^3 \right\} \\
&\quad - C_F C_A n_f \left\{ \frac{716509}{4374} - \frac{148}{3}\zeta_5 - \frac{12356}{81}\zeta_3 - \frac{51053}{243}\zeta_2 + \frac{392}{9}\zeta_2\zeta_3 + \frac{1372}{45}\zeta_2^2 \right\}.
\end{aligned} \tag{5.41}$$

Here, $C_A = N_c$ and $C_F = \frac{N_c^2-1}{2N_c}$ are the quadratic Casimirs of the adjoint and fundamental representations of $SU(N_c)$, respectively, while n_f denoted the number of quark flavors. Note, that the constants in Eq. (5.41) are also related to the threshold exponent $\mathbf{D}^q(a_s(q^2(1-z)^2))$ via Eq. (46) of [423].

The results for $\overline{\mathcal{G}}_{d,i}^{q,(j)}$ for $i = 1, 2$ have been obtained from the NLO and NNLO CFs expanded to sufficient order in ϵ [109, 171, 175]. We find that these results are identical to the corresponding ones for the rapidity distribution of pairs of leptons in DY production [272–274, 405, 424, 441, 470, 496–499], see also [150, 404, 405], where a conjecture on the relation between these two processes in the threshold limit had

been proposed. Assuming that this conjecture holds true beyond NNLO, we have used $\overline{\mathcal{G}}_{d,3}^{q,(1)}$ of the rapidity distribution for the DY process also for SIDIS at N³LO.

The all order result given in Eq. (5.35) is useful to obtain predictions for the SV part of the CFs order by order a_s . However, to study the numerical impact of the all order result, we need to perform a resummation in Mellin space. This can be achieved by expressing the summations given in Eq. (5.35) in the integral form. The integral representation for $\Phi_{d,q}^{\text{SV}}$ for the DY process is given in [272] and the same can be used for SIDIS in Eq. (5.35):

$$\begin{aligned} \Phi_{d,q}^{\text{SV}}(\hat{a}_s, Q^2, \mu^2, x', z', \epsilon) = & \left[\frac{1}{2} \delta(\bar{z}') \left(\frac{1}{\bar{x}'} \left\{ \int_{\mu_F^2}^{Q^2 \bar{x}'} \frac{d\lambda^2}{\lambda^2} A^q(a_s(\lambda^2)) + \overline{G}_d^q(a_s(Q^2 \bar{x}'), \epsilon) \right\} \right) \right]_+ \\ & + Q^2 \frac{d}{dQ^2} \left[\left(\frac{1}{4\bar{x}'\bar{z}'} \left\{ \int_{\mu_F^2}^{Q^2 \bar{x}'\bar{z}'} \frac{d\lambda^2}{\lambda^2} A^q(a_s(\lambda^2)) + \overline{G}_d^q(a_s(Q^2 \bar{x}'\bar{z}'), \epsilon) \right\} \right) \right]_+ \\ & + \frac{1}{2} \delta(\bar{x}') \delta(\bar{z}') \sum_{i=1}^{\infty} \hat{a}_s^i \left(\frac{Q^2}{\mu^2} \right)^{i\frac{\epsilon}{2}} S_\epsilon^i \hat{\phi}_{d,q}^{\text{SV},(i)}(\epsilon) \\ & + \frac{1}{2} \delta(\bar{z}') \left(\frac{1}{\bar{x}'} \right)_+ \sum_{i=1}^{\infty} \hat{a}_s^i \left(\frac{\mu_F^2}{\mu^2} \right)^{i\frac{\epsilon}{2}} S_\epsilon^i \overline{K}_d^{q,(i)}(\epsilon) \Big] + (x' \leftrightarrow z'), \quad (5.42) \end{aligned}$$

In complete analogy to the SV part, using the renormalization group, the coefficients $\hat{\varphi}_{d,\xi,q}^{\text{NSV},(i)}$ in the NSV solution $\Phi_{d,q}^{\text{NSV}}$, Eq. (5.37) can be expanded as follows, for $\xi = x', z'$,

$$\begin{aligned} \hat{\varphi}_{d,\xi,q}^{\text{NSV},(1)}(\xi, \epsilon) &= \frac{1}{\epsilon} \overline{\mathcal{G}}_{d,\xi,1}^q(\xi, \epsilon), \\ \hat{\varphi}_{d,\xi,q}^{\text{NSV},(2)}(\xi, \epsilon) &= \frac{1}{\epsilon^2} (-\beta_0 \overline{\mathcal{G}}_{d,\xi,1}^q(\xi, \epsilon)) + \frac{1}{2\epsilon} \overline{\mathcal{G}}_{d,\xi,2}^q(\xi, \epsilon), \\ \hat{\varphi}_{d,\xi,q}^{\text{NSV},(3)}(\xi, \epsilon) &= \frac{1}{\epsilon^3} \left(\frac{4}{3} \beta_0^2 \overline{\mathcal{G}}_{d,\xi,1}^q(\xi, \epsilon) \right) + \frac{1}{\epsilon^2} \left(-\frac{1}{3} \beta_1 \overline{\mathcal{G}}_{d,\xi,1}^q(\xi, \epsilon) - \frac{4}{3} \beta_0 \overline{\mathcal{G}}_{d,\xi,2}^q(\xi, \epsilon) \right) \\ &\quad + \frac{1}{3\epsilon} \overline{\mathcal{G}}_{d,\xi,3}^q(\xi, \epsilon), \\ \hat{\varphi}_{d,\xi,q}^{\text{NSV},(4)}(\xi, \epsilon) &= \frac{1}{\epsilon^4} (-2\beta_0^3 \overline{\mathcal{G}}_{d,\xi,1}^q(\xi, \epsilon)) + \frac{1}{\epsilon^3} \left(\frac{4}{3} \beta_0 \beta_1 \overline{\mathcal{G}}_{d,\xi,1}^q(\xi, \epsilon) + 3\beta_0^2 \overline{\mathcal{G}}_{d,\xi,2}^q(\xi, \epsilon) \right) \\ &\quad + \frac{1}{\epsilon^2} \left(-\frac{1}{6} \beta_2 \overline{\mathcal{G}}_{d,\xi,1}^q(\xi, \epsilon) - \frac{1}{2} \beta_1 \overline{\mathcal{G}}_{d,\xi,2}^q(\xi, \epsilon) - \frac{3}{2} \beta_0 \overline{\mathcal{G}}_{d,\xi,3}^q(\xi, \epsilon) \right) \end{aligned}$$

$$+ \frac{1}{4\epsilon} \bar{\mathcal{G}}_{d,\xi,4}^q(\xi, \epsilon). \quad (5.43)$$

In order to cancel the collinear poles from the AP kernels, the quantities $\bar{\mathcal{G}}_{d,\xi,i}^q(\xi, \epsilon)$ can be further decomposed as

$$\begin{aligned} \bar{\mathcal{G}}_{d,x',i}^q(x', \epsilon) &= 2L_i^q(x') + \bar{\chi}_{d,x',i}^q(x') + \sum_{j=1}^{\infty} \epsilon^j \bar{\mathcal{G}}_{d,x',i}^{q,(j)}(x'), \\ \bar{\mathcal{G}}_{d,z',i}^q(z', \epsilon) &= 2\tilde{L}_i^q(z') + \bar{\chi}_{d,z',i}^q(z') + \sum_{j=1}^{\infty} \epsilon^j \bar{\mathcal{G}}_{d,z',i}^{q,(j)}(z') \end{aligned} \quad (5.44)$$

with $L_i^q(x') = C_i^q \ln(1 - x') + D_i^q$ and $\tilde{L}_i^q(z') = \tilde{C}_i^q \ln(1 - z') + \tilde{D}_i^q$ and

$$\bar{\chi}_{d,\xi,i}^q(\xi) = \bar{\chi}_{d,i}^q \Big|_{(\bar{\mathcal{G}}_{d,i}^{q,(j)} \rightarrow \bar{\mathcal{G}}_{d,\xi,i}^{q,(j)}(\xi))}, \quad (5.45)$$

where $\bar{\chi}_{d,i}^q$ is given in Eq. (5.40). The coefficients $C_i^q(\tilde{C}_i^q)$ and $D_i^q(\tilde{D}_i^q)$ are related to the cusp A_i^q and virtual B_i^q anomalous dimensions in the following way [265, 500–502], see also [503]. For space-like splitting functions one has

$$\begin{aligned} C_1^q &= 0, & C_2^q &= (A_1^q)^2, & C_3^q &= 2A_1^q A_2^q, \\ C_4^q &= (A_2^q)^2 + 2A_1^q A_3^q, \end{aligned} \quad (5.46)$$

$$\begin{aligned} D_1^q &= -A_1^q, & D_2^q &= -A_2^q - A_1^q(-B_1^q + \beta_0), \\ D_3^q &= -A_3^q - A_1^q(-B_2^q + \beta_1) - A_2^q(-B_1^q + \beta_0), \\ D_4^q &= -A_4^q - A_1^q(-B_3^q + \beta_2) - A_2^q(-B_2^q + \beta_1) - A_3^q(-B_1^q + \beta_0). \end{aligned} \quad (5.47)$$

and for the time-like ones,

$$\begin{aligned} \tilde{C}_1^q &= 0, & \tilde{C}_2^q &= -\left(A_1^q\right)^2, & \tilde{C}_3^q &= -2A_1^q A_2^q, \\ \tilde{C}_4^q &= -\left(A_2^q\right)^2 - 2A_1^q A_3^q, \end{aligned} \quad (5.48)$$

$$\begin{aligned}
\tilde{D}_1^q &= -A_1^q, & \tilde{D}_2^q &= -A_2^q - A_1^q(B_1^q + \beta_0), \\
\tilde{D}_3^q &= -A_3^q - A_1^q(B_2^q + \beta_1) - A_2^q(B_1^q + \beta_0), \\
\tilde{D}_4^q &= -A_4^q - A_1^q(B_3^q + \beta_2) - A_2^q(B_2^q + \beta_1) - A_3^q(B_1^q + \beta_0).
\end{aligned} \tag{5.49}$$

The renormalised coefficients $\overline{\mathcal{G}}_{d,\xi,i}^{q,(j)}(\xi)$ in the above equations are parametrized in terms of $\ln^k(1-\xi)$, $k = 0, 1, \dots$ and all the terms vanishing as $\xi \rightarrow 1$ are dropped

$$\overline{\mathcal{G}}_{d,\xi,i}^{q,(j)}(\xi) = \sum_{k=0}^{i+j-1} \overline{\mathcal{G}}_{d,\xi,i}^{q,(j,k)} \ln^k(1-\xi). \tag{5.50}$$

The leading term in $\ln(1-\xi)$ at every order in a_s depends on the power of a_s , but also the power of ϵ . The leading power of $\ln(1-\xi)$ can be determined by expanding the partonic cross sections to high accuracy in ϵ at every order in a_s . One can also use the mass factorised results such as the CFs to determine them. In the former approach, we have computed the partonic cross section at NLO to an accuracy of ϵ up to third order and at NNLO to first power in ϵ . We expect that the observed pattern for those logarithms persists at higher orders and we can extrapolate to all orders in $\hat{a}_s$ and ϵ by fixing the highest power for $\ln(1-\xi)$ to be $i+j-1$ in Eq. (5.50).

For a resummation to all orders an integral form for $\Phi_{d,q}^{\text{NSV}}$ is needed to study its numerical impact. In order to do this, we decompose $\Phi_{d,q}^{\text{NSV}}$ as a sum of a singular part and a finite part. The singular part can be obtained by setting all the terms to zero in Eq. (5.44) except the first one, $2L_i^q$ and $2\tilde{L}_i^q$. It contains the correct terms that will cancel against NSV terms of the AP kernels. We write $\Phi_{d,q}^{\text{NSV}} = \Phi_{d,q,s}^{\text{NSV}} + \Phi_{d,q,f}^{\text{NSV}}$, where the first term is singular as $\epsilon \rightarrow 0$ and contains only L_i^q as well as $\tilde{L}_i^q$ and the second one contains the finite remainder. This decomposition facilitates to express $\Phi_{d,q}^{\text{NSV}}$ in an integral form as follows:

$$\Phi_{d,q}^{\text{NSV}} = \frac{1}{2} \delta(\bar{x}') \int_{\mu_F^2}^{Q^2 \bar{z}'} \frac{d\lambda^2}{\lambda^2} \tilde{L}^q(a_s(\lambda^2), z') + \frac{1}{2} \left(\frac{1}{\bar{x}'} \tilde{L}^q(a_s(Q^2 \bar{x}' \bar{z}'), z') \right)_+$$

$$\begin{aligned}
& + \frac{1}{2} \delta(\bar{x}') \varphi_{d,z',f}^q(a_s(Q^2 \bar{z}'), z') + \frac{1}{2} \left(\frac{1}{\bar{x}'} Q^2 \frac{d}{dQ^2} \varphi_{d,z',f}^q(a_s(Q^2 \bar{x}' \bar{z}'), z') \right) + \\
& + \frac{1}{2} \delta(\bar{x}') \sum_{i=1}^{\infty} \hat{a}_s^i \left(\frac{\mu_F^2}{\mu^2} \right)^{i \frac{\epsilon}{2}} S_{\epsilon}^i \varphi_{d,z',s}^{(i)}(z', \epsilon) + \left(\tilde{L}^q \leftrightarrow L^q, x' \leftrightarrow z' \right). \quad (5.51)
\end{aligned}$$

In the above equation, the term containing $\varphi_{d,\xi,s}^{(i)}$ is singular while the remaining ones are all finite as $\epsilon \rightarrow 0$. The fact that $\Phi_{d,q}^{\text{NSV}}$ is renormalization group invariant implies that $\varphi_{d,\xi,s}^q(a_s(\mu_F^2), \xi) = \sum_{i=1}^{\infty} \hat{a}_s^i \left(\frac{\mu_F^2}{\mu^2} \right)^{i \frac{\epsilon}{2}} S_{\epsilon}^i \varphi_{d,\xi,s}^{(i)}(\xi, \epsilon)$ satisfies the equations

$$\begin{aligned}
\mu_F^2 \frac{d}{d\mu_F^2} \varphi_{d,x',s}^q(a_s(\mu_F^2), x') &= L^q(a_s(\mu_F^2), x'), \\
\mu_F^2 \frac{d}{d\mu_F^2} \varphi_{d,z',s}^q(a_s(\mu_F^2), z') &= \tilde{L}^q(a_s(\mu_F^2), z'), \quad (5.52)
\end{aligned}$$

where

$$L^q(a_s(\mu_F^2), x') = \sum_{i=1}^{\infty} a_s^i(\mu_F^2) L_i^q(x'), \quad \tilde{L}^q(a_s(\mu_F^2), z') = \sum_{i=1}^{\infty} a_s^i(\mu_F^2) \tilde{L}_i^q(z'). \quad (5.53)$$

Having fixed the divergent part of $\Phi_{d,q}^{\text{NSV}}$ completely, we need to understand all order structure of the finite piece $\varphi_{d,\xi,f}^q$. Using Eq. (5.50), we can expand this functions in powers of renormalised coupling a_s :

$$\varphi_{d,\xi,f}^q(a_s(\lambda^2), \xi) = \sum_{i=1}^{\infty} a_s^i(\lambda^2) \sum_{k=0}^i \bar{\varphi}_{q,\xi,i}^{(k)} \ln^k(1 - \xi), \quad (5.54)$$

where the highest power of $\ln(1 - \xi)$ aligns at each order in a_s with that in Eq. (5.50). The coefficients $\bar{\varphi}_{q,\xi,i}^{(k)}$ can be expressed in terms of their unrenormalised counter part $\bar{\mathcal{G}}_{d,\xi,i}^{q,(j,k)}$'s in Eq. (5.50) as:

$$\begin{aligned}
\bar{\varphi}_{q,\xi,1}^{(k)} &= \bar{\mathcal{G}}_{d,\xi,1}^{q,(1,k)}, \quad k = 0, 1 \\
\bar{\varphi}_{q,\xi,2}^{(k)} &= \left(\frac{1}{2} \bar{\mathcal{G}}_{d,\xi,2}^{q,(1,k)} + \beta_0 \bar{\mathcal{G}}_{d,\xi,1}^{q,(2,k)} \right), \quad k = 0, 1, 2 \\
\bar{\varphi}_{q,\xi,3}^{(k)} &= \left(\frac{1}{3} \bar{\mathcal{G}}_{d,\xi,3}^{q,(1,k)} + \frac{2}{3} \beta_1 \bar{\mathcal{G}}_{d,\xi,1}^{q,(2,k)} + \frac{2}{3} \beta_0 \bar{\mathcal{G}}_{d,\xi,2}^{q,(2,k)} + \frac{4}{3} \beta_0^2 \bar{\mathcal{G}}_{d,\xi,1}^{q,(3,k)} \right), \quad k = 0, 1, 2, 3
\end{aligned}$$

$$\begin{aligned}\overline{\varphi}_{q,\xi,4}^{(k)} = & \left(\frac{1}{4}\overline{\mathcal{G}}_{d,\xi,4}^{q,(1,k)} + \frac{1}{2}\beta_2\overline{\mathcal{G}}_{d,\xi,1}^{q,(2,k)} + \frac{1}{2}\beta_1\overline{\mathcal{G}}_{d,\xi,2}^{q,(2,k)} + \frac{1}{2}\beta_0\overline{\mathcal{G}}_{d,\xi,3}^{q,(2,k)} + 2\beta_0\beta_1\overline{\mathcal{G}}_{d,\xi,1}^{q,(3,k)} \right. \\ & \left. + \beta_0^2\overline{\mathcal{G}}_{d,\xi,2}^{q,(3,k)} + 2\beta_0^3\overline{\mathcal{G}}_{d,\xi,1}^{q,(4,k)} \right), \quad k = 0, 1, 2, 3, 4 \quad (5.55)\end{aligned}$$

The structure of divergent and finite pieces of $\Phi_{d,q}^{\text{NSV}}$ allows us to determine the coefficients $\overline{\mathcal{G}}_{d,\xi,i}^{q,(j,k)}$. Since our final result depends on $\overline{\varphi}_{q,\xi,i}^{(k)}$ we can directly determine them by comparison with the fixed order results for the CFs, known to NNLO level [171–173, 175, 176, 184] and they are listed below:

$$\begin{aligned}\overline{\varphi}_{q,x',1}^{(0)} &= C_F \left\{ -4 \right\}, \quad \overline{\varphi}_{q,x',1}^{(1)} = 0, \\ \overline{\varphi}_{q,x',2}^{(0)} &= C_F C_A \left\{ \frac{1108}{27} - 28\zeta_3 - \frac{44}{3}\zeta_2 \right\} - C_F n_f \left\{ \frac{52}{27} - \frac{8}{3}\zeta_2 \right\} - C_F^2 \left\{ 8\zeta_2 \right\}, \\ \overline{\varphi}_{q,x',2}^{(1)} &= C_F C_A \left\{ -10 \right\} + C_F^2 \left\{ 10 \right\}, \quad \overline{\varphi}_{q,x',2}^{(2)} = C_F^2 \left\{ 4 \right\}, \quad (5.56)\end{aligned}$$

$$\begin{aligned}\overline{\varphi}_{q,z',1}^{(0)} &= C_F \left\{ 4 \right\}, \quad \overline{\varphi}_{q,z',1}^{(1)} = 0, \\ \overline{\varphi}_{q,z',2}^{(0)} &= C_F C_A \left\{ \frac{1492}{27} - 28\zeta_3 - \frac{68}{3}\zeta_2 \right\} - C_F n_f \left\{ \frac{364}{27} - \frac{8}{3}\zeta_2 \right\} - C_F^2 \left\{ 16\zeta_2 \right\}, \\ \overline{\varphi}_{q,z',2}^{(1)} &= C_F C_A \left\{ 10 \right\} - C_F^2 \left\{ 10 \right\}, \quad \overline{\varphi}_{q,z',2}^{(2)} = C_F^2 \left\{ -4 \right\}, \quad (5.57)\end{aligned}$$

Note that the constants $\overline{\varphi}_{q,x',i}^{(k)}$ are different from $\overline{\varphi}_{q,z',i}^{(k)}$ unlike those that appearing in rapidity distributions of the DY process, see [274].

In this section, we established the master formula for the diagonal coefficient functions and analyzed its constituent building blocks, namely the quark form factor, the mass-factorization kernels, and the soft function. We reviewed the renormalization group equations and differential equations governing each of these ingredients, highlighting their universal infrared structure. Exploiting these properties together with the known fixed-order results, we derived the all-order structure of the soft-virtual (SV) and next-to-soft-virtual (NSV) contributions to the soft function. Furthermore, we obtained integral representations for both the SV and NSV exponents, which pro-

vide the foundation for the Mellin-space threshold resummation developed in the following section.

5.4 All order result

Having established the all-order structure of the constituent building blocks of the master formula, we now combine them to obtain the all-order expression for the diagonal coefficient functions. Substituting the integral representations for $\Phi_{d,q}^{\text{SV}}$ in Eq. (5.42), for $\Phi_{d,q}^{\text{NSV}}$ in Eq. (5.51), the solutions to the form factor in Eq. (5.24) and the AP kernels in Eq. (5.26) into Eq. (5.17). We find that all the soft and collinear singularities cancel among themselves leaving SV and NSV parts of the CFs IR finite.

$$(\Delta)\mathcal{C}_{J,qq}^{\text{SV+NSV}} = \mathcal{C} \exp \left(\Psi_d^q(Q^2, \mu_F^2, x', z', \epsilon) \right) \Big|_{\epsilon=0}, \quad (5.58)$$

where the IR finite expression Ψ_d^q takes a simple form

$$\begin{aligned} \Psi_d^q = & \frac{\delta(\bar{x}')}{2} \left(\int_{\mu_F^2}^{Q^2 \bar{z}'} \frac{d\lambda^2}{\lambda^2} \tilde{\mathcal{P}}^q(a_s(\lambda^2), \bar{z}') + \mathcal{Q}^q(a_s(Q_2^2), \bar{z}') \right)_+ \\ & + \frac{1}{4} \left(\frac{1}{\bar{x}'} \left\{ \tilde{\mathcal{P}}^q(a_s(Q_{12}^2), \bar{z}') + 2\tilde{L}^q(a_s(Q_{12}^2), \bar{z}') \right. \right. \\ & \left. \left. + Q^2 \frac{d}{dQ^2} \left(\mathcal{Q}^q(a_s(Q_2^2), \bar{z}') + 2\varphi_{d,z',f}^q(a_s(Q_2^2), \bar{z}') \right) \right\} \right)_+ \\ & + \frac{1}{2} \delta(\bar{x}') \delta(\bar{z}') \ln \left(g_{d,0}^q(a_s(\mu_F^2)) \right) + (x' \leftrightarrow z'). \end{aligned} \quad (5.59)$$

Here, we use the short-hands $\bar{x}' = (1 - x')$ and $\bar{z}' = (1 - z')$, $Q_1^2 = Q^2 \bar{x}'$, $Q_2^2 = Q^2 \bar{z}'$ and $Q_{12}^2 = Q^2 \bar{x}' \bar{z}'$. The subscript $+$ indicates the standard plus distribution. In the

above equation, $\mathcal{P}^q, \tilde{\mathcal{P}}^q$ are related diagonal splitting functions given in Eq. (5.28),

$$\begin{aligned}\mathcal{P}^q(a_s, \bar{x}') &= P_{q \leftarrow q}(\mu_s^2, \bar{x}') - 2B^q(a_s)\delta(\bar{x}'), \\ \tilde{\mathcal{P}}^q(a_s, \bar{z}') &= \tilde{P}_{q \leftarrow q}(\mu_s^2, \bar{z}') - 2B^q(a_s)\delta(\bar{z}'),\end{aligned}\tag{5.60}$$

and $\mathcal{Q}_d^q(a_s, \bar{z}') = \frac{2}{\bar{z}'} G_d^q(a_s) + 2 \varphi_{d,z',f}^q(a_s, \bar{z}')$ and similar for x' . Note that $g_{d,0}^q$ is process-dependent and receives contributions only from the form factor and finite parts of $\Phi_{d,q}^{\text{SV}}$.

The result for $(\Delta)\mathcal{C}_{J,qq}^{\text{SV+NSV}}$ in Eq. (5.59) is valid to all orders in a_s . The exponent Ψ_d^q contains universal (process independent) quantities such as the QCD β function and anomalous dimensions A^q, B^q, f^q etc. and process dependent quantities $G_d^q, \varphi_{d,\xi,f}^q$ and $g_{d,0}^q$. Each of them can be expanded in powers of a_s , hence Ψ_d^q is expanded as

$$\Psi_d^q(Q^2, \mu_F^2) = \sum_{i=1}^{\infty} a_s^i(\mu_R^2) \Psi_d^{q,(i)}(Q^2, \mu_F^2, \mu_R^2),\tag{5.61}$$

where we have suppressed the dependence on x', z' in Ψ_d^q and $\Psi_d^{q,(i)}$.

The result in Eq. (5.58) is the main result. It sums up towers of SV and NSV terms to all orders in a_s in those CFs, which dominate near threshold. The particular logarithmic structure of Ψ_d^q given in Eq. (5.59) allows us to predict certain SV and NSV terms to any order in a_s , i.e., a_s^n for the diagonal CFs for all $n \geq 1$, provided Ψ_d^q is known up to order a_s^m with $n > m$. The achievable accuracy of those predictions for $\Psi_d^{q,(i)}$ s for $i = 1, 2, 3$ and for general $i = n$ is summarized in Tabs. 5.1 and 5.2. For example, if we know only $\Psi_d^{q,(1)}$, we can predict the following terms for $(\Delta)\mathcal{C}_{J,cc}^{(2)}$, i.e., for the SV part, $\{\delta_{\bar{x}'} \mathcal{D}_{\bar{z}'}^3, \delta_{\bar{z}'} \mathcal{D}_{\bar{x}'}^3\}$ and $\{\mathcal{D}_{\bar{x}'}^i \mathcal{D}_{\bar{z}'}^j\}$ for $i + j = 2$ and, likewise, for the NSV one $\{\delta_{\bar{x}'} \mathcal{L}_{\bar{z}'}^3, \delta_{\bar{z}'} \mathcal{L}_{\bar{x}'}^3\}$, and $\{\mathcal{D}_{\bar{x}'}^i \mathcal{L}_{\bar{z}'}^j, \mathcal{D}_{\bar{z}'}^i \mathcal{L}_{\bar{x}'}^j\}$ for $i + j = 2$. If, in addition, we allow for terms present in $\Psi_d^{q,(2)}$ which depend only on information about $\Psi_d^{q,(1)}$, then, because of the renormalization group equations, we can predict, for the SV part also $\{\delta_{\bar{x}'} \mathcal{D}_{\bar{z}'}^2, \delta_{\bar{z}'} \mathcal{D}_{\bar{x}'}^2\}$ and $\{\mathcal{D}_{\bar{x}'}^i \mathcal{D}_{\bar{z}'}^j\}$ for $i + j = 1$, and for the NSV

GIVEN				PREDICTIONS FOR SV		
$\Psi_d^{q,(1)}$	$\Psi_d^{q,(2)}$	$\Psi_d^{q,(3)}$	$\Psi_d^{q,(n)}$	$(\Delta)\mathcal{C}_{J,cc}^{(2)}$	$(\Delta)\mathcal{C}_{J,cc}^{(3)}$	$(\Delta)\mathcal{C}_{J,cc}^{(i)}$
$\delta_{\bar{x}'}\delta_{\bar{z}'}^j, \mathcal{D}_{\bar{x}'}^j\mathcal{D}_{\bar{z}'}^k$ $\mathcal{D}_{\bar{x}'}^{j'}\delta_{\bar{z}'}^j, \mathcal{D}_{\bar{z}'}^{j'}\delta_{\bar{x}'}^k$ $j+k=0$ $j'=1,0$				$\mathcal{D}_{\bar{x}'}^j\mathcal{D}_{\bar{z}'}^k,$ $\mathcal{D}_{\bar{x}'}^{j'}\delta_{\bar{z}'}^j, \mathcal{D}_{\bar{z}'}^{j'}\delta_{\bar{x}'}^k$ $j+k=2,1$ $j'=3,2$	$\mathcal{D}_{\bar{x}'}^j\mathcal{D}_{\bar{z}'}^k,$ $\mathcal{D}_{\bar{x}'}^{j'}\delta_{\bar{z}'}^j, \mathcal{D}_{\bar{z}'}^{j'}\delta_{\bar{x}'}^k$ $j+k=4,3$ $j'=5,4$	$\mathcal{D}_{\bar{x}'}^j\mathcal{D}_{\bar{z}'}^k, \mathcal{D}_{\bar{x}'}^{j'}\delta_{\bar{z}'}^j, \mathcal{D}_{\bar{z}'}^{j'}\delta_{\bar{x}'}^k$ $j+k=2i-2, 2i-3$ $j'=2i-1, 2i-2$
	$\delta_{\bar{x}'}\delta_{\bar{z}'}^j, \mathcal{D}_{\bar{x}'}^j\mathcal{D}_{\bar{z}'}^k$ $\mathcal{D}_{\bar{x}'}^{j'}\delta_{\bar{z}'}^j, \mathcal{D}_{\bar{z}'}^{j'}\delta_{\bar{x}'}^k$ $j+k=2,1,0$ $j'=3,\dots,0$				$\mathcal{D}_{\bar{x}'}^j\mathcal{D}_{\bar{z}'}^k,$ $\mathcal{D}_{\bar{x}'}^{j'}\delta_{\bar{z}'}^j, \mathcal{D}_{\bar{z}'}^{j'}\delta_{\bar{x}'}^k$ $j+k=4,3,2,1$ $j'=5,4,3,2$	$\mathcal{D}_{\bar{x}'}^j\mathcal{D}_{\bar{z}'}^k, \mathcal{D}_{\bar{x}'}^{j'}\delta_{\bar{z}'}^j, \mathcal{D}_{\bar{z}'}^{j'}\delta_{\bar{x}'}^k$ $j+k=2i-2,\dots,2i-4,2i-5$ $j'=2i-1,\dots,2i-3,2i-4$
		$\delta_{\bar{x}'}\delta_{\bar{z}'}^j, \mathcal{D}_{\bar{x}'}^j\mathcal{D}_{\bar{z}'}^k$ $\mathcal{D}_{\bar{x}'}^{j'}\delta_{\bar{z}'}^j, \mathcal{D}_{\bar{z}'}^{j'}\delta_{\bar{x}'}^k$ $j+k=4,\dots,0$ $j'=5,\dots,0$				$\mathcal{D}_{\bar{x}'}^j\mathcal{D}_{\bar{z}'}^k, \mathcal{D}_{\bar{x}'}^{j'}\delta_{\bar{z}'}^j, \mathcal{D}_{\bar{z}'}^{j'}\delta_{\bar{x}'}^k$ $j+k=2i-2,\dots,2i-5,\dots,2i-7$ $j'=2i-1,\dots,2i-4,\dots,2i-6$
			$\delta_{\bar{x}'}\delta_{\bar{z}'}^j, \mathcal{D}_{\bar{x}'}^j\mathcal{D}_{\bar{z}'}^k$ $\mathcal{D}_{\bar{x}'}^{j'}\delta_{\bar{z}'}^j, \mathcal{D}_{\bar{z}'}^{j'}\delta_{\bar{x}'}^k$ $j+k=2n-2,\dots,0$ $j'=2n-1,\dots,0$			$\mathcal{D}_{\bar{x}'}^j\mathcal{D}_{\bar{z}'}^k, \mathcal{D}_{\bar{x}'}^{j'}\delta_{\bar{z}'}^j, \mathcal{D}_{\bar{z}'}^{j'}\delta_{\bar{x}'}^k$ $j+k=2i-2,\dots,2i-n-2,\dots,2i-2n-1$ $j'=2i-1,\dots,2i-n-1,\dots,2i-2n$

Table 5.1: Towers of SV Distributions $(\delta_{\bar{x}'}, \delta_{\bar{z}'}, \mathcal{D}_{\bar{x}'}, \mathcal{D}_{\bar{z}'})$ that can be predicted for $(\Delta)\mathcal{C}_{J,cc}^{(i)}$ for $c = q, \bar{q}$ given $\Psi_d^{q,(n)}$, $j, k \geq 0$ and $\delta_{\bar{\xi}} = \delta(1 - \xi)$, $\mathcal{D}_{\bar{\xi}}^j = \left[\frac{\ln^j(1-\xi)}{1-\xi} \right]_+$ with $\xi = x', z'$.

GIVEN, SV +				PREDICTIONS FOR NSV		
$\Psi_d^{q,(1)}$	$\Psi_d^{q,(2)}$	$\Psi_d^{q,(3)}$	$\Psi_d^{q,(n)}$	$(\Delta)\mathcal{C}_{J,cc}^{(2)}$	$(\Delta)\mathcal{C}_{J,cc}^{(3)}$	$(\Delta)\mathcal{C}_{J,cc}^{(i)}$
$\mathcal{L}_{\bar{x}'}^{j'}\delta_{\bar{z}'}^j, \mathcal{L}_{\bar{z}'}^{j'}\delta_{\bar{x}'}^k$ $\mathcal{D}_{\bar{x}'}^j\mathcal{L}_{\bar{z}'}^k,$ $\mathcal{D}_{\bar{z}'}^j\mathcal{L}_{\bar{x}'}^k$ $j+k=0$ $j'=1,0$				$\mathcal{D}_{\bar{x}'}^j\mathcal{L}_{\bar{z}'}^k, \mathcal{D}_{\bar{z}'}^j\mathcal{L}_{\bar{x}'}^k$ $\mathcal{L}_{\bar{x}'}^{j'}\delta_{\bar{z}'}^j, \mathcal{L}_{\bar{z}'}^{j'}\delta_{\bar{x}'}^k$ $j+k=2$ $j'=3$	$\mathcal{D}_{\bar{x}'}^j\mathcal{L}_{\bar{z}'}^k, \mathcal{D}_{\bar{z}'}^j\mathcal{L}_{\bar{x}'}^k$ $\mathcal{L}_{\bar{x}'}^{j'}\delta_{\bar{z}'}^j, \mathcal{L}_{\bar{z}'}^{j'}\delta_{\bar{x}'}^k$ $j+k=4$ $j'=5$	$\mathcal{D}_{\bar{x}'}^j\mathcal{L}_{\bar{z}'}^k, \mathcal{D}_{\bar{z}'}^j\mathcal{L}_{\bar{x}'}^k, \mathcal{L}_{\bar{x}'}^{j'}\delta_{\bar{z}'}^j, \mathcal{L}_{\bar{z}'}^{j'}\delta_{\bar{x}'}^k$ $j+k=2i-2$ $j'=2i-1$
	$\mathcal{L}_{\bar{x}'}^{j'}\delta_{\bar{z}'}^j, \mathcal{L}_{\bar{z}'}^{j'}\delta_{\bar{x}'}^k$ $\mathcal{D}_{\bar{x}'}^j\mathcal{L}_{\bar{z}'}^k,$ $\mathcal{D}_{\bar{z}'}^j\mathcal{L}_{\bar{x}'}^k$ $j+k=2,1,0$ $j'=3,\dots,0$				$\mathcal{D}_{\bar{x}'}^j\mathcal{L}_{\bar{z}'}^k, \mathcal{D}_{\bar{z}'}^j\mathcal{L}_{\bar{x}'}^k$ $\mathcal{L}_{\bar{x}'}^{j'}\delta_{\bar{z}'}^j, \mathcal{L}_{\bar{z}'}^{j'}\delta_{\bar{x}'}^k$ $j+k=4,3,2$ $j'=5,4$	$\mathcal{D}_{\bar{x}'}^j\mathcal{L}_{\bar{z}'}^k, \mathcal{D}_{\bar{z}'}^j\mathcal{L}_{\bar{x}'}^k, \mathcal{L}_{\bar{x}'}^{j'}\delta_{\bar{z}'}^j, \mathcal{L}_{\bar{z}'}^{j'}\delta_{\bar{x}'}^k$ $j+k=2i-2, 2i-3, 2i-4$ $j'=2i-1, 2i-2$
		$\mathcal{L}_{\bar{x}'}^{j'}\delta_{\bar{z}'}^j, \mathcal{L}_{\bar{z}'}^{j'}\delta_{\bar{x}'}^k$ $\mathcal{D}_{\bar{x}'}^j\mathcal{L}_{\bar{z}'}^k,$ $\mathcal{D}_{\bar{z}'}^j\mathcal{L}_{\bar{x}'}^k$ $j+k=4,\dots,0$ $j'=5,\dots,0$				$\mathcal{D}_{\bar{x}'}^j\mathcal{L}_{\bar{z}'}^k, \mathcal{D}_{\bar{z}'}^j\mathcal{L}_{\bar{x}'}^k, \mathcal{L}_{\bar{x}'}^{j'}\delta_{\bar{z}'}^j, \mathcal{L}_{\bar{z}'}^{j'}\delta_{\bar{x}'}^k$ $j+k=2i-2,\dots,2i-5,2i-6$ $j'=2i-1,\dots,2i-3$
			$\mathcal{L}_{\bar{x}'}^{j'}\delta_{\bar{z}'}^j, \mathcal{L}_{\bar{z}'}^{j'}\delta_{\bar{x}'}^k$ $\mathcal{D}_{\bar{x}'}^j\mathcal{L}_{\bar{z}'}^k, \mathcal{D}_{\bar{z}'}^j\mathcal{L}_{\bar{x}'}^k$ $j+k=2n-2,\dots,0$ $j'=2n-1,\dots,0$			$\mathcal{D}_{\bar{x}'}^j\mathcal{L}_{\bar{z}'}^k, \mathcal{D}_{\bar{z}'}^j\mathcal{L}_{\bar{x}'}^k, \mathcal{L}_{\bar{x}'}^{j'}\delta_{\bar{z}'}^j, \mathcal{L}_{\bar{z}'}^{j'}\delta_{\bar{x}'}^k$ $j+k=2i-2,\dots,2i-n-2,\dots,2i-2n$ $j'=2i-1,\dots,2i-n$

Table 5.2: Towers of NSV logarithms that can be predicted for $(\Delta)\mathcal{C}_{J,cc}^{(i)}$ for $c = q, \bar{q}$ given $\Psi_d^{q,(n)}$, $j, k \geq 0$ and $\delta_{\bar{\xi}} = \delta(1 - \xi)$, $\mathcal{D}_{\bar{\xi}}^j = \left[\frac{\ln^j(1-\xi)}{1-\xi} \right]_+$ and $\mathcal{L}_{\bar{\xi}}^j = \ln^j(1 - \xi)$ with $\xi = x', z'$.

part $\{\mathcal{D}_{\bar{x}'}^1 \mathcal{L}_{\bar{z}'}^0, \mathcal{D}_{\bar{z}'}^1 \mathcal{L}_{\bar{x}'}^0\}$. Knowledge on higher-order corrections to the anomalous dimensions leads to predictions for the SV terms $\{\delta_{\bar{x}'} \mathcal{D}_{\bar{z}'}^i, \delta_{\bar{z}'} \mathcal{D}_{\bar{x}'}^i\}$ for $i = 0, 1$ and $\{\mathcal{D}_{\bar{x}'}^0 \mathcal{D}_{\bar{z}'}^0\}$ and for the NSV terms $\{\mathcal{D}_{\bar{x}'}^0 \mathcal{L}_{\bar{z}'}^i, \mathcal{D}_{\bar{z}'}^0 \mathcal{L}_{\bar{x}'}^i\}$ for $i = 0, 1$. We elaborate on these predictions in Appendix-E, where explicit third and fourth order results in a_s using the $\Psi_d^{q,(i)}$ s at $i = 1, 2$ and together with partial results on $\Psi_d^{q,(i)}$ s for $i > 2$.

The all-order expression derived in this section constitutes the central result of the present work. By combining the universal infrared structure of the quark form factor, the mass-factorization kernels, and the soft function, we have assembled all the ingredients entering the master formula, thereby establishing the framework that systematically resums the threshold-enhanced soft-virtual (SV) and next-to-soft-virtual (NSV) contributions. Moreover, the predictive structure of the exponent Ψ_d^q enables the determination of higher-order threshold logarithms beyond the currently available fixed-order calculations.

5.5 Resummation in Mellin space

The formalism for the SV and NSV terms applied in the previous section is useful for obtaining results in (x', z') space at a given order a_s^n , provided that the exponent Ψ_d^q is known to order a_s^m , where $m = 1, \dots, n-1$. It is impractical, though, for studying the numerical impact at all orders in a_s , because it involves iterated convolutions among distributions as well as among distributions and powers of $\ln(1 - \xi)$ terms, which become difficult to evaluate at higher orders in a_s . All-order resummation of our result in Eq. (5.58) is therefore carried out in Mellin space spanned by two complex numbers $N_i, i = 1, 2$, taking double Mellin moments with respect to $N_i, i = 1, 2$ of CF given in Eq. (5.58). In Mellin space, the convolution $\mathcal{C}$ of the exponential in Eq. (5.58) becomes an exponential of the double Mellin moment of the exponent

Ψ_d^q , i.e.,

$$\begin{aligned}
(\Delta)\mathcal{C}_{J,qq}^{\vec{N}} &= \mathcal{N} \int_0^1 dx' x'^{N_1-1} \int_0^1 dz' z'^{N_2-1} (\Delta)\mathcal{C}_{qq}^{\text{SV}+\text{NSV}}(x', z') \\
&= \exp \left(\mathcal{N} \int_0^1 dx' x'^{N_1-1} \int_0^1 dz' z'^{N_2-1} \Psi_d^q(x', z') \right) \\
&= \exp \left(G_{d,q}^{\vec{N}} \right), \tag{5.62}
\end{aligned}$$

where we have suppressed the dependence on the scales Q^2 and μ_F^2 . In Mellin $\vec{N}$ -space, $\vec{N} = (N_1, N_2)$, the threshold limits of the (x', z') space, namely $\{x', z'\} \rightarrow \{1, 1\}$, correspond to taking both $\{N_1, N_2\} \rightarrow \{\infty, \infty\}$ and the limits on N_1 and N_2 are applied simultaneously. The symbol $\mathcal{N}$ in Eq. (5.62) indicates that we retain only the (N_1, N_2) space versions of SV and NSV terms, which are denoted as $\overline{\text{SV}}$ and $\overline{\text{NSV}}$, respectively. Recall that, in the large- N limit, the Mellin moments of the threshold distributions exhibit the following structure,

$$\begin{aligned}
\delta(1 - \xi) &\rightarrow 1, \\
D_\xi^i &\rightarrow \ln^{i+1}(N) + \cdots + \frac{1}{N} \left(\ln^i(N) + \cdots \right) + \mathcal{O} \left(\frac{1}{N^2} \right), \\
\ln^i(1 - \xi) &\rightarrow \frac{1}{N} \left(\ln^i(N) + \cdots \right) + \mathcal{O} \left(\frac{1}{N^2} \right). \tag{5.63}
\end{aligned}$$

Here, the above relations are schematic and are provided only to demonstrate the characteristic logarithmic behavior in the large- N limit. Note, $\overline{\text{SV}}$ terms are of the form $\ln^i(N_1) \ln^j(N_2)$ with $i, j = 0, \dots, \infty$. $\overline{\text{NSV}}$ terms, on the other hand, include corrections of the type $1/N_i$. They are of the form $\ln^i(N_1)/N_1 \ln^j(N_2)$ or $\ln^i(N_1) \ln^j(N_2)/N_2$ where $i, j = 0, \dots, \infty$. All other terms are classified as $\overline{\text{BNSV}}$. We use the overline notations to distinguish the $\vec{N}$ -space approximations for those directly obtained in (x', z') space, because the inverse Mellin transform of $\overline{\text{SV}}$ terms in (x', z') space yields SV terms as well as NSV and BNSV terms. Similarly, the inverse Mellin transform of $\overline{\text{NSV}}$ terms will produce NSV and BNSV terms in (x', z') space.

The Mellin moments of Eq. (5.42) contain terms of the type $\omega = a_s(\mu_R^2)\beta_0 \ln(N_1 N_2)$ as well as single logarithms $\omega_i = a_s(\mu_R^2)\beta_0 \ln(N_i)$, where large logarithms $\ln(N_i)$ and the strong coupling $a_s(\mu_R^2)$ at moderate values combine into an effective expansion parameter of $\mathcal{O}(1)$, spoiling the reliability of perturbative predictions, if truncated at specific order in a_s . A systematic reorganization of the $\vec{N}$ -space in the exponent sums all the terms containing ω , ω_i etc using the resummed expression for strong coupling a_s as described in Appendix-E of [179], which was derived using [504].

By rewriting $G_{d,q}^{\vec{N}} = \bar{G}_{d,q}^{\vec{N}} + G_{d,q}^{\vec{N}=\vec{1}}$ and defining $\tilde{g}_{d,0}^q = \exp(G_{d,q}^{\vec{N}=\vec{1}})$, we obtain

$$(\Delta)\mathcal{C}_{J,qq}^{\vec{N}} = \tilde{g}_{d,0}^q(Q^2, \mu_F^2) \exp\left(\bar{G}_{d,q}^{\vec{N}}(Q^2, \mu_F^2)\right). \quad (5.64)$$

We expand these $\vec{N}$ -independent constants as $\tilde{g}_{d,0}^q = \sum_{i=0}^{\infty} a_s^i(\mu_R^2) \tilde{g}_{d,0,i}^q(Q^2, \mu_F^2, \mu_R^2)$, so that the resummed result takes the following form,

$$\begin{aligned} \bar{G}_{d,q}^{\vec{N}} = & g_{d,1}^q(\omega) \ln N_1 + \sum_{i=0}^{\infty} a_s^i \left(\frac{1}{2} g_{d,i+2}^q(\omega) + \frac{1}{N_1} \bar{g}_{d,i}^q(\omega) \right) \\ & + \frac{1}{N_1} \left(h_{d,0}^q(\omega, N_1) + \sum_{i=1}^{\infty} a_s^i h_{d,i}^q(\omega, \omega_1, N_1) \right) + (N_1 \leftrightarrow N_2, \omega_1 \leftrightarrow \omega_2), \end{aligned} \quad (5.65)$$

where

$$\begin{aligned} h_{d,0}^q(\omega, N_l) &= h_{d,0,0}^q(\omega) + h_{d,0,1}^q(\omega) \ln N_l, \\ h_{d,i}^q(\omega, \omega_l, N_l) &= \sum_{k=0}^{i-1} h_{d,i,k}^q(\omega, \omega_l) \ln^k N_l + \tilde{h}_{d,i,i}^q(\omega, \omega_l) \ln^i N_l. \end{aligned} \quad (5.66)$$

The functions $g_{d,i}^q$ and $\bar{g}_{d,i}^q$ are derived from $\Phi_{d,q}^{\text{SV}}$, as given in Eq. (5.42), and $h_{d,0}^q$ and $h_{d,i}^q$ originate from $\Phi_{d,q}^{\text{NSV}}$, as given in Eq. (5.51).

For brevity, we refrain from displaying these resummation exponents explicitly here. Their expressions are collected in the Appendix-H of [179].

5.6 Physical Evolution Kernel

The ingredients of SIDIS structure functions, CFs as well as the PDFs and FFs are defined in a factorization scheme, but structure functions themselves, being physical observables are scheme independent. This inherent scheme independence allows to derive a scheme-invariant combination of CFs and splitting functions by constructing a system of differential equations among the structure functions [97, 346, 505, 506]. Such physical evolution equations have been employed previously in refs. [507–509] to obtain certain NSV terms for the CFs of inclusive DIS. With an ansatz based on the known results for the CFs and the AP kernels from fixed order computations, predictions for the second and third orders CFs of structure functions in inclusive DIS were made [509], finding agreement for some of the color factors. A systematic construction of physical evolution kernels (PEK), relying on the observation about the logarithmic structure of, namely the single-logarithmic enhancement in $\ln(1-z)$ at large z to all orders, has been performed for the CFs of inclusive DIS, semi-inclusive e^+e^- annihilation and the DY process in [462] (also see refs. [463, 491]). By conjecturing that this behavior holds true at every order in a_s , constraints on the structure of the corresponding leading $\ln(1-z)$ terms in the kernel could be derived and predictions for power suppressed contributions, including NSV logarithms at higher orders in a_s , were obtained, in agreement with known third-order results for DY and Higgs production [510, 511].

Following ref. [462], we have established physical evolution equations for the structure functions F_1 , F_2 , and g_1 to analyze the PEK in the SV and NSV limits. In these limits, we have found that the evolution equations simplify significantly, with only diagonal splitting functions and diagonal CFs contributing to the PEK. Setting $\mu_F^2 = Q^2$ for convenience, we find

$$\begin{aligned}
Q^2 \frac{d}{dQ^2} (g_1) F_J &= \left\{ \frac{1}{2} (\Delta) P_{q \leftarrow q} (a_s) + \frac{1}{2} \tilde{P}_{q \leftarrow q} (a_s) \right. \\
&\quad \left. + \beta(a_s) \frac{d(\Delta) \mathcal{C}_{J,qq}(a_s)}{da_s} \otimes \left((\Delta) \mathcal{C}_{J,qq}(a_s) \right)^{-1} \right\} \otimes (g_1) F_J \\
&= (\Delta) K_J \otimes (g_1) F_J \\
&= \sum_{l=0}^{\infty} a_s^{l+1} (\Delta) K_{J,l} \otimes (g_1) F_J, \tag{5.67}
\end{aligned}$$

where $a_s = a_s(Q^2)$. Note that the kernels $K_{J,l}$ in the differential equations contain scheme-dependent CFs and splitting functions. However, because of the scheme invariance of the structure functions, the kernels also have to be invariant under scheme transformations. Since, in the SV + NSV limit, the polarized and unpolarized coefficient functions, as well as the corresponding splitting functions, coincide for $J = 1, 2$, we suppress the symbol Δ and J throughout this section. Using Eq. (5.5), and expanding the QCD β function and the splitting functions in powers of a_s , we get,

$$\begin{aligned}
K_0 &= \frac{1}{2} P_0^q + \frac{1}{2} \tilde{P}_0^q, \\
K_1 &= \frac{1}{2} P_1^q + \frac{1}{2} \tilde{P}_1^q - \beta_0 \mathcal{C}_q^{(1)}, \\
K_2 &= \frac{1}{2} P_2^q + \frac{1}{2} \tilde{P}_2^q - \beta_1 \mathcal{C}_q^{(1)} - 2\beta_0 \mathcal{C}_q^{(2)} + \beta_0 \mathcal{C}_q^{(1)} \otimes^2, \\
K_3 &= \frac{1}{2} P_3^q + \frac{1}{2} \tilde{P}_3^q - \beta_2 \mathcal{C}_q^{(1)} - 2\beta_1 \mathcal{C}_q^{(2)} - 3\beta_0 \mathcal{C}_q^{(3)} + 3\beta_0 \mathcal{C}_q^{(2)} \otimes \mathcal{C}_q^{(1)} + \beta_1 \mathcal{C}_q^{(1)} \otimes^2 \\
&\quad - \beta_0 \mathcal{C}_q^{(1)} \otimes^3, \\
K_4 &= \frac{1}{2} P_4^q + \frac{1}{2} \tilde{P}_4^q - \beta_3 \mathcal{C}_q^{(1)} - 2\beta_2 \mathcal{C}_q^{(2)} - 3\beta_1 \mathcal{C}_q^{(3)} - 4\beta_0 \mathcal{C}_q^{(4)} + 4\beta_0 \mathcal{C}_q^{(3)} \otimes \mathcal{C}_q^{(1)} \\
&\quad + 2\beta_0 \mathcal{C}_q^{(2)} \otimes^2 + 3\beta_1 \mathcal{C}_q^{(2)} \otimes \mathcal{C}_q^{(1)} - 4\beta_0 \mathcal{C}_q^{(2)} \otimes \mathcal{C}_q^{(1)} \otimes^2 + \beta_2 \mathcal{C}_q^{(1)} \otimes^2 - \beta_1 \mathcal{C}_q^{(1)} \otimes^3 \\
&\quad + \beta_0 \mathcal{C}_q^{(1)} \otimes^4. \tag{5.68}
\end{aligned}$$

In the above, we have used short-hand notation $\mathcal{C}_q^{(l)}$ for $\mathcal{C}_{J,qq}^{(l)}$ and $\mathcal{C}_q^{(l)} \otimes^i$, for the

$(i-1)$ -fold convolution of $\mathcal{C}_q^{(l)}$ with itself, i.e., $\mathcal{C}_q^{(1)} \otimes^2 = \mathcal{C}_q^{(1)} \otimes \mathcal{C}_q^{(1)}$ etc. Following the approach of ref. [462] and using CFs known to second order [171–173, 175, 176, 184] in a_s , we obtain K_l for $l = 0, 1, 2$ in $\vec{N}$ -space, The results are given in Appendix-G.

Some observations from looking at the structure of K_l for $l = 0, 1, 2$,

- In the SV part of K_l , the highest power of logarithms N_i is constrained, for example for the logarithms $\ln^i(N_1) \ln^j(N_2)$, we find $0 \leq i + j \leq l + 1$.
- In the NSV part of K_l , the power of highest logarithms is constrained, for example, for the logarithms $\frac{1}{N_1} \ln^i(N_1) \ln^j(N_2)$ or $\frac{1}{N_2} \ln^i(N_1) \ln^j(N_2)$, we have the limit on i, j as $0 \leq i + j \leq l$.

Thus, also the SIDIS PEK shows a single-logarithmic enhancement, both in (x', z') space as well as in $\vec{N}$ space, similar to what was observed in ref. [462] in the case of PEKs from inclusive cross-sections. If we conjecture that this logarithm structure persists at every order in a_s for K_l , then we can determine certain SV and NSV logarithms at a given order l for $\mathcal{C}_q^{(l)}$ from the knowledge of AP kernels and CFs from previous order in a_s , i.e., results for all orders up to a_s^k where $k < l$.

The validation of the SIDIS PEK predictions against the known second-order CFs can be readily performed. We use K_0 and K_1 , i.e., the PEKs known from the NLO CFs and NLO splitting functions. Then, for SV terms, the maximum sum of logarithmic powers is $(i + j)|_{\max} = 3$ for terms of the form $\ln^i(N_1) \ln^j(N_2)$. For NSV terms, the constraint is $(i + j)|_{\max} = 2$ for logarithms of the form $\frac{1}{N_1} \ln^i(N_1) \ln^j(N_2)$ or $\frac{1}{N_2} \ln^i(N_1) \ln^j(N_2)$. By substituting explicit results for $P_2^q, \tilde{P}_2^q$ and $\mathcal{C}_q^{(1)}$ in K_2 of Eq. (5.68), and applying the general structure of SV and NSV terms specified in Eq. (5.8), we impose the condition that all terms with $i + j > 3$ for SV and $i + j > 2$ for NSV must vanish. This process yields a set of 13 equations relating the second-order coefficients $C_{J,ab}^{(2),\xi_1\xi_2}$ in Eq. (5.8). The solutions to these equations provide the NNLO coefficients for terms such as $\delta_{\vec{x}'} \{ \mathcal{D}_{\vec{z}'}^i, \mathcal{L}_{\vec{z}'}^i \}$ with $i = 3$ and $\{ \mathcal{D}_{\vec{x}'}^i \mathcal{D}_{\vec{z}'}^j, \mathcal{D}_{\vec{x}'}^i \mathcal{L}_{\vec{z}'}^j \}$

with $i+j = 2$, along with similar terms where $x' \leftrightarrow z'$. We find that these predictions are in complete agreement with the results obtained from explicit computations [171–173, 175, 176, 184].

Next, by using known NNLO results, we can predict the third and fourth-order results for CFs, i.e., classes of logarithms for $\mathcal{C}_q^{(3)}$ and $\mathcal{C}_q^{(4)}$. For SV terms in K_3 , we consider logarithms of the form $\ln^i(N_1) \ln^j(N_2)$ with the constraint $(i+j)|_{\max} = 4$, and for NSV logarithms $\frac{1}{N_1} \ln^i(N_1) \ln^j(N_2)$ or $\frac{1}{N_2} \ln^i(N_1) \ln^j(N_2)$, the constraint is $(i+j)|_{\max} = 3$. By imposing that there are no SV logarithms for $i+j > 4$ and no NSV logarithms exist for $i+j > 3$, we obtain a system of 35 linear equations that relate the coefficients $C_{J,ab}^{(3),\xi_1\xi_2}$. Solving for these coefficients, we can predict 35 different logarithms at N³LO level. For example, at third order, for the CF $\mathcal{C}_q^{(3)}$ in (x', z') -space, we can predict terms such as $\delta_{\bar{x}'}\{\mathcal{D}_{\bar{z}'}^i, \mathcal{L}_{\bar{z}'}^i\}$ for $i = 4, 5$ and $\{\mathcal{D}_{\bar{x}'}^i \mathcal{D}_{\bar{z}'}^j, \mathcal{D}_{\bar{x}'}^i \mathcal{L}_{\bar{z}'}^j\}$ for $i+j = 3, 4$ and similarly for $x' \leftrightarrow z'$. We have found that all these predictions are in complete agreement with those obtained using the resummation approach.

Similarly, we can determine the coefficients of highest logarithms in $\mathcal{C}_q^{(4)}$ by observing that the SV logarithms of the form $\ln^i(N_1) \ln^j(N_2)$ are constrained by $(i+j)|_{\max} = 5$ and for NSV logarithms, $\frac{1}{N_1} \ln^i(N_1) \ln^j(N_2)$ or $\frac{1}{N_2} \ln^i(N_1) \ln^j(N_2)$, the constraint is $(i+j)|_{\max} = 4$. These constraints yield a system of 66 equations, with which we can predict 47 SV and NSV logarithms in $\mathcal{C}_q^{(4)}$, namely terms of the form $\delta_{\bar{x}'}\{\mathcal{D}_{\bar{z}'}^i, \mathcal{L}_{\bar{z}'}^i\}$ for $i = 6, 7$ and $\{\mathcal{D}_{\bar{x}'}^i \mathcal{D}_{\bar{z}'}^j, \mathcal{D}_{\bar{x}'}^i \mathcal{L}_{\bar{z}'}^j\}$ for $i+j = 5, 6$, including analogous terms where $x' \leftrightarrow z'$. These predictions are also in agreement with the ones obtained via the resummation approach. However, the remaining 19 equations require information from $\mathcal{C}_q^{(3)}$ and hence we cannot predict them using this current approach.

Alternatively, the physical evolution kernel can be derived within the resummation formalism. Using Eq. (5.58), together with the perturbative expansion in Eq. (5.61),

we obtain

$$K_l = Q^2 \frac{d}{dQ^2} \Psi_d^{q,(l+1)} \quad (5.69)$$

In this section, we analyzed the threshold behavior of the physical evolution kernels (PEK) for the SIDIS structure functions. Exploiting their logarithmic structure, we obtained independent predictions for the threshold-enhanced SV and NSV contributions. The agreement of these predictions with those derived from the master formula provides a non-trivial validation of the all-order resummation framework. Having established the consistency of the formalism through two independent approaches, we now proceed to investigate its phenomenological implications.

5.7 Phenomenology

We illustrate the impact of resummed SV and NSV contributions on the structure functions F_1 and g_1 for the EIC at a center-of-mass energy of $\sqrt{s} = 140$ GeV. In the following, we perform resummation at various logarithmic accuracies, namely $\overline{\text{LL}}$, $\overline{\text{NLL}}$ and $\overline{\text{NNLL}}$, where the bar denotes the inclusion of both SV and NSV logarithms. As shown in the first row of Tab. 5.3, the resummed result at $\overline{\text{LL}}$ accuracy requires the resummed exponents $\{\tilde{g}_{d,0,0}^q, g_{d,1}^q, \bar{g}_{d,0}^q, h_{d,0}^q\}$. They systematically resum SV logarithms of the form $\{\ln^i N_1 \ln^j N_2\}$ (where $i + j = 2n$) and NSV logarithms like $\{\frac{\ln^i N_1}{N_1} \ln^j N_2, \frac{\ln^i N_2}{N_2} \ln^j N_1\}$ (where $i + j = 2n - 1$) at n th order in a_s , i.e., a_s^n for all $n > 1$:

$$(\Delta) \mathcal{C}_{J,qq,\vec{N}}^{\overline{\text{LL}}} = \left(\tilde{g}_{d,0,0}^q \right) \exp \left[g_{d,1}^q(\omega) \ln N_1 + \frac{1}{N_1} \left(\bar{g}_{d,0}^q(\omega) + h_{d,0}^q(\omega, N_1) \right) + (N_1 \leftrightarrow N_2) \right]. \quad (5.70)$$

Similarly, for the resummed result at $\overline{\text{NLL}}$ accuracy, as detailed in the second row of Tab. 5.3, we require the additional resummation exponents $\{\tilde{g}_{d,0,1}^q, g_{d,2}^q, \bar{g}_{d,1}^q, h_{d,1}^q\}$ alongside the $\overline{\text{LL}}$ exponents. This suffices to sum up the next-to-leading SV logarithms and next-to-highest NSV logarithms to all orders. Specifically, this includes SV logarithms of the form $\{\ln^i N_1 \ln^j N_2\}$ (where $i+j = \{2n-1, 2n-2\}$) and NSV logarithms of the form $\{\frac{\ln^i N_1}{N_1} \ln^j N_2, \frac{\ln^i N_2}{N_2} \ln^j N_1\}$ (where $i+j = 2n-2$ with $n > 2$), i.e.,

$$\begin{aligned}
(\Delta)C_{J,qq,\vec{N}}^{\overline{\text{NLL}}} = & \left(\tilde{g}_{d,0,0}^q + a_s \tilde{g}_{d,0,1}^q \right) \exp \left[g_{d,1}^q(\omega) \ln N_1 + \frac{1}{2} g_{d,2}^q(\omega) \right. \\
& + \frac{1}{N_1} \left(\bar{g}_{d,0}^q(\omega) + a_s \bar{g}_{d,1}^q(\omega) + h_{d,0}^q(\omega, N_1) + a_s h_{d,1}^q(\omega, \omega_1, N_1) \right) \\
& \left. + (N_1 \leftrightarrow N_2, \omega_1 \leftrightarrow \omega_2) \right]. \tag{5.71}
\end{aligned}$$

GIVEN	PREDICTIONS - SV and NSV Logarithms					Logarithmic Accuracy
Resummed Exponents Up To	$(\Delta)C_{J,qq,\vec{N}}^{(2)}$	$(\Delta)C_{J,qq,\vec{N}}^{(3)}$	$(\Delta)C_{J,qq,\vec{N}}^{(4)}$	$\dots$	$(\Delta)C_{J,qq,\vec{N}}^{(n)}$	
$\tilde{g}_{d,0,0}^q, g_{d,1}^q, \bar{g}_{d,0}^q, h_{d,0}^q$	$L_1^i L_2^j _{i+j=4}$ $L_{N_1}^i L_2^j _{i+j=3}$ $L_1^i L_{N_2}^j _{i+j=3}$	$L_1^i L_2^j _{i+j=6}$ $L_{N_1}^i L_2^j _{i+j=5}$ $L_1^i L_{N_2}^j _{i+j=5}$	$L_1^i L_2^j _{i+j=8}$ $L_{N_1}^i L_2^j _{i+j=7}$ $L_1^i L_{N_2}^j _{i+j=7}$	$\dots$	$L_1^i L_2^j _{i+j=2n}$ $L_{N_1}^i L_2^j _{i+j=2n-1}$ $L_1^i L_{N_2}^j _{i+j=2n-1}$	$\overline{\text{LL}}$
$\tilde{g}_{d,0,1}^q, g_{d,2}^q, \bar{g}_{d,1}^q, h_{d,1}^q$		$L_1^i L_2^j _{i+j=6,5,4}$ $L_{N_1}^i L_2^j _{i+j=5,4}$ $L_1^i L_{N_2}^j _{i+j=5,4}$	$L_1^i L_2^j _{i+j=8,7,6}$ $L_{N_1}^i L_2^j _{i+j=7,6}$ $L_1^i L_{N_2}^j _{i+j=7,6}$	$\dots$	$L_1^i L_2^j _{i+j=2n,\dots,2n-2}$ $L_{N_1}^i L_2^j _{i+j=2n-1,2n-2}$ $L_1^i L_{N_2}^j _{i+j=2n-1,2n-2}$	$\overline{\text{NLL}}$
$\tilde{g}_{d,0,2}^q, g_{d,3}^q, \bar{g}_{d,2}^q, h_{d,2}^q$			$L_1^i L_2^j _{i+j=8,\dots,4}$ $L_{N_1}^i L_2^j _{i+j=7,\dots,5}$ $L_1^i L_{N_2}^j _{i+j=7,\dots,5}$	$\dots$	$L_1^i L_2^j _{i+j=2n,\dots,2n-4}$ $L_{N_1}^i L_2^j _{i+j=2n-1,\dots,2n-3}$ $L_1^i L_{N_2}^j _{i+j=2n-1,\dots,2n-3}$	$\overline{\text{NNLL}}$

Table 5.3: The set of resummed exponents required to predict the tower of NSV logarithm in $C_{J,qq,\vec{N}}^{(n)}$, $L_1^i = \ln^i(N_1)$, $L_{N_1}^i = \frac{\ln^i(N_1)}{N_1}$, $L_2^j = \ln^j(N_2)$, $L_{N_2}^j = \frac{\ln^j(N_2)}{N_2}$.

According to the third row of Tab. 5.3, we include the resummation exponents $\{\tilde{g}_{d,0,2}^q, g_{d,3}^q, \bar{g}_{d,2}^q, h_{d,2}^q\}$ alongside the $\overline{\text{LL}}$ and $\overline{\text{NLL}}$ terms to achieve $\overline{\text{NNLL}}$ accuracy. This set resums SV logarithms of the form $\{\ln^i N_1 \ln^j N_2\}$ (where $i+j = \{2n-3, 2n-4\}$) and NSV logarithms of the form $\{\frac{\ln^i N_1}{N_1} \ln^j N_2, \frac{\ln^i N_2}{N_2} \ln^j N_1\}$ with $i+j =$

$2n - 3, n > 3$.

$$\begin{aligned}
(\Delta)\mathcal{C}_{J,qq,\vec{N}}^{\overline{\text{NNLL}}} = & \left(\tilde{g}_{d,0,0}^q + a_s \tilde{g}_{d,0,1}^q + a_s^2 \tilde{g}_{d,0,2}^q \right) \exp \left[g_{d,1}^q(\omega) \ln N_1 \right. \\
& + \frac{1}{2} \left(g_{d,2}^q(\omega) + a_s g_{d,3}^q(\omega) \right) + \frac{1}{N_1} \left(\bar{g}_{d,0}^q(\omega) + a_s \bar{g}_{d,1}^q(\omega) + a_s^2 \bar{g}_{d,2}^q(\omega) \right. \\
& + h_{d,0}^q(\omega, N_1) + a_s h_{d,1}^q(\omega, \omega_1, N_1) + a_s^2 h_{d,2}^q(\omega, \omega_1, N_1) \left. \right) \\
& \left. + (N_1 \leftrightarrow N_2, \omega_1 \leftrightarrow \omega_2) \right]. \tag{5.72}
\end{aligned}$$

The resummed results are matched to the respective fixed-order results as follows:

$$\begin{aligned}
(g_1)F_J^{\text{N}^n\text{LO}+\overline{\text{N}^n\text{LL}}} = & (g_1)F_J^{\text{N}^n\text{LO}} \\
& + \sum_{cc} \int_{c_1-i\infty}^{c_1+i\infty} \frac{dN_1}{2\pi i} \int_{c_2-i\infty}^{c_2+i\infty} \frac{dN_2}{2\pi i} (\Delta) f_{\frac{c}{P},N_1}(\mu_F^2) D_{\frac{H'}{c},N_2}(\mu_F^2) \\
& \times \left((\Delta)\mathcal{C}_{J,cc,\vec{N}}^{\overline{\text{N}^n\text{LL}}} - (\Delta)\mathcal{C}_{J,cc,\vec{N}} \Big|_{\text{tr}^n} \right). \tag{5.73}
\end{aligned}$$

The first term in Eq. (5.73) represents the fixed-order contributions up to N^nLO accuracy. The second term corresponds to the resummed result at $\overline{\text{N}^n\text{LL}}$ accuracy. This term is derived by subtracting its fixed-order expansion, truncated up to order a_s^n , from the full resummed result, which precisely avoids double-counting of threshold logarithms. Therefore, the latter encapsulates the all-order SV and NSV resummed contributions in perturbation theory starting from a_s^{n+1} onward. The subscript ‘trⁿ’ denotes the n^{th} -order ‘truncated’ part of the resummed result which is already contained in the fixed-order expressions. The CFs required for $(g_1)F_J^{\text{N}^n\text{LO}}$ in the first term are known up to NNLO [109, 171–173, 175, 176, 184].

For the unpolarized structure function (F_1), we have employed the ABMP16 PDF sets [39] and NNFF10PIp FF sets [64] at their respective orders, except for the LO where we use NLO PDF set. For the polarized structure function (g_1), we have used the polarized BDSSV24NLO PDFs at LL and NLL accuracies, and BDSSV24NNLO

PDFs at NNLL accuracy. The strong coupling a_s is taken as provided through the LHAPDF interface [51] with $n_f = 3$ active massless quark flavors throughout. We have used an in-house FORTRAN code to perform the double Mellin inversion for the resummed contributions, and we have adopted the so-called minimal prescription [512] to handle the Landau pole in the Mellin inversion routines. The parton densities in $\vec{N}$ -space are obtained from their xz -space counterparts following the procedure described in Appendix-B of [513].

In Figs. 5.1 and 5.2, we present the structure functions F_1 and g_1 for the EIC at $\sqrt{s} = 140$ GeV center-of-mass energy as a function of x after integrating over the kinematic ranges $y \in [0.5, 0.9]$ and $z \in [0.2, 0.85]$. The displayed curves correspond to fixed-order QCD predictions up to NNLO accuracy and the resummed cross sections to NNLO+ $\overline{\text{NNLL}}$ accuracy. The associated bands indicates the variation of the μ_R^2 and μ_F^2 scales independently by a factor of two, i.e. $\mu_R^2, \mu_F^2 \in [Q_{\text{avg}}^2/2, 2Q_{\text{avg}}^2]$ with the constraint $1/2 \leq \mu_R^2/\mu_F^2 \leq 2$ in the so-called seven-point scale variation, where $Q_{\text{avg}}^2 = xy_{\text{avg}}s$.

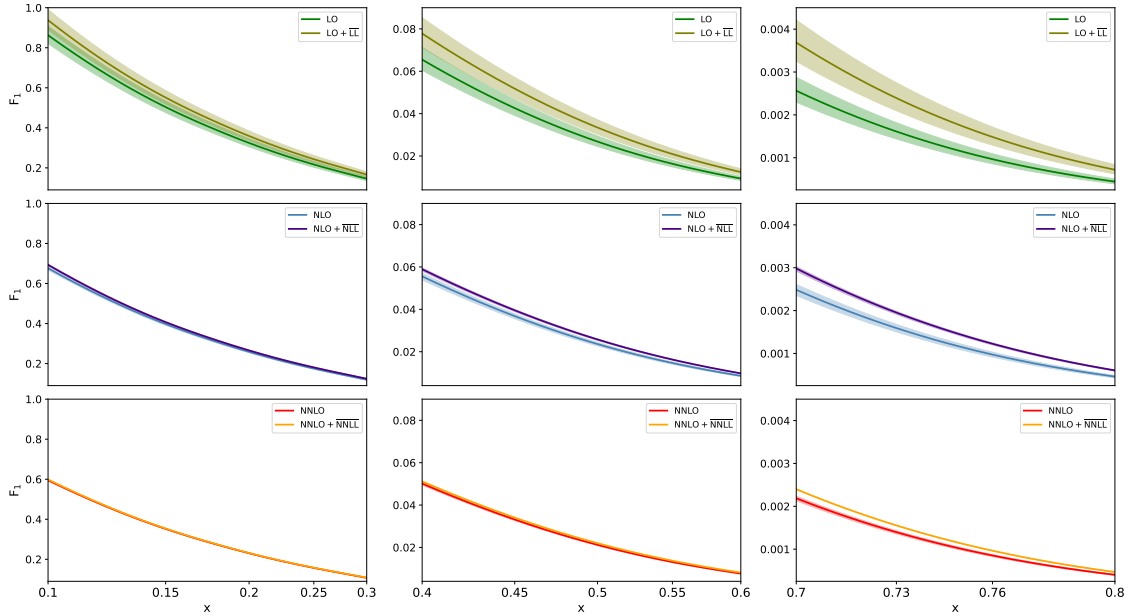


Figure 5.1: Seven-point scale variation of the structure function F_1 as a function of x (log-scale) for the EIC at $\sqrt{s} = 140$ GeV.

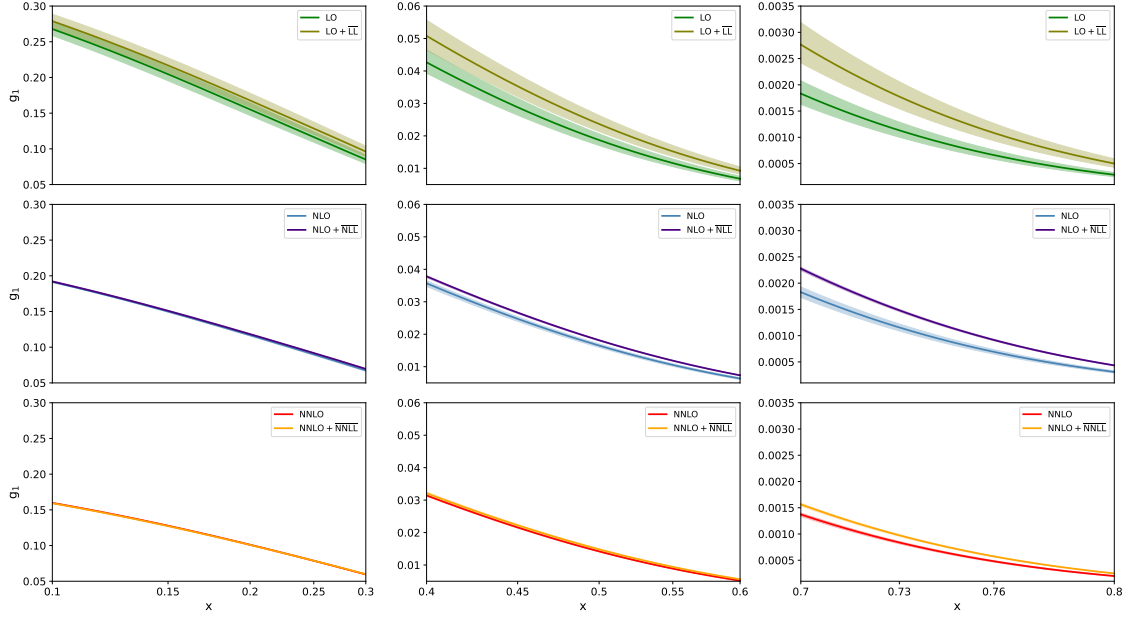


Figure 5.2: Seven-point scale variation of structure function g_1 as a function x (log-scale) for the EIC at $\sqrt{s} = 140$ GeV.

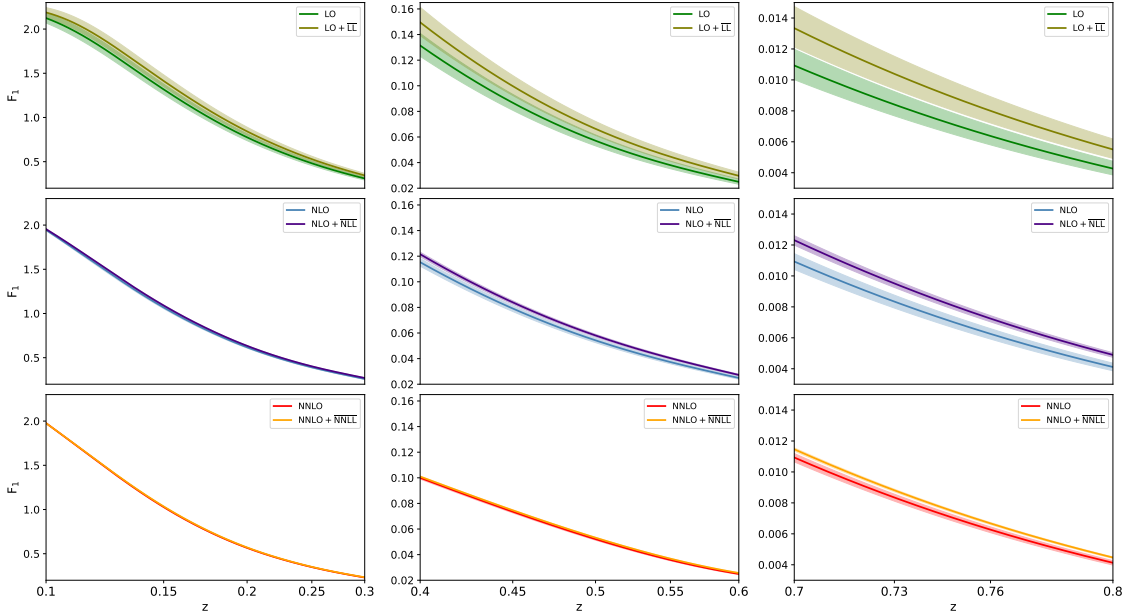


Figure 5.3: Seven-point scale variation of the structure function F_1 as a function of z (log-scale) for the EIC at $\sqrt{s} = 140$ GeV.

Figs. 5.3 and 5.4 display again F_1 and g_1 for the EIC at $\sqrt{s} = 140$ GeV, now as a function of z after integrating over the kinematic ranges $x \in [0.1, 0.8]$ and

$y \in [0.5, 0.9]$, and again showing predictions both at fixed-order NNLO and at NNLO+ $\overline{\text{NNLL}}$ accuracies. The corresponding bands illustrate the uncertainty from a seven-point scale variation, where μ_R^2 and μ_F^2 are independently varied by a factor of two, i.e. $\mu_R^2, \mu_F^2 \in [Q_{\text{avg}}^2/2, 2Q_{\text{avg}}^2]$, where $Q_{\text{avg}}^2 = x_{\text{avg}}y_{\text{avg}}s$.

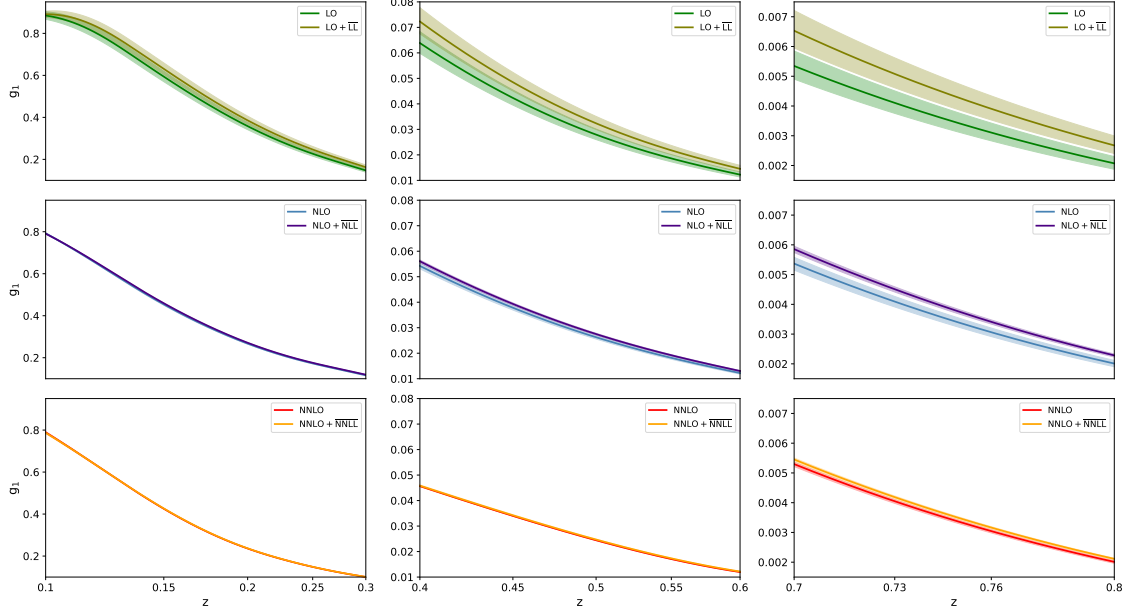


Figure 5.4: Seven-point scale variation of structure function g_1 for $z(\text{log-scale})$ for the EIC at $\sqrt{s} = 140$ GeV.

Figs. 5.1 and 5.3 (5.2 and 5.4) demonstrate an increase of the cross-sections that incorporate the SV+NSV resummed results together with the fixed-order predictions as the logarithmic accuracy improves. In addition, we find that the uncertainty band, obtained from variations of the renormalization and factorization scales, shrinks considerably from LO+ $\overline{\text{LL}}$ to NNLO+ $\overline{\text{NNLL}}$ accuracy. This improvement in scale independence is more significant in the large- x or large- z regions e.g. $x > 0.7$ or $z > 0.7$, due to dominance of the threshold resummation.

The impact of resummation on F_1 and g_1 is illustrated for three distinct values of z ($z=\{0.7, 0.8, 0.9\}$) in Fig. 5.5 respectively, when compare to the fixed perturbative QCD predictions and keeping all other parameters consistent with those in Fig. 5.3 e.g. x and y have been integrated over the kinematic ranges $x \in [0.1, 0.8]$ and

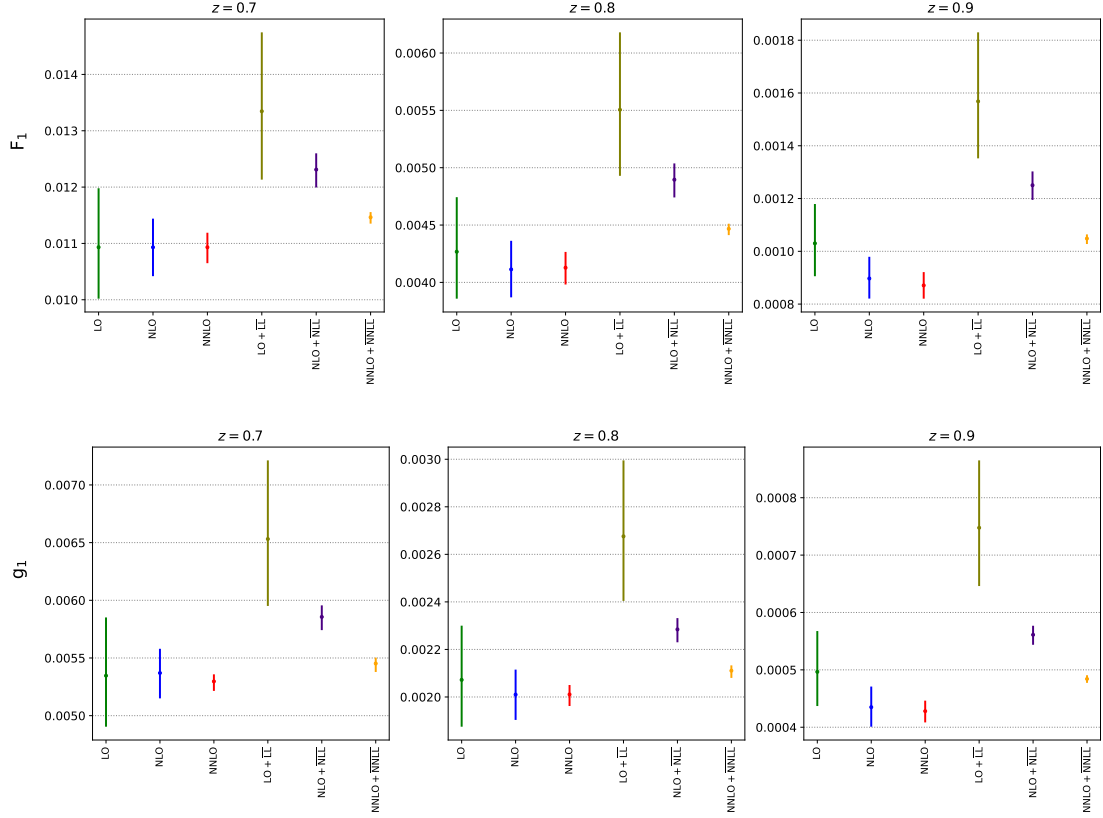


Figure 5.5: Various perturbative contributions to F_1 (upper) and g_1 (lower) at different z values for the EIC at $\sqrt{s} = 140$ GeV.

$y \in [0.5, 0.9]$. In all these plots Fig. 5.5, the vertical lines represent a seven-point μ_R^2, μ_F^2 scale variation. Note, that there is a significant scale dependence in the LO+LL predictions in Fig. 5.5, which arises because the LO contribution inherently lacks renormalization scale dependence. It is then introduced solely by the LL terms without counteracting contributions. These plots clearly demonstrate how, in the large x and/or large z regions, the contribution of resummed terms is significant. Furthermore, they illustrate, how resummed predictions substantially reduce the theoretical uncertainties arising from the choice of μ_R and μ_F .

Finally, in Tabs. 5.4 and 5.5, we present the explicit results for F_1 at a few values of x and z after integrating y and z or x , respectively, and setting $\mu_R^2 = \mu_F^2 = Q_{\text{avg}}^2$ as was done for the Figs. 5.1 and 5.3. A similar table can be constructed for the polarized case; however, we omit it for brevity.

x	F_1					
	LO	NLO	NNLO	LO+ $\overline{\text{LL}}$	NLO+ $\overline{\text{NLL}}$	NNLO+ $\overline{\text{NNLL}}$
0.15	$0.5044^{+5.971\%}_{-5.389\%}$	$0.3980^{+1.237\%}_{-1.557\%}$	$0.3526^{+0.570\%}_{-0.700\%}$	$0.5518^{+6.393\%}_{-5.740\%}$	$0.4077^{+0.715\%}_{-0.934\%}$	$0.3541^{+0.475\%}_{-0.357\%}$
0.25	$0.2168^{+7.160\%}_{-6.375\%}$	$0.1751^{+1.758\%}_{-2.104\%}$	$0.1569^{+0.719\%}_{-0.899\%}$	$0.2433^{+7.698\%}_{-6.809\%}$	$0.1807^{+0.919\%}_{-1.189\%}$	$0.1579^{+0.484\%}_{-0.397\%}$
0.45	$0.0426^{+9.307\%}_{-8.104\%}$	$0.0368^{+2.984\%}_{-3.301\%}$	$0.0331^{+1.180\%}_{-1.452\%}$	$0.0518^{+10.294\%}_{-8.862\%}$	$0.0395^{+1.121\%}_{-1.492\%}$	$0.0341^{+0.244\%}_{-0.360\%}$
0.6	$0.0094^{+10.991\%}_{-9.400\%}$	$0.0087^{+4.157\%}_{-4.360\%}$	$0.0077^{+1.738\%}_{-2.044\%}$	$0.0125^{+12.509\%}_{-10.521\%}$	$0.0098^{+1.269\%}_{-1.740\%}$	$0.0082^{+0.123\%}_{-0.347\%}$
0.75	$0.0012^{+13.053\%}_{-10.968\%}$	$0.0012^{+5.773\%}_{-5.787\%}$	$0.0010^{+2.618\%}_{-2.957\%}$	$0.0017^{+15.374\%}_{-12.620\%}$	$0.0014^{+1.604\%}_{-2.160\%}$	$0.0011^{+0.349\%}_{-0.465\%}$

Table 5.4: Values of resummed structure function F_1 at various orders in comparison to the fixed order results at the central scale $\mu_R^2 = \mu_F^2 = Q_{\text{avg}}^2$ as function of x (see text for integration ranges of y, z).

z	F_1					
	LO	NLO	NNLO	LO+ $\overline{\text{LL}}$	NLO+ $\overline{\text{NLL}}$	NNLO+ $\overline{\text{NNLL}}$
0.15	$1.3176^{+4.645\%}_{-4.259\%}$	$1.0682^{+1.051\%}_{-1.263\%}$	$1.0282^{+0.441\%}_{-0.554\%}$	$1.4127^{+4.927\%}_{-4.497\%}$	$1.0908^{+0.522\%}_{-0.669\%}$	$1.0350^{+0.214\%}_{-0.176\%}$
0.25	$0.4817^{+5.822\%}_{-5.261\%}$	$0.3909^{+1.479\%}_{-1.712\%}$	$0.3476^{+0.609\%}_{-0.744\%}$	$0.5286^{+6.257\%}_{-5.619\%}$	$0.4020^{+0.759\%}_{-0.950\%}$	$0.3507^{+0.270\%}_{-0.304\%}$
0.45	$0.0866^{+7.581\%}_{-6.726\%}$	$0.0790^{+2.765\%}_{-2.945\%}$	$0.0741^{+1.096\%}_{-1.291\%}$	$0.0997^{+8.307\%}_{-7.299\%}$	$0.0838^{+1.494\%}_{-1.715\%}$	$0.0752^{+0.439\%}_{-0.540\%}$
0.6	$0.0251^{+8.644\%}_{-7.598\%}$	$0.0251^{+3.797\%}_{-3.905\%}$	$0.0247^{+1.790\%}_{-2.003\%}$	$0.0299^{+9.544\%}_{-8.297\%}$	$0.0275^{+1.972\%}_{-2.208\%}$	$0.0255^{+0.680\%}_{-0.817\%}$
0.75	$0.0070^{+10.248\%}_{-8.889\%}$	$0.0069^{+5.253\%}_{-5.220\%}$	$0.0069^{+2.755\%}_{-2.980\%}$	$0.0087^{+11.255\%}_{-9.656\%}$	$0.0079^{+2.588\%}_{-2.828\%}$	$0.0073^{+0.877\%}_{-1.093\%}$

Table 5.5: Values of resummed structure function F_1 at various orders in comparison to the fixed order results at the central scale $\mu_R^2 = \mu_F^2 = Q_{\text{avg}}^2$ as function of z (see text for integration ranges of x, y).

5.8 Summary

In this chapter, we have developed a threshold-resummation framework for semi-inclusive deep-inelastic scattering (SIDIS), enabling the systematic all-order resummation of threshold-enhanced soft-virtual (SV) and next-to-soft-virtual (NSV) logarithms. Such logarithms appear in fixed-order perturbative predictions and must be resummed to obtain reliable theoretical predictions in the relevant kinematic region. The threshold region in SIDIS is characterized by the scaling variables x' and z' tend to unity. In this limit, the fixed-order perturbative predictions of the CFs are then dominated by the plus and delta function distributions (SV terms) as well as $\log^j(1-x')$ or $\log^j(1-z')$ (NSV terms) with $j = 0, 1, 2, \dots$. This is a situation similar to the case of rapidity distributions in the Drell-Yan process. Based on the insights there, we have developed a formalism, using collinear factorisation and renormalisation group equations, to achieve the resummation of these threshold logarithms (SV as well as NSV) both in (x', z') space as well as in the space of the conjugate Mellin variables $\vec{N} = (N_1, N_2)$. In Mellin space, these threshold logarithms show up as $\ln^i(N_1) \ln^j(N_2)$ for SV as well as $\ln^i(N_1) \ln^j(N_2)/N_2$, $\ln^i(N_1) \ln^j(N_2)/N_1$ where $\{i, j\} = 0, 1, 2, \dots$ and they can be systematically resummed to all orders in a_s .

The compact expressions for the resummed results encapsulate both SV and NSV logarithms in $\vec{N}$ -space and allow for phenomenological studies with EIC kinematics. Upon expansion in a_s the resummed result generates predictions for the full SV and partial NSV terms for the CFs $(\Delta)\mathcal{C}_{J,qq}^{(3),SV}$, $(\Delta)\mathcal{C}_{J,qq}^{(3),NSV}$ third order in (x', z') space. At fourth order, using the recently obtained results for four-loop quark virtual and eikonal anomalous dimensions B_4^q and f_4^q , we have predicted all SV terms in $(\Delta)\mathcal{C}_{J,qq}^{(4),SV}$ except the coefficient of $\delta_{\bar{x}'}\delta_{\bar{z}'}$. The derivation of the NSV terms has been corroborated by an independent approach that uses PEKs for the structure functions, and we have confirmed our predictions both at third and fourth order. Finally, we have demonstrated the numerical importance of the resummed thresh-

old logarithms for structure functions F_1 and g_1 at EIC energies. We have shown, that at each logarithmic order the resummed contributions are larger than the corresponding fixed order ones. Moreover, including these logarithms to all orders through resummation reduces the dependence on the renormalisation and factorisation scales and hence improves the reliability of our predictions. These results demonstrate the importance of threshold resummation for achieving precision QCD predictions for SIDIS at the EIC.

Chapter 6

Neutral and Charged Current SIDIS

Electroweak interactions provide an additional avenue for probing the partonic structure of hadrons beyond purely electromagnetic scattering. With the increasing kinematic reach and precision of modern lepton-hadron scattering experiments, particularly at the forthcoming Electron-Ion Collider, the inclusion of neutral-current (NC) and charged-current (CC) interactions becomes essential for precision studies of semi-inclusive deep-inelastic scattering (SIDIS). These processes offer complementary sensitivity to the flavor and spin structure of the nucleon. Building upon the SIDIS formalism developed in the previous chapters, this chapter presents the complete NNLO QCD coefficient functions for polarized and unpolarized SIDIS with both NC and CC electroweak interactions. We also examine the correspondence between coefficient functions associated with different electroweak currents, providing important consistency checks of the calculation, and investigate the phenomenological impact of the NNLO corrections for kinematics relevant to the EIC.

6.1 Introduction

Semi-inclusive deep inelastic scattering (SIDIS) serves as a key process for investigating the partonic structure of hadrons, the dynamics of quarks and gluons and simultaneously providing insight into the fragmentation mechanisms that produce the observed final-state hadrons. Within the framework of QCD factorization, these non-perturbative aspects are described through parton distribution functions (PDFs), which describe the partonic content of hadrons, and fragmentation functions (FFs), which characterize the formation of hadrons from partons [123, 144, 145].

The discussion in the previous chapters focused primarily on electromagnetic interactions mediated by a virtual photon exchange. However, the broad kinematic range and unprecedented precision along with high luminosity of the of the forthcoming Electron-Ion Collider (EIC) will enable studies in a regime where electroweak effects become increasingly important [145], see also [514–516]. At sufficiently large momentum transfer, neutral-current (NC) processes receive contributions from both photon and Z -boson exchange, together with their interference, while charged-current (CC) processes proceed through the exchange of $W^\pm$ bosons. These interactions enrich the structure of the SIDIS cross section through additional couplings and structure functions (SFs), providing sensitivity to the chiral and flavor structure of the nucleon.

The inclusion of NC and CC interactions significantly broadens the physics program of SIDIS. In particular, electroweak interactions offer opportunities to disentangle individual quark and antiquark flavor contributions, allowing a more precise determination of flavor-separated parton distributions, helicity distributions, and parity-violating asymmetries that are inaccessible in purely electromagnetic scattering. Consequently, the combined analysis of electromagnetic, neutral-current, and charged-current SIDIS measurements offers substantially improved constraints on parton distribution and fragmentation functions and pro-

vides a more comprehensive understanding of the flavor and spin structure of hadrons [39–43, 62, 65, 68, 69, 77, 79, 139–143, 170, 187].

In this chapter, we extend the SIDIS formalism developed in the previous chapters to include both neutral-current and charged-current interactions. We derive the corresponding electroweak structure functions and the complete NNLO QCD coefficient functions for polarized and unpolarized scattering, thereby providing the theoretical ingredients required for precision phenomenological studies.

We first describe the methodology and present the computation of the NNLO coefficient functions. This is followed by a discussion of the various checks and comparisons performed to validate the calculation, including the correspondence between coefficient functions associated with different electroweak currents. Finally, we investigate the phenomenological impact of the NNLO corrections for kinematics relevant to the Electron-Ion Collider.

6.2 Methodology

The general theoretical framework of SIDIS, including the QCD factorization formalism, the definition of the hadronic structure functions, and their decomposition in terms of perturbatively calculable coefficient functions, was presented in Chapter 2. Subsequently, Chapter 3 developed the computational framework for the calculation of the next-to-next-to-leading-order QCD coefficient functions associated with the polarized electromagnetic structure function g_1 . In the present chapter, the same theoretical formalism and computational setup are employed and extended to neutral-current and charged-current interactions, leading to a unified treatment of the complete polarized and unpolarized electroweak SIDIS coefficient functions.

Within the QCD factorization framework, the hadronic structure functions are expressed as convolutions of perturbatively calculable coefficient functions (CFs) with

universal parton distribution functions (PDFs) and fragmentation functions (FFs),

$$\begin{aligned}
(\Delta)\mathcal{F}_i^j(x, z, Q^2) &= \sum_{a,b} \int_x^1 \frac{dx_1}{x_1} (\Delta)f_{a/H}(x_1, \mu_F^2) \int_z^1 \frac{dz_1}{z_1} D_{H'/b}(z_1, \mu_F^2) \\
&\times (\Delta)\mathcal{C}_{i,ab}^j\left(\frac{x}{x_1}, \frac{z}{z_1}, \mu_F^2, Q^2\right).
\end{aligned} \tag{6.1}$$

where $(\Delta)f_{a/H}$ and $D_{H'/b}$ denote the (polarized) parton distribution and fragmentation functions, respectively, while $(\Delta)\mathcal{C}_{i,ab}^j$ are the perturbatively calculable coefficient functions describing the short-distance partonic dynamics.

The present calculation builds upon the computational framework developed in Chapter 3. The procedure involves the generation of Feynman diagrams, the algebraic simplification of amplitudes through Dirac algebra, Lorentz contractions, and color-factor decomposition, the reduction of loop and phase-space integrals to a basis of master integrals (MIs), and the subsequent substitution of the MIs in the squared amplitudes. The extension to neutral- and charged-current interactions introduces several new features compared to the electromagnetic case. In particular, in the electromagnetic calculation Dirac matrix γ^5 appears only through the helicity projectors of polarized external fermions but in electroweak interactions introduce additional axial-vector couplings that generate γ^5 contributions at the interaction vertices. As a result, a consistent treatment of γ^5 within dimensional regularization, together with the associated renormalization factors, becomes essential. Furthermore, the interplay of vector and axial-vector couplings gives rise to a richer structure of coefficient functions and structure functions, leading to a broader class of electroweak observables.

At the partonic level, these contributions appear in the matrix element squared $|M_{ab}|_{j,\mu\nu}^2$, see Eq. (2.28), where the γ_5 matrix arises due to the axial-vector coupling as well as from spin dependent (anti-)quark states. In addition, we encounter Levi-Civita tensor from polarization of gluons and also from the projectors in Eq. (2.29).

Since both the γ_5 matrix and the Levi-Civita tensor are intrinsically four-dimensional objects, a prescription is required to define them in $d = 4 + \epsilon$ dimensions. Several such prescriptions have been proposed [23, 209–221], see also [222–231, 517], however, none is known to preserve the chiral Ward identity automatically. In this work, for the axial-vector coupling, we employ Larin’s prescription [211] to define γ_5 in $d = 4 + \epsilon$,

$$\gamma_\mu \gamma_5 = \frac{i}{6} \epsilon_{\mu\nu\sigma\lambda} \gamma^\nu \gamma^\sigma \gamma^\lambda. \quad (6.2)$$

and to project out the polarization of initial quarks we use, (see [185, 518, 519]),

$$\not{p}_a \gamma_5 = \frac{i}{2 p_a \cdot q} \epsilon_{\mu\nu\sigma\lambda} \gamma^\mu \gamma^\nu p_a^\sigma q^\lambda \not{p}_a. \quad (6.3)$$

With the above identities, we have encountered a maximum of four Levi-Civita tensors which need to be contracted in a particular order see [185, 221, 228]:

- Those coming from the projector and the polarized parton are contracted first.
- Then we contract the tensors arising from the axial-vector couplings.
- Finally, the remaining Levi-Civita tensors (from polarized partons and the vertex) are contracted.

The contraction is expressed in terms of a determinant containing metric tensors defined in d dimensions, see Eq. (3.16). The results obtained in Larin’s scheme are transformed to the standard $\overline{\text{MS}}$ scheme through a renormalization scheme transformation. The associated renormalization constants [220, 232, 233] used for this scheme transformation restore the Ward identity and ensure that the final coefficient functions are defined in the $\overline{\text{MS}}$ scheme.

The ultraviolet (UV) divergences arising from the loop corrections are removed through the standard renormalization of the strong coupling constant in the $\overline{\text{MS}}$

scheme. In addition, since Eq. (6.2) is employed to define the γ_5 matrix at the axial-vector interaction vertices, an additional overall renormalization is required. This is achieved by multiplying the renormalized amplitudes with the corresponding $\overline{\text{MS}}$ scheme counter renormalization factor $Z_{A5} = Z_A Z_5$ [211, 275] to each vertex involving γ_5 , before performing mass factorization. Expanding Z_{A5} in powers of a_s as $Z_{A5} = 1 + \sum_{k=1} a_s^k(\mu_R^2) Z_{A5}^{(k)}$, where

$$\begin{aligned} Z_{A5}^{(1)} &= C_F \left(-4 + 5\epsilon - \epsilon^2 \left(\frac{11}{2} - \frac{1}{2}\zeta_2 \right) \right), \\ Z_{A5}^{(2)} &= C_F^2(22) - C_A C_F \left(\frac{44}{3\epsilon} + \frac{107}{9} \right) + C_F n_f \left(\frac{8}{3\epsilon} + \frac{2}{9} \right). \end{aligned} \quad (6.4)$$

Following UV renormalization, the soft singularities originating from virtual and real-emission subprocesses cancel among themselves in accordance with the Kinoshita-Lee-Nauenberg theorem. The remaining collinear singularities associated with the initial- and final-state partons are removed through mass factorization by absorbing them into the PDFs and FFs via the space-like and time-like Altarelli-Parisi kernels, respectively. This procedure is performed at the factorization scale μ_F and is expressed as

$$d(\Delta) \hat{\sigma}_{i,ab}^j(\epsilon) = (\Delta) \Gamma_{c \leftarrow a}(\epsilon, \mu_F^2) \otimes (\Delta) \mathcal{C}_{i,cd}^j(\epsilon, \mu_F^2) \tilde{\otimes} \tilde{\Gamma}_{b \leftarrow d}(\epsilon, \mu_F^2), \quad (6.5)$$

where summation over the intermediate parton indices c and d is implied. The symbols $\otimes$ and $\tilde{\otimes}$ denote convolutions over the momentum fractions associated with the PDFs and FFs, respectively, see Eq. (3.22).

For the unpolarized SFs, Eq. (6.5) yields the CFs in the $\overline{\text{MS}}$ and the counter terms in Eq. (6.4) completely remove the scheme dependence from Larin's prescription. In the case of polarized SFs, these counter terms remove the scheme dependence from the γ_5 matrices that are present in the vertices. The treatment of the γ_5 matrix that enters through the polarization of incoming partons requires an additional finite

renormalization to obtain the CFs in $\overline{\text{MS}}$ scheme. This is done in two steps. We first perform mass factorization for the polarized CFs using the space-like polarized AP kernels computed in Larin's scheme and then perform a suitable scheme transformations to convert these Larin scheme CFs to $\overline{\text{MS}}$ ones. Following the procedure discussed in Chapter 3, the finite renormalization constants Z_{ab} [220, 232, 233] are used to transform the CFs, defined in the Larin scheme, denoted by $\Delta\mathcal{C}_{i,ab}^L$ to those in the $\overline{\text{MS}}$ scheme, $\Delta\mathcal{C}_{i,ab}$, according to

$$\Delta\mathcal{C}_{1,ab}(\mu_F^2) = (Z^{-1}(\mu_F^2))_{ad} \otimes \Delta\mathcal{C}_{1,db}^L(\mu_F^2). \quad (6.6)$$

where summation over the intermediate parton index d is implied. The explicit expressions for the finite renormalization constants are presented in Eqs. (3.32)-(3.35).

After obtaining the polarized and unpolarized coefficient functions, they are substituted into Eq. (6.1) to construct the corresponding hadronic structure functions. The resulting coefficient functions satisfy several non-trivial relations, whose origin can be understood by comparing the underlying electroweak interactions. Such comparisons also provide important consistency checks of the present calculation.

6.3 Comparison of the Coefficient Functions

The NNLO coefficient functions presented in the previous chapters involve both vector and axial-vector couplings of the electroweak gauge bosons. Owing to the presence of the axial-vector current, the treatment of γ_5 in dimensional regularization plays an important role in establishing the relation between different coefficient functions. In this section, we compare the coefficient functions obtained for different electroweak interactions and identify the diagram responsible for their differences. Throughout this comparison, we consider an even number of massless quark flavors;

hence, all quark triangle diagrams vanish identically and do not contribute. Furthermore, the overall electroweak coupling factors are omitted from the coefficient functions to facilitate a direct comparison.

The comparison is carried out in two stages. We first compare the coefficient functions for the unpolarized structure functions obtained from photon and Z -boson exchange, namely $\mathcal{C}_i^{\gamma\gamma}$ and $\mathcal{C}_i^{ZZ}$ for $i = 1, 2$. This comparison is performed at the level of the finite coefficient functions after ultraviolet renormalization and mass factorization, and illustrates how the presence of two γ_5 matrices at the electroweak vertices of the squared amplitude in the ZZ case affects the final result. Although the discussion is presented for the unpolarized coefficient functions, the same conclusions apply to the corresponding polarized coefficient functions.

We next compare the coefficient functions contributing to the parity-violating structure function F_3 with those contributing to the polarized structure function g_1 , namely $\mathcal{C}_3^{ZZ}$ and $\Delta\mathcal{C}_1^{\gamma\gamma}$ respectively. In this case, the γ_5 matrix originates from different parts of the amplitude, for $\mathcal{C}_3^{ZZ}$ it is associated with the axial-vector coupling of the exchanged electroweak boson, whereas for $\Delta\mathcal{C}_1^{\gamma\gamma}$ it arises from the polarized projector of the incoming quark (or antiquark). Whenever the γ_5 matrix can be anti-commuted along the fermion line using the naive anti-commutation relation, the corresponding contributions to $\mathcal{C}_3^{ZZ}$ and $\Delta\mathcal{C}_1^{\gamma\gamma}$ can be mapped onto each other. At NNLO, the comparison also requires excluding the mass-factorization terms associated with the diagram for which such an anti-commutation is not possible. With these contributions removed, the remaining coefficient functions are found to agree.

In both comparisons, the differences between the corresponding coefficient functions arise from NNLO diagram in which the γ_5 matrices cannot be related by the naive anticommutation procedure. A common feature of these differences is that they are all proportional to the color factor $C_F T_F$. We begin by comparing the coefficient functions for photon and Z -boson exchange contributing to the unpolarized structure

functions.

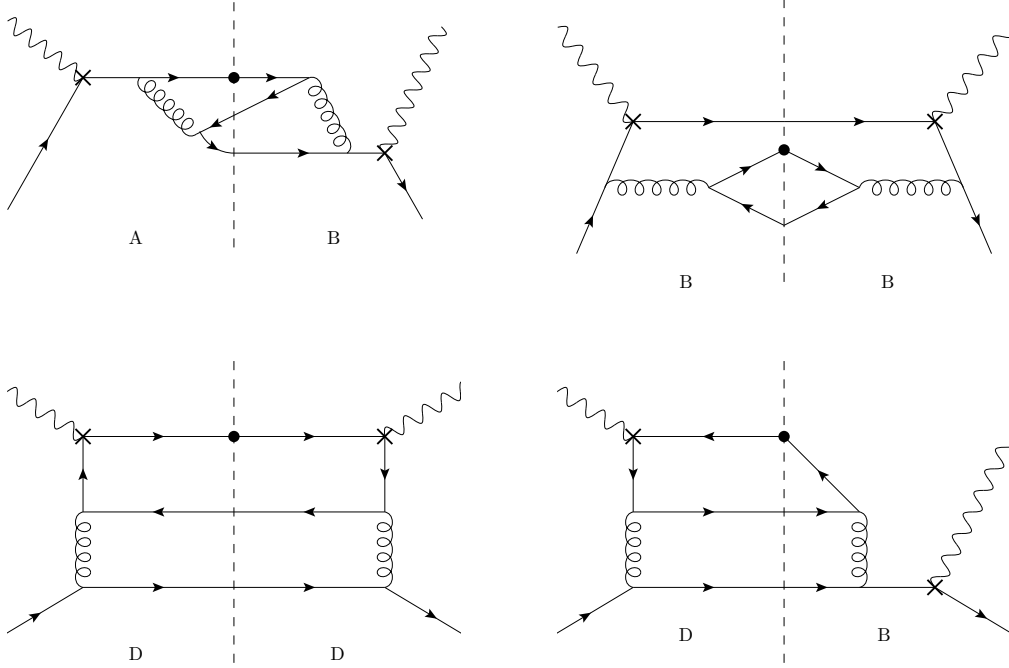


Figure 6.1: Representative diagrams illustrating the naive anti-commutation of the γ_5 matrix (marked by $\times$) through the fermion line. The fragmenting parton is indicated by a dot.

6.3.1 Comparison of $\mathcal{C}_i^{\gamma\gamma}$ and $\mathcal{C}_i^{ZZ}$

For the axial-vector contribution, the squared amplitudes contain two γ_5 matrices. Whenever these matrices belong to the same fermion trace, they can be brought together by repeatedly using the naive anti-commutation relation,

$$\{\gamma^\mu, \gamma_5\} = 0, \quad (6.7)$$

after which the identity $(\gamma_5)^2 = 1$ can be applied. Consequently, these contributions become identical to the corresponding vector-current coefficient functions. At NLO, after including the finite renormalization factor Z_{A5} , the coefficient functions $\mathcal{C}_i^{\gamma\gamma}$ and $\mathcal{C}_i^{ZZ}$ are identical for all partonic channels. At NNLO, the coefficient functions also remain identical for channels with a gluon in the initial and/or fragmenting state.

Therefore, in the following we restrict the discussion to quark-initiated channels.

At NNLO, for channels with a quark pair in the final state, see Figure 3.8, this correspondence holds diagram by diagram for all real-emission topologies of types A, B, C, and D, together with all interference contributions except the BD and AC interference diagrams. Figure 6.1 illustrates this property: for the first three diagrams, the two γ_5 insertions (marked by $\times$) can be moved to the same position along the fermion chain by repeated use of the naive anti-commutation relation. This is, however, not possible for the last diagram, where the two γ_5 matrices belong to different fermion traces. In contrast, for the double-virtual (VV), real-virtual (RV), and double real-gluon-emission contributions, the correspondence between the vector- and axial-vector parts does not hold diagram by diagram. Instead, the agreement is recovered only after summing all these contributions and including the axial-current renormalization factor Z_{A5} . Furthermore, the coefficient functions are identical for channels with a gluon in the initial and/or fragmenting state. Therefore, only quark-initiated channels are discussed below.

As a consequence, the non-singlet coefficient function $\mathcal{C}_{i,q\bar{q}}^{ZZ,(2)}$ differs from $\mathcal{C}_{i,q\bar{q}}^{\gamma\gamma,(2)}$ only through the BD interference diagrams. In these diagrams, the two γ_5 matrices belong to different fermion traces and therefore cannot be brought together using the naive anti-commutation relation, leading to a genuine difference between the vector and axial-vector coefficient functions.

An analogous situation occurs in the $q\bar{q}$ channel, where the unmatched contributions again arise from diagram topologies in which the two γ_5 matrices belong to different fermion traces. Likewise, in the flavor-changing qq' channel, the difference between $\mathcal{C}_{I,qq'}^{ZZ}$ and $\mathcal{C}_{I,qq'}^{\gamma\gamma}$ originates solely from the AC interference diagrams, for which the same argument applies.

Therefore, after ultraviolet renormalization, mass factorization, and the inclusion of the renormalization factor Z_{A5} , the only differences between the vector and axial-

vector coefficient functions arise in quark-initiated channels from NNLO diagram in which the two γ_5 matrices cannot be brought together into the same fermion trace.

6.3.2 Comparison between $\mathcal{C}_3^{ZZ}$ and $\Delta\mathcal{C}_1^{\gamma\gamma}$

The correspondence between $\mathcal{C}_3^{ZZ}$ and $\Delta\mathcal{C}_1^{\gamma\gamma}$ is examined similarly to the previous comparison, with the analysis carried out separately for the qq , $q\bar{q}$, and qq' channels. Since the γ_5 matrix in $\Delta\mathcal{C}_1^{\gamma\gamma}$ originates from the spin-dependent (polarized) projector of the incoming quark (or antiquark), such a comparison is restricted to quark-initiated processes. No analogous comparison can be made for gluon-initiated channels because the polarized gluon projector does not contain γ_5 . The comparison relies on anti-commuting the γ_5 matrix from the polarized projector along the fermion line to the electroweak interaction vertex using the naive commutation relation. Figure 6.2 illustrates this procedure. In the first two representative diagrams in a row, the γ_5 originating from the polarized external quark can be moved along the same fermion chain to the virtual gauge-boson vertex by repeated use of the naive anticommutation relation. Consequently, the resulting Dirac structures become identical to those of the corresponding axial-vector contribution in the ZZ channel, establishing the correspondence between the two coefficient functions.

In contrast, for channels with a fragmenting gluon, the correspondence holds and, after including the appropriate finite renormalization at NLO, the coefficient functions are found to agree. In contrast, for channels with a fragmenting gluon and the NLO coefficient functions agree after including the appropriate renormalization.

At NNLO, besides identifying the diagram for which the γ_5 matrix cannot be anti-commuted to the electroweak vertex, it is also necessary to exclude the corresponding mass-factorization contributions. For the remaining contributions, the correspondence between $\mathcal{C}_3^{ZZ}$ and $\Delta\mathcal{C}_1^{\gamma\gamma}$ is recovered only after combining the VV, RV, and

double real-gluon-emission contributions and including the renormalization factors Z_{A5} and Z_{ab} .

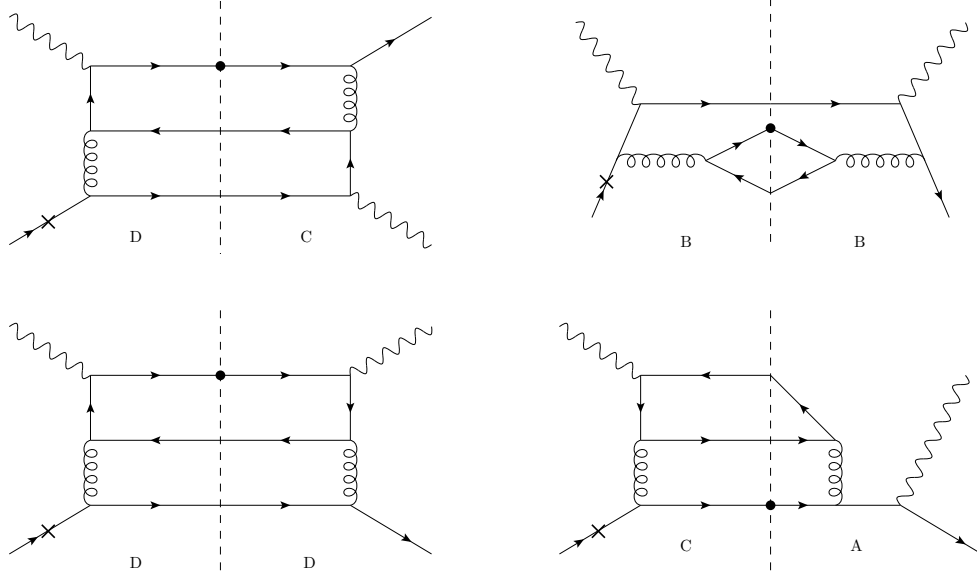


Figure 6.2: Representative diagrams illustrating that the γ_5 originating from the polarized external quark (marked by $\times$) can be brought to the interaction vertex by repeated application of the naive anti-commutation relation. The fragmenting parton is indicated by a filled dot.

For the qq channel, the comparison holds for all contributions except the D^2 and BD diagrams, including their associated mass factorization terms, for which the γ_5 matrix cannot be anti-commuted to the electroweak vertex along the fermion line. Consequently, the naive correspondence between the two coefficient functions does not hold for these contributions. After removing these contributions and including the corresponding renormalization factors Z_{A5} and Z -factor, the remaining parts of the two coefficient functions are in agreement.

In the $q\bar{q}$ channel, the unmatched contributions arise from D^2 and BD together with the corresponding mass-factorization terms. These are of the same type as in qq channel. Similarly, in the flavor-changing qq' channel, the only unmatched contribution originates from the AC interference diagrams and its associated mass-factorization term, with the same origin as in the previous channels. After excluding

these contributions and including the renormalization factors, the corresponding CFs agree.

This completes the comparison of the NNLO coefficient functions across the different electroweak channels, providing a non-trivial check of our results and confirm the treatment of γ_5 in dimensional regularization.

Checks: We have further performed several additional checks to validate our results. At NLO, our findings are in complete agreement with [74, 129]. In the soft plus virtual (SV) limit, where double-distribution terms alone contribute, the contributions of the $qq, \overline{q}q$ channel for NC and $u\overline{b}, \overline{b}u$ channel for CC survive and they are found to be identical. Recently, NNLO QCD predictions for both NC and CC processes have been published [183, 184]. We find complete analytical agreement for all terms containing distributions for all the channels and numerical agreement for the regular parts. Furthermore, all coefficient functions have been expressed in terms of single-valued polylogarithms. This allows to perform numerical computation over the entire kinematic range of x' and z' .

We now turn to the phenomenological implications of these findings.

6.4 Phenomenology

In this section, we investigate the numerical impact of the newly computed unpolarized NNLO coefficient functions on the neutral-current and charged-current SIDIS structure functions for different values of the scaling variables x and z . The structure functions are evaluated as convolutions of the perturbatively calculable coefficient functions with the corresponding PDFs and FFs. and expand the structure functions

in powers of the strong coupling constant as, (here setting $\mu_R^2 = \mu_F^2 = Q^2$)

$$\mathcal{F}_i^j = \sum_{k=0}^{\infty} a_s^k(\mu_R^2) \mathcal{F}_i^{j,(k)}(\mu_R^2). \quad (6.8)$$

In case of γ exchange, the SFs $\mathcal{F}_i^{\gamma\gamma}$, $i = 1, 2$ up to a_s^2 read

$$\mathcal{F}_i^{\gamma\gamma,(0)} = \sum_q e_q^2 H_{qq} \hat{\otimes} C_{I,qq}^{\gamma\gamma,(0)}, \quad (6.9)$$

$$\mathcal{F}_i^{\gamma\gamma,(1)} = \sum_q e_q^2 \left(H_{qq} \hat{\otimes} C_{I,qq}^{\gamma\gamma,(1)} + H_{qg} \hat{\otimes} C_{I,qg}^{\gamma\gamma,(1)} + H_{gq} \hat{\otimes} C_{I,gq}^{\gamma\gamma,(1)} \right), \quad (6.10)$$

$$\begin{aligned} \mathcal{F}_i^{\gamma\gamma,(2)} = & \sum_q e_q^2 H_{qq} \hat{\otimes} C_{I,qq}^{\gamma\gamma,(2),\text{NS}} + \sum_{q,q_k} e_q^2 \left(H_{qq} \hat{\otimes} C_{I,qq}^{\gamma\gamma,(2),\text{PS}} + H_{gg} \hat{\otimes} C_{I,gg}^{\gamma\gamma,(2)} \right) \\ & + \sum_q e_q^2 \left(H_{qg} \hat{\otimes} C_{I,qg}^{\gamma\gamma,(2)} + H_{gq} \hat{\otimes} C_{I,gq}^{\gamma\gamma,(2)} + H_{q\bar{q}} \hat{\otimes} C_{I,q\bar{q}}^{\gamma\gamma,(2)} \right) \\ & + \sum_q \sum_{q' \neq q} \left(e_q^2 H_{qq'}^+ \hat{\otimes} C_{I,qq'}^{\gamma\gamma,(2),[1]} + e_{q'}^2 H_{qq'}^+ \hat{\otimes} C_{I,qq'}^{\gamma\gamma,(2),[2]} + e_q e_{q'} H_{qq'}^- \hat{\otimes} C_{I,qq'}^{\gamma\gamma,(2),[3]} \right). \end{aligned} \quad (6.11)$$

For γZ interference, the SFs $\mathcal{F}_i^{\gamma Z}$, $i = 1, 2$ up to a_s^2 are given by

$$-\mathcal{F}_i^{\gamma Z,(0)} = \sum_q 2e_q \bar{g}_{V_q} H_{qq} \hat{\otimes} C_{I,qq}^{\gamma\gamma,(0)}, \quad (6.12)$$

$$-\mathcal{F}_i^{\gamma Z,(1)} = \sum_q 2e_q \bar{g}_{V_q} \left(H_{qq} \hat{\otimes} C_{I,qq}^{\gamma\gamma,(1)} + H_{qg} \hat{\otimes} C_{I,qg}^{\gamma\gamma,(1)} + H_{gq} \hat{\otimes} C_{I,gq}^{\gamma\gamma,(1)} \right), \quad (6.13)$$

$$\begin{aligned} -\mathcal{F}_i^{\gamma Z,(2)} = & \sum_q 2e_q \bar{g}_{V_q} H_{qq} \hat{\otimes} C_{I,qq}^{\gamma\gamma,(2),\text{NS}} + \sum_{q,q_k} 2e_{q_k} \bar{g}_{V_{q_k}} \left(H_{qq} \hat{\otimes} C_{I,qq}^{\gamma\gamma,(2),\text{PS}} + H_{gg} \hat{\otimes} C_{I,gg}^{\gamma\gamma,(2)} \right) \\ & + \sum_q 2e_q \bar{g}_{V_q} \left(H_{qg} \hat{\otimes} C_{I,qg}^{\gamma\gamma,(2)} + H_{gq} \hat{\otimes} C_{I,gq}^{\gamma\gamma,(2)} + H_{q\bar{q}} \hat{\otimes} C_{I,q\bar{q}}^{\gamma\gamma,(2)} \right) \\ & + \sum_q \sum_{q' \neq q} \left(2e_q \bar{g}_{V_q} H_{qq'}^+ \hat{\otimes} C_{I,qq'}^{\gamma\gamma,(2),[1]} + 2e_{q'} \bar{g}_{V_{q'}} H_{qq'}^+ \hat{\otimes} C_{I,qq'}^{\gamma\gamma,(2),[2]} \right. \\ & \left. + \left(e_{q'} \bar{g}_{V_q} + e_q \bar{g}_{V_{q'}} \right) H_{qq'}^- \hat{\otimes} C_{I,qq'}^{\gamma\gamma,(2),[3]} \right), \end{aligned} \quad (6.14)$$

In case of Z -boson exchange, the SFs $\mathcal{F}_i^{ZZ}$, $i = 1, 2$ up to a_s^2 we have

$$\mathcal{F}_i^{ZZ,(0)} = \sum_q \left(\bar{g}_{V_q}^2 + \bar{g}_{A_q}^2 \right) H_{qq} \hat{\otimes} C_{I,qq}^{\gamma\gamma,(0)}, \quad (6.15)$$

$$\mathcal{F}_i^{ZZ,(1)} = \sum_q \left(\bar{g}_{V_q}^2 + \bar{g}_{A_q}^2 \right) \left(H_{qq} \hat{\otimes} C_{I,qq}^{\gamma\gamma,(1)} + H_{qg} \hat{\otimes} C_{I,qg}^{\gamma\gamma,(1)} + H_{gq} \hat{\otimes} C_{I,gq}^{\gamma\gamma,(1)} \right), \quad (6.16)$$

$$\begin{aligned} \mathcal{F}_i^{ZZ,(2)} = & \sum_q H_{qq} \hat{\otimes} \left(\bar{g}_{V_q}^2 C_{I,qq}^{\gamma\gamma,(2),\text{NS}} + \bar{g}_{A_q}^2 C_{I,qq}^{AA,(2),\text{NS}} \right) \\ & + \sum_{q,q_k} \left(\bar{g}_{V_{q_k}}^2 + \bar{g}_{A_{q_k}}^2 \right) \left(H_{qq} \hat{\otimes} C_{I,qq}^{\gamma\gamma,(2),\text{PS}} + H_{gg} \hat{\otimes} C_{I,gg}^{\gamma\gamma,(2)} \right) \\ & + \sum_q \left(\bar{g}_{V_q}^2 + \bar{g}_{A_q}^2 \right) \left(H_{qg} \hat{\otimes} C_{I,qg}^{\gamma\gamma,(2)} + H_{gq} \hat{\otimes} C_{I,gq}^{\gamma\gamma,(2)} \right) \\ & + \sum_q H_{q\bar{q}} \hat{\otimes} \left(\bar{g}_{V_q}^2 C_{I,q\bar{q}}^{\gamma\gamma,(2)} + \bar{g}_{A_q}^2 C_{I,q\bar{q}}^{AA,(2)} \right) \\ & + \sum_q \sum_{q' \neq q} \left(\left(\bar{g}_{V_q}^2 + \bar{g}_{A_q}^2 \right) H_{qq'}^+ \hat{\otimes} C_{I,qq'}^{\gamma\gamma,(2),[1]} + \left(\bar{g}_{V_{q'}}^2 + \bar{g}_{A_{q'}}^2 \right) H_{qq'}^+ \hat{\otimes} C_{I,qq'}^{\gamma\gamma,(2),[2]} \right. \\ & \left. + \bar{g}_{V_q} \bar{g}_{V_{q'}} H_{qq'}^- \hat{\otimes} C_{I,qq'}^{\gamma\gamma,(2),[3]} + \bar{g}_{A_q} \bar{g}_{A_{q'}} H_{qq'}^+ \hat{\otimes} C_{I,qq'}^{AA,(2),[3]} \right), \end{aligned} \quad (6.17)$$

where H_{ab} are given by,

$$\begin{aligned} H_{qq} &= f_q(x) D_q(z) + f_{\bar{q}}(x) D_{\bar{q}}(z), \quad H_{q\bar{q}} = f_q(x) D_{\bar{q}}(z) + f_{\bar{q}}(x) D_q(z), \\ H_{qg} &= f_q(x) D_g(z) + f_{\bar{q}}(x) D_g(z), \quad H_{gq} = f_g(x) D_q(z) + f_g D_{\bar{q}}(z), \\ H_{qq'}^\pm &= f_q(x) D_{q'}(z) \pm f_q(x) D_{\bar{q}'}(z) \pm f_{\bar{q}}(x) D_{q'}(z) + f_{\bar{q}}(x) D_{\bar{q}'}(z), \\ H_{gg} &= f_g(x) D_g(z). \end{aligned} \quad (6.18)$$

Here, $\bar{g}_{V_f}$ and $\bar{g}_{A_f}$ are defined in Eqs. (2.13), (2.14). For CC SIDIS, the SFs $\mathcal{F}_i^{W^-}$, $i = 1, 2$ are found to be

$$\frac{1}{2} \mathcal{F}_i^{W^-, (0)} = \sum_{u,b} |\bar{V}_{ub}|^2 (H_{ub} + H_{\bar{b}\bar{u}}) \hat{\otimes} C_{I,qq}^{\gamma\gamma,(0)}, \quad (6.19)$$

$$\frac{1}{2} \mathcal{F}_i^{W^-, (1)} = \sum_{u,b} |\bar{V}_{ub}|^2 \left((H_{ub} + H_{\bar{b}\bar{u}}) \hat{\otimes} C_{I,qq}^{\gamma\gamma,(1)} + (H_{ug} + H_{\bar{b}g}) \hat{\otimes} C_{I,qg}^{\gamma\gamma,(1)} \right)$$

$$+ \left(H_{gb} + H_{g\bar{u}} \right) \hat{\otimes} C_{I,gq}^{\gamma\gamma,(1)}, \quad (6.20)$$

$$\begin{aligned} \frac{1}{2} \mathcal{F}_i^{W^-, (2)} = & \sum_{\mathbf{u}, \mathbf{b}} |\bar{V}_{\mathbf{u}\mathbf{b}}|^2 (H_{\mathbf{u}\mathbf{b}} + H_{\bar{\mathbf{b}}\bar{\mathbf{u}}}) \hat{\otimes} C_{I,qq}^{W^-, (2), [1]} \\ & + \sum_{\mathbf{u}, \mathbf{b}} \left(\left(\sum_{\beta} |\bar{V}_{\mathbf{u}\beta}|^2 \right) H_{\mathbf{u}\mathbf{b}} + \left(\sum_{\alpha} |\bar{V}_{\alpha\mathbf{b}}|^2 \right) H_{\bar{\mathbf{b}}\bar{\mathbf{u}}} \right) \hat{\otimes} C_{I,qq'}^{\gamma\gamma, (2), [1]} \\ & + \sum_{\mathbf{u}, \mathbf{b}} \left(\left(\sum_{\alpha} |\bar{V}_{\alpha\mathbf{b}}|^2 \right) H_{\mathbf{u}\mathbf{b}} + \left(\sum_{\beta} |\bar{V}_{\mathbf{u}\beta}|^2 \right) H_{\bar{\mathbf{b}}\bar{\mathbf{u}}} \right) \hat{\otimes} C_{I,qq'}^{\gamma\gamma, (2), [2]} \\ & + \sum_{\mathbf{u}, \mathbf{b}} |\bar{V}_{\mathbf{u}\mathbf{b}}|^2 (H_{\mathbf{u}g} + H_{\bar{\mathbf{b}}g}) \hat{\otimes} C_{I,gg}^{\gamma\gamma, (2)} + \sum_{\mathbf{u}, \mathbf{b}} |\bar{V}_{\mathbf{u}\mathbf{b}}|^2 (H_{\mathbf{u}\mathbf{u}} + H_{\bar{\mathbf{b}}\bar{\mathbf{b}}}) \hat{\otimes} C_{I,qq}^{W^-, (2), [2]} \\ & + \left(\sum_{\alpha, \beta} |\bar{V}_{\alpha\beta}|^2 \right) \left(\sum_{\mathbf{u}} H_{\mathbf{u}\mathbf{u}} + \sum_{\mathbf{b}} H_{\bar{\mathbf{b}}\bar{\mathbf{b}}} \right) \hat{\otimes} C_{I,qq}^{\gamma\gamma, (2), \text{PS}} \\ & + \sum_{\mathbf{u}, \mathbf{b}} |\bar{V}_{\mathbf{u}\mathbf{b}}|^2 (H_{\bar{\mathbf{b}}\mathbf{b}} + H_{\mathbf{u}\bar{\mathbf{u}}}) \hat{\otimes} C_{I,qq}^{W^-, (2), [3]} + \sum_{\mathbf{u}, \mathbf{b}} |\bar{V}_{\mathbf{u}\mathbf{b}}|^2 (H_{\mathbf{u}\bar{\mathbf{u}}} + H_{\bar{\mathbf{b}}\mathbf{b}}) \hat{\otimes} C_{I,q\bar{q}}^{W^-, (2), [1]} \\ & + \left(\sum_{\alpha, \beta} |\bar{V}_{\alpha\beta}|^2 \right) \left(\sum_{\mathbf{b}} H_{\bar{\mathbf{b}}\mathbf{b}} + \sum_{\mathbf{u}} H_{\mathbf{u}\bar{\mathbf{u}}} \right) \hat{\otimes} C_{I,qq}^{\gamma\gamma, (2), \text{PS}} \\ & + \sum_{\mathbf{u}, \mathbf{b}} \left(\left(\sum_{\beta} |\bar{V}_{\mathbf{u}\beta}|^2 \right) H_{\mathbf{u}\bar{\mathbf{b}}} + \left(\sum_{\alpha} |\bar{V}_{\alpha\mathbf{b}}|^2 \right) H_{\bar{\mathbf{b}}\mathbf{u}} \right) \hat{\otimes} C_{I,qq'}^{\gamma\gamma, (2), [1]} \\ & + \sum_{\mathbf{u}, \mathbf{b}} |\bar{V}_{\mathbf{u}\mathbf{b}}|^2 (H_{\mathbf{u}\bar{\mathbf{b}}} + H_{\bar{\mathbf{b}}\mathbf{u}}) \hat{\otimes} C_{I,q\bar{q}}^{W^-, (2), [2]} + \sum_{\mathbf{u}, \mathbf{b}} |\bar{V}_{\mathbf{u}\mathbf{b}}|^2 (H_{\bar{\mathbf{b}}\mathbf{u}} + H_{\mathbf{u}\bar{\mathbf{b}}}) \hat{\otimes} C_{I,q\bar{q}}^{W^-, (2), [3]} \\ & + \sum_{\mathbf{u}, \mathbf{b}} \left(\left(\sum_{\beta} |\bar{V}_{\mathbf{u}\beta}|^2 \right) H_{\bar{\mathbf{b}}\mathbf{u}} + \left(\sum_{\alpha} |\bar{V}_{\alpha\mathbf{b}}|^2 \right) H_{\mathbf{u}\bar{\mathbf{b}}} \right) \hat{\otimes} C_{I,qq'}^{\gamma\gamma, (2), [2]} \\ & + \left(\sum_{\mathbf{u}, \mathbf{u}'} \left(\sum_{\beta} |\bar{V}_{\mathbf{u}\beta}|^2 \right) H_{\mathbf{u}\mathbf{u}'} + \sum_{\mathbf{b}, \mathbf{b}'} \left(\sum_{\alpha} |\bar{V}_{\alpha\mathbf{b}}|^2 \right) H_{\bar{\mathbf{b}}\bar{\mathbf{b}}'} \right) \hat{\otimes} C_{I,qq'}^{\gamma\gamma, (2), [1]} \\ & + \left(\sum_{\mathbf{b}, \mathbf{b}'} \left(\sum_{\alpha} |\bar{V}_{\alpha\mathbf{b}'}|^2 \right) H_{\bar{\mathbf{b}}\mathbf{b}'} + \sum_{\mathbf{u}, \mathbf{u}'} \left(\sum_{\beta} |\bar{V}_{\mathbf{u}\beta}|^2 \right) H_{\mathbf{u}\bar{\mathbf{u}}'} \right) \hat{\otimes} C_{I,qq'}^{\gamma\gamma, (2), [2]} \\ & + \sum_{\mathbf{u}, \mathbf{b}} |\bar{V}_{\mathbf{u}\mathbf{b}}|^2 (H_{g\mathbf{b}} + H_{g\bar{\mathbf{u}}}) \hat{\otimes} C_{I,gq}^{\gamma\gamma, (2)} + \sum_{\mathbf{u}, \mathbf{b}} |\bar{V}_{\mathbf{u}\mathbf{b}}|^2 H_{gg} \hat{\otimes} C_{I,gg}^{\gamma\gamma, (2)} \\ & + \left(\sum_{\mathbf{u}, \mathbf{u}'} \left(\sum_{\beta} |\bar{V}_{\mathbf{u}\beta}|^2 \right) H_{\mathbf{u}\bar{\mathbf{u}}'} + \sum_{\mathbf{b}, \mathbf{b}'} \left(\sum_{\alpha} |\bar{V}_{\alpha\mathbf{b}}|^2 \right) H_{\bar{\mathbf{b}}\mathbf{b}'} \right) \hat{\otimes} C_{I,qq'}^{\gamma\gamma, (2), [1]} \\ & + \left(\sum_{\mathbf{u}, \mathbf{u}'} \left(\sum_{\beta} |\bar{V}_{\mathbf{u}\beta}|^2 \right) H_{\mathbf{u}\bar{\mathbf{u}}'} + \sum_{\mathbf{b}, \mathbf{b}'} \left(\sum_{\alpha} |\bar{V}_{\alpha\mathbf{b}'}|^2 \right) H_{\bar{\mathbf{b}}\mathbf{b}'} \right) \hat{\otimes} C_{I,qq'}^{\gamma\gamma, (2), [2]}. \quad (6.21) \end{aligned}$$

with up-and down-type quarks, $\mathbf{u}, \alpha = \{u, c, (t)\}$ and $\mathbf{b}, \beta = \{d, s, (b)\}$. The symbol $\hat{\otimes}$ denotes the convolutions in both variables x and z and here $H_{ab} = f_a(x)D_b(z)$

with $\overline{V}_{ff'}$ is defined in Eq. (2.15).

We now illustrate the numerical impact of the NC and CC contributions to the unpolarized SF $\mathcal{F}_1$ as functions of the scaling variables x in Figs. 6.3 and 6.4, at a center-of-mass energy $\sqrt{s} = 140$ GeV anticipated at the EIC. NNPDF31 PDFs [277] and NNFF10 FFs [64] are used consistently at LO, NLO, and NNLO, with $n_f = 4$ active quark flavors. Here y is integrated over $[0.5, 0.9]$ and z over $[0.2, 0.85]$. The average momentum transfer is defined as $Q_{\text{avg}}^2 = s x y_{\text{avg}}$, with the central scale choice $\mu_R = \mu_F = Q_{\text{avg}}$. $\mathcal{F}_1^{\text{NC}}$ and $\mathcal{F}_1^{\text{CC}}$.

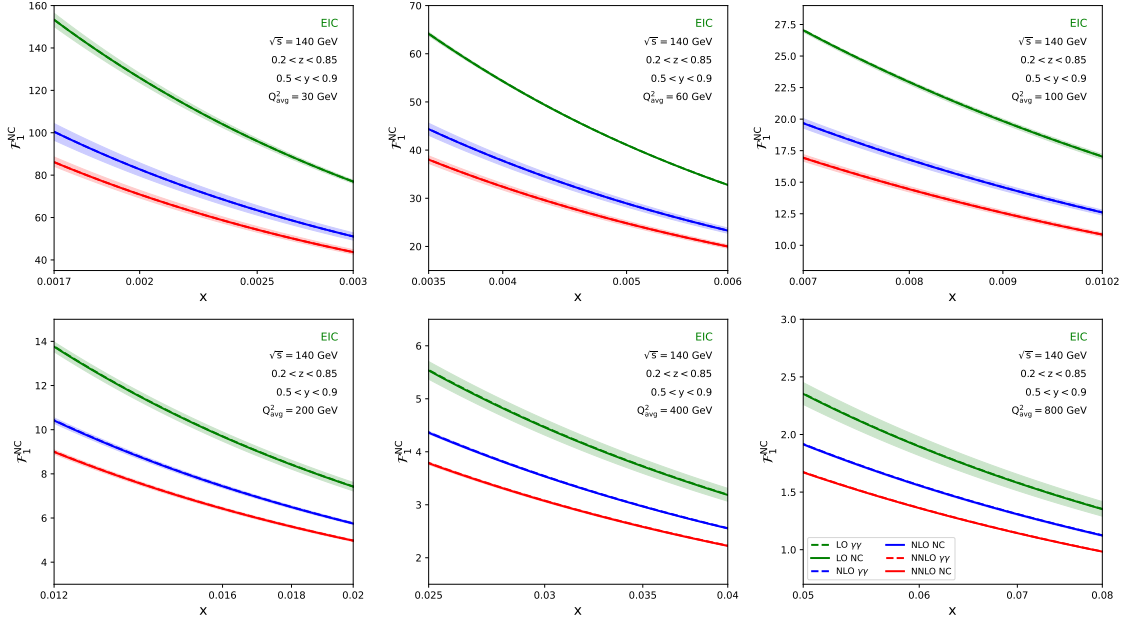


Figure 6.3: Variation of $\mathcal{F}_1^{\text{NC}}$ with the renormalization and factorization scales as a function of x for six different values of Q^2 .

To study the dependence of the predictions on the choice of renormalization and factorization scales over a range of momentum transfers, we present in Figs. 6.3 and 6.4 the seven-point scale variation of the structure functions $\mathcal{F}_1^{\text{NC}}$ and $\mathcal{F}_1^{\text{CC}}$ as functions of x . The results are shown for six representative values of the momentum transfer, $Q_{\text{avg}}^2 = \{30, 60, 100, 200, 400, 800\} \text{ GeV}^2$. For each value of Q^2 , the corresponding range of x is determined by demanding the inelasticity variable $y = Q^2/(xs)$ to lie in the interval $0.5 \leq y \leq 0.9$. The renormalization and factorization scales

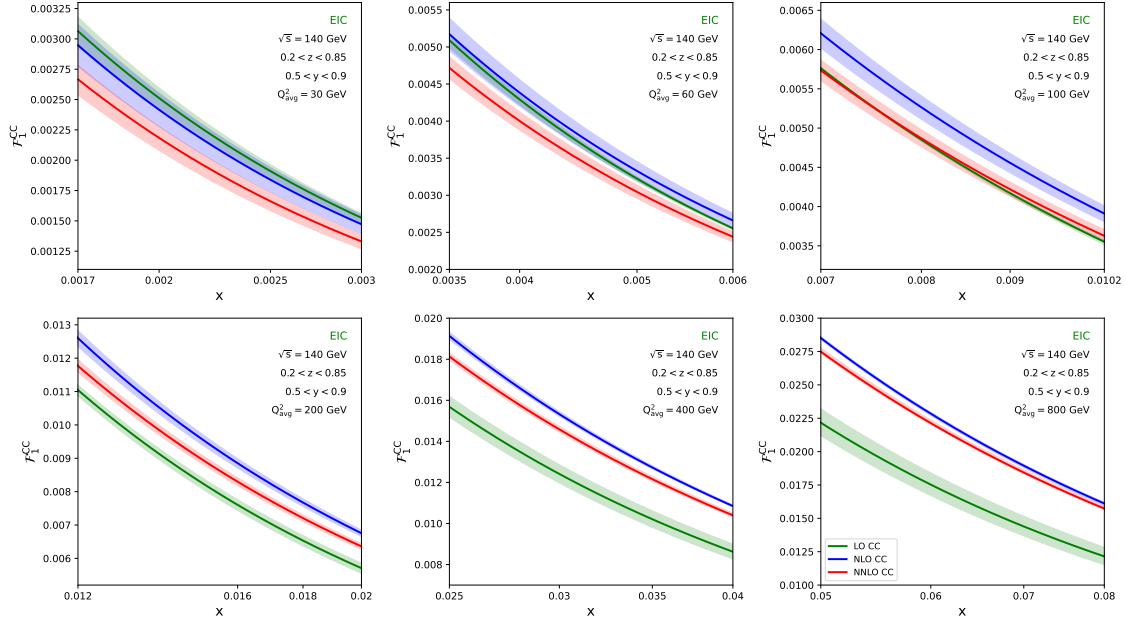


Figure 6.4: Variation of $\mathcal{F}_1^{\text{CC}}$ with the renormalization and factorization scales as a function of x for six different values of Q^2 .

are varied independently by a factor of two, with $\mu_R^2, \mu_F^2 \in [Q^2/2, 2Q^2]$, subject to the constraint $1/2 \leq \mu_R^2/\mu_F^2 \leq 2$, corresponding to the standard seven-point scale variation.

The large uncertainty bands of the LO predictions, particularly for the $\mathcal{F}_1^{\text{NC}}$ and $\mathcal{F}_1^{\text{CC}}$ structure functions, arise primarily from the factorization scale dependence of the PDFs and FFs. The results shown in Figs. 6.3 and 6.4 clearly demonstrate that the inclusion of higher order QCD corrections substantially reduces the μ_F dependence. The renormalization scale dependence can be meaningfully assessed only from NLO onwards, as illustrated by the plots on the left and in the center. A comparison of the NLO and NNLO uncertainty bands reveals a significant reduction in the μ_R dependence at NNLO. Together with the observed improvement in the convergence of the perturbative series for SIDIS, this reduced scale sensitivity provides strong support for the robustness of our theoretical framework.

We now illustrate the numerical impact of the NC and CC contributions to the unpolarized SF $\mathcal{F}_1$ as functions of the scaling variable z in Figs. 6.5 and 6.6, at a

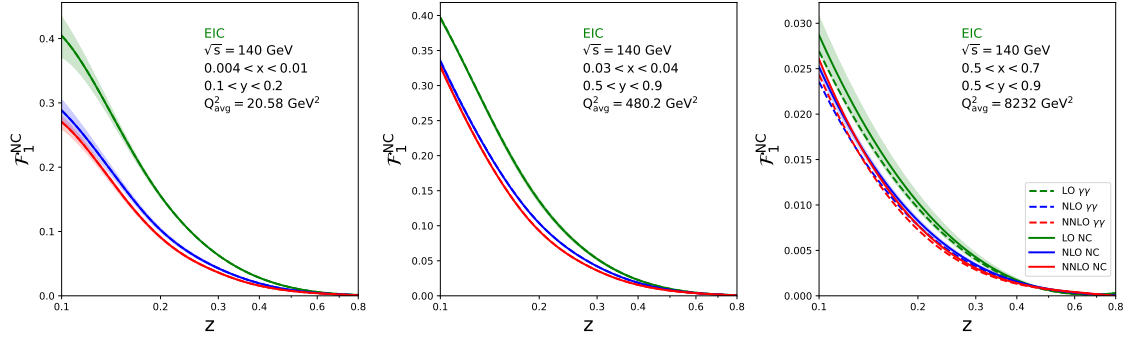


Figure 6.5: Variation of $\mathcal{F}_1^{\text{NC}}$ with the renormalization and factorization scales as a function of z for three values of Q^2 .

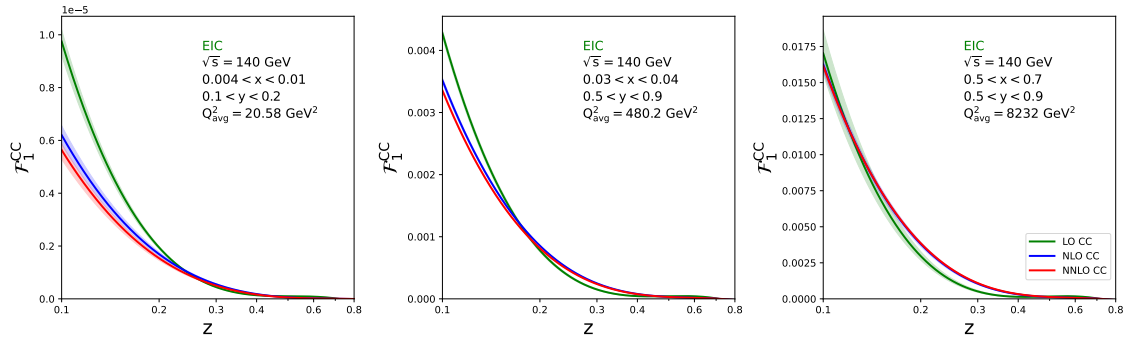


Figure 6.6: Variation of $\mathcal{F}_1^{\text{CC}}$ with the renormalization and factorization scales as a function of z for three values of Q^2 .

center-of-mass energy $\sqrt{s} = 140$ GeV anticipated at the EIC. NNPDF31 PDFs [277] and NNFF10 FFs [64] are used consistently at LO, NLO, and NNLO, with $n_f = 4$ active quark flavors. For these plots, x is integrated over $[0.1, 0.8]$ and y over $[0.5, 0.9]$. The average momentum transfer is defined as $Q_{\text{avg}}^2 = s x_{\text{avg}} y_{\text{avg}}$, with the central scale choice $\mu_R = \mu_F = Q_{\text{avg}}$.

The shaded bands in all panels correspond to the seven-point variation of the renormalization and factorization scales, $\mu_R^2, \mu_F^2 \in [Q_{\text{avg}}^2/2, 2Q_{\text{avg}}^2]$ with the constraint $1/2 \leq \mu_R^2/\mu_F^2 \leq 2$, capturing the combined uncertainty from scale choices after integration over different ranges of x and y , such that each range gives a fixed value of Q_{avg} , as indicated in each plot. The bands in the plots represent the seven-point scale variation around Q_{avg}^2 . As before, the dependence on the renormalization and factorization scales is significantly reduced upon the inclusion of the NLO and NNLO

QCD corrections. The results show that NNLO QCD corrections are significant and play a crucial role in reducing theoretical uncertainties from the choice of μ_R and μ_F . The scale variation bands shrink notably from LO to NLO and NNLO, demonstrating improved perturbative convergence and enhanced stability at higher orders. At NNLO accuracy, the perturbative expansion exhibits both apparent convergence and robustness against scale variations, providing a reliable baseline for precision predictions of SIDIS observables.

Figs. 6.3 and 6.5 show that the photon-mediated contribution dominates in the NC channel. This behavior can be understood from the propagator structure: the photon contribution scales as $1/Q^2$, whereas the Z -boson contribution is suppressed by the massive propagator $1/(Q^2 + M_Z^2)$, which reduces its impact for $Q^2 < M_Z^2$. In addition, the Z -boson couplings to fermions involve both vector and axial-vector components with weaker effective strengths compared to the electromagnetic coupling, further suppressing its contribution. A similar suppression is observed for the CC structure function in Figs. 6.4 and 6.6. This suppression mainly arises from the massive propagator $1/(Q^2 + M_W^2)$, as well as purely left-handed charged-current interaction of W -boson couplings restricting the contributing fermionic configurations and reducing the overall magnitude relative to photon exchange.

6.5 Summary

In this chapter, we presented the complete NNLO QCD coefficient functions for unpolarized and polarized SIDIS, including both neutral-current and charged-current electroweak interactions. We investigated the correspondence between coefficient functions associated with different electroweak currents, identifying the origin of the genuine differences arising from the treatment of γ_5 in dimensional regularization. These comparisons provide important consistency checks of our calculation and are

in agreement with recent independent results.

The phenomenological analysis demonstrates that the NNLO corrections have a significant impact on SIDIS observables over the kinematic region relevant to the Electron-Ion Collider (EIC). The different electroweak channels exhibit complementary sensitivities to the underlying partonic structure, allowing flavor-dependent information on parton distribution functions and fragmentation functions to be disentangled through polarization and charged-current/neutral-current asymmetries.

Overall, the results presented in this chapter establish a complete NNLO framework for precision studies of SIDIS. Combined with the broad kinematic coverage and particle identification capabilities of the EIC, they open the door to precision tests of QCD and electroweak interactions in semi-inclusive processes. These results will improve the extraction of PDFs and FFs, providing more precise, improved constraints on the flavor structure of the nucleon and support future investigations of nucleon structure and the proton spin at the EIC.

Chapter 7

Conclusion

The work presented in the thesis has been devoted to the development of precision perturbative QCD predictions for semi-inclusive deep-inelastic scattering (SIDIS), with particular emphasis on next-to-next-to leading order (NNLO) corrections, the analytic evaluation of master integrals, threshold resummation beyond fixed order, and the extension to neutral-current and charged-current electroweak interactions. SIDIS is one of the key processes for the future Electron-Ion Collider, since it provides simultaneous access to the partonic structure of the incoming nucleon through parton distribution functions and to the hadronization of final-state partons through fragmentation functions. The high precision expected at the EIC makes equally precise theoretical predictions essential. The work presented in this thesis addresses this need by providing higher-order perturbative ingredients required for precision SIDIS phenomenology. These results establish a substantially improved perturbative foundation for precision SIDIS phenomenology and provide the ingredients needed to fully exploit the anticipated accuracy of future EIC measurements.

Chapter 1 introduced the basic theoretical framework of Quantum Chromodynamics. After motivating QCD as the non-Abelian gauge theory of the strong interaction, the chapter reviewed the QCD Lagrangian, the corresponding Feynman rules, and

the general structure of perturbative calculations. The role of ultraviolet renormalization was discussed, together with the appearance of infrared singularities in perturbative QCD. These concepts therefore provide the general field-theoretic framework needed for the fixed-order and resummed calculations developed in the later chapters.

Chapter 2 presented the theoretical preliminaries of semi-inclusive deep-inelastic scattering. Starting from inclusive DIS, the chapter reviewed how lepton-hadron scattering provides direct information about the partonic structure of hadrons. The discussion was then extended to semi-inclusive processes, where an identified hadron is observed in the final state. This additional measurement makes SIDIS sensitive not only to parton distribution functions, but also to fragmentation functions. The SIDIS kinematics, scaling variables, hadronic tensor, and structure functions were introduced. The QCD factorization formula was discussed, in which the measured structure functions are expressed as convolutions of parton distribution functions, fragmentation functions, and perturbatively calculable coefficient functions. This chapter established the notation and theoretical setup used throughout the thesis.

Having established the SIDIS framework, in Chapter 3, we turned to the main fixed-order calculation of the thesis. This chapter was devoted to the computation of the NNLO QCD corrections to polarized SIDIS, providing the first complete result for the corresponding coefficient functions at this order. The relevant partonic subprocesses contributing at different perturbative orders were identified, including the double-virtual, real-virtual, and double-real contributions at NNLO. The chapter described the loop and phase-space integrals entering the calculation, the pole structure of the partonic results, and the procedure of mass factorization needed to obtain finite coefficient functions. The inclusion of higher-order corrections was shown to be essential for reducing the dependence on unphysical scales like renormalization and factorization scales and for improving the reliability of theoretical

predictions. The phenomenological impact of the NNLO corrections was also discussed, demonstrating their importance for future precision analyses of SIDIS.

Chapter 4 focused on the evaluation of the master integrals required for the NNLO calculation. The integrals arising from the double-virtual (VV), real-virtual (RV), and double-real (RR) contributions were discussed separately. Reverse unitarity was used to treat phase-space integrals within the framework of integration-by-parts reduction. For the RV case, the analytic continuation required to obtain results in the physical SIDIS region was described. The RR contribution required the evaluation of new master integrals, which were computed using different methods. These included direct phase-space parametrizations and the differential equation method, together with the construction of canonical bases and the techniques required to obtain analytic solutions. The results of this chapter provide one of the central technical ingredients of the complete NNLO calculation.

Building on the fixed-order NNLO results, Chapter 5 extended the analysis beyond fixed-order perturbation theory by developing the threshold resummation framework for SIDIS. Near partonic threshold, the perturbative coefficient functions contain enhanced logarithmic contributions arising from soft and collinear configurations of QCD radiation, which can become dominant in the threshold limit i.e. $x' \rightarrow 1$ and $z' \rightarrow 1$. Using QCD factorization, renormalization-group invariance, the finiteness of coefficient functions, and the transcendentality structure of the one- and two-loop results, the chapter systematically obtained the an all-order expression for the diagonal coefficient functions in the threshold limit. A master formula was derived to organize the soft-plus-virtual (SV) and next-to-SV logarithmic contributions to all orders in the strong coupling. The all-order structure was further studied in Mellin space, where the resummation was achieved up to $\overline{\text{NNLL}}$ accuracy. The physical evolution kernel was also discussed as an alternative approach for understanding the structure of threshold logarithms. The resummed results were expanded to ob-

tain predictions for threshold-enhanced terms beyond NNLO, up to fourth order in perturbation theory. The phenomenological studies presented in this chapter illustrated the relevance of threshold-enhanced contributions in the kinematic regions important for SIDIS.

While the preceding chapters focused on QCD corrections to photon-mediated SIDIS, the broad kinematic reach and polarized beams of the EIC make neutral-current and charged-current SIDIS important. These processes provide complementary probes for disentangling the flavor and spin structure of the nucleon. This motivated Chapter 6, where the NNLO analysis was extended to SIDIS mediated by electroweak currents. The methodology for including photon, Z boson, photon- Z interference, and $W^\pm$ exchange contributions was described. The chapter presented the corresponding coefficient functions for polarized and unpolarized processes. The treatment of axial-vector couplings and γ_5 in dimensional regularization was discussed, together with the corresponding renormalization factors. Several comparisons among the coefficient functions were performed, including the relation between photon and Z mediated contributions and the comparison between certain parity-violating and polarized coefficient functions. These comparisons provided non-trivial checks of the calculation and of the treatment of axial-vector couplings. The chapter also presented phenomenology relevant for future EIC studies, showing the importance of electroweak SIDIS channels for flavor separation and precision analyses.

Taken together, the results of this thesis fill an important gap in the perturbative description of SIDIS. Prior to this work, the coefficient functions for SIDIS were known completely only up to NLO, while only approximate NNLO results (in the threshold limit) were available in the literature. This thesis completes the NNLO QCD description of polarized SIDIS by providing the full coefficient functions at this order, together with the master integrals required for their analytic computation and a systematic framework for threshold resummation beyond fixed order. Together

with the extension to neutral-current and charged-current electroweak SIDIS, these results establish a substantially improved theoretical foundation for precision SIDIS phenomenology.

The complete NNLO coefficient functions obtained in this thesis enable SIDIS analyses at the accuracy required for precision extractions of parton distribution functions, polarized parton distributions, and fragmentation functions. The improved perturbative stability and reduced residual scale dependence will be essential for reliable phenomenological studies and global QCD analyses in the EIC era.

Several future directions naturally follow from this work. An important next step is the implementation of the complete NNLO coefficient functions in phenomenological programs and global QCD analyses. This will make it possible to quantify the impact of the NNLO corrections on the extraction of PDFs, polarized PDFs, and fragmentation functions using existing SIDIS measurements and the high-precision data expected from the EIC. Such studies will be particularly important for assessing the reduction of perturbative uncertainties, improving quark-flavor separation, and obtaining more precise information on the spin and flavor structure of the nucleon.

Another important direction is the systematic inclusion of mixed QCD-QED and QCD-electroweak corrections. As the experimental precision of SIDIS measurements increases, electroweak effects may become relevant at a level comparable to the remaining QCD uncertainties. A complete precision framework will therefore require a consistent combination of QCD, QED, and electroweak corrections, together with the corresponding coupled evolution of parton distribution and fragmentation functions.

A longer term direction is the extension of the fixed-order calculation to $N^3\text{LO}$ in QCD. Although technically challenging, the threshold resummation framework developed in this thesis already predicts important soft-virtual and next-to-soft contributions at this order and higher, providing useful approximations and checks for

future complete calculations. Further progress may be achieved by matching higher-accuracy resummation to the NNLO results and extending the analysis beyond diagonal partonic channels.

Appendix A

Analytical Continuation in RV Integrals

The hypergeometric functions (HFs) appearing in our calculation are generally expressed through their standard series representation, which converges only within a restricted domain of the argument. In several kinematic regions, however, the arguments of these functions may lie outside the convergence region, thereby requiring an analytic continuation to region where argument is less than 1. In addition, the accompanying prefactors of HFs containing non-integer powers can also develop branch cut structures and therefore require careful treatment.

To perform the continuation consistently, it is necessary to keep track of the appropriate branch structure in the complex plane. This is achieved by introducing the Feynman $+i0$ prescription for the kinematic variables, which enables an unambiguous identification of the branch and ensures the correct analytic continuation across branch cuts. To illustrate the procedure, we discuss two representative examples below.

We begin with the first example and analyse the analytic structure of the prefactor

and the argument of the hypergeometric function appearing in

$$F_\epsilon \left(\frac{1-z'}{1-x'} \right) = \left(\frac{z'-x'}{1-x'} \right)^{-\epsilon/2} \tilde{F}_\epsilon \left(\frac{1-z'}{x'-z'} \right). \quad (\text{A.1})$$

where, F_ϵ is defined in Eq. (4.26) and $\tilde{F}_\epsilon$ in Eq. (4.30). Note, in the region $x' > z'$, the prefactor develops a branch structure and also the argument of the hypergeometric function (HF) exceeds unity. Hence, we have to analytically continued the HF to an argument less than unity. Using the Feynman $+i0$ prescription for the kinematic variables i.e. $x' \equiv x' - i0$ and $z' \equiv z' - i0$, we can determine the appropriate branch of the complex plane unambiguously. For the prefactor we write

$$\begin{aligned} \frac{z'-x'}{1-x'} &\equiv \frac{z'-x'}{1-x'+i0} \\ &= \frac{z'-x'}{1-x'} \left(1 - \frac{i0}{1-x'} \right) = \frac{z'-x'}{1-x'} - i0 \frac{z'-x'}{(1-x')^2}. \end{aligned} \quad (\text{A.2})$$

Similarly, for the argument of the hypergeometric function,

$$\begin{aligned} \frac{1-z'}{x'-z'} &\equiv \frac{1-z'+i0}{x'-z'} \\ &= \frac{1-z'}{x'-z'} \left(1 + i0 \frac{1}{1-z'} \right) = \frac{1-z'}{x'-z'} + i0 \frac{1}{x'-z'}. \end{aligned} \quad (\text{A.3})$$

The sign of the infinitesimal imaginary part depends on the either $x' > z'$ or $x' < z'$. Hence we decompose the expression into different kinematic regions using step functions,

$$\begin{aligned} \frac{z'-x'}{1-x'} &= \theta(z'-x') \left(\frac{z'-x'}{1-x'} - i0 \right) + \theta(x'-z') \left(-\frac{x'-z'}{1-x'} + i0 \right) \\ &= \left| \frac{z'-x'}{1-x'} \right| \left\{ \theta(z'-x')(1-i0) + \theta(x'-z')(-1+i0) \right\}. \end{aligned} \quad (\text{A.4})$$

Using this decomposition, we obtain

$$F_\epsilon \left(\frac{1-z'}{1-x'} \right) = \left| \frac{z'-x'}{1-x'} \right|^{-\epsilon/2} \left\{ \theta(z'-x') \tilde{F}_\epsilon \left(\frac{1-z'}{x'-z'} - i0 \right) + \theta(x'-z') (-1+i0)^{-\epsilon/2} \tilde{F}_\epsilon \left(\frac{1-z'}{x'-z'} + i0 \right) \right\}. \quad (\text{A.5})$$

After fixing the branches of the prefactors and of the hypergeometric functions, we perform the expansion of the latter about $\epsilon = 0$ and the resulting polylogarithms are then continued to the required kinematic region using the same branch prescription, see Eqs. (C.6) and Eqs. (C.11)-(C.12).

Let us discuss one more example.

$$F_\epsilon \left(\frac{x'(1-x')}{z'(1-z')} \right) = \left(\frac{(z'-x')(1-z'-x')}{z'(1-z')} \right)^{-\frac{\epsilon}{2}} \tilde{F}_\epsilon \left(\frac{x'(1-x')}{(x'-z')(1-z'-x')} \right) \quad (\text{A.6})$$

Following the procedure as in the previous example, we first consider the prefactor:

$$\begin{aligned} \frac{(z'-x')(1-z'-x')}{z'(1-z')} &\equiv \frac{(z'-x')(1-z'-x'+i0)}{(z'-i0)(1-z'+i0)} \\ &= \frac{(z'-x')(1-z'-x')}{z'(1-z')} \left(1 + \frac{i0}{1-z'-x'} + \frac{i0}{z'} - \frac{i0}{1-z'} \right) \\ &= \frac{(z'-x')(1-z'-x')}{z'(1-z')} + i0 \frac{(z'-x')}{z'(1-z')} \\ &\quad + i0 \frac{(z'-x')(1-z'-x')}{(z')^2(1-z')} - i0 \frac{(z'-x')(1-z'-x')}{z'(1-z')^2} \\ &= \frac{(z'-x')(1-z'-x')}{z'(1-z')} \\ &\quad + i0 \frac{((1-z')(1-z'-x') + x'z')(z'-x')}{(z')^2(1-z')^2} \end{aligned} \quad (\text{A.7})$$

and similarly for the argument of hypergeometric function

$$\begin{aligned} \frac{x'(1-x')}{(x'-z')(1-z'-x')} &\equiv \frac{(x'-i0)(1-x'+i0)}{(x'-z')(1-z'-x'+i0)} \\ &= \frac{x'(1-x')}{(x'-z')(1-z'-x')} \left(1 - \frac{i0}{x'} + \frac{i0}{1-x'} - \frac{i0}{1-z'-x'} \right) \end{aligned}$$

$$\begin{aligned}
&= \frac{x'(1-x')}{(x'-z')(1-z'-x')} - i0 \frac{(1-x')}{(x'-z')(1-z'-x')} \\
&\quad + i0 \frac{x'}{(x'-z')(1-z'-x')} - i0 \frac{x'(1-x')}{(x'-z')(1-z'-x')^2} \\
&= \frac{x'(1-x')}{(x'-z')(1-z'-x')} + i0 \frac{((1-x')(1-z'-x') + x'z')}{(z'-x')(1-z'-x')^2}
\end{aligned} \tag{A.8}$$

Note for both prefactor as well as argument of HF, the sign of the imaginary part depends on either $x' > z'$ or $x' < z'$ or $x' + z' > 1$ or $x' + z' < 1$. Consequently, we decompose the expression into four different regions as,

$$\begin{aligned}
\frac{(z'-x')(1-z'-x')}{z'(1-z')} &= \left| \frac{(z'-x')(1-z'-x')}{z'(1-z')} \right| \left\{ \theta(z'-x')\theta(1-z'-x')(1+i0) \right. \\
&\quad + \theta(z'-x')\theta(z'+x'-1)(-1+i0) \\
&\quad + \theta(x'-z')\theta(z'+x'-1)(1-i0) \\
&\quad \left. + \theta(x'-z')\theta(1-z'-x')(-1-i0) \right\}
\end{aligned} \tag{A.9}$$

Using the above decomposition, we obtain,

$$\begin{aligned}
F_\epsilon \left(\frac{x'(1-x')}{z'(1-z')} \right) &= \left(\frac{(z'-x')(1-z'-x')}{z'(1-z')} \right)^{-\frac{\epsilon}{2}} \tilde{F}_\epsilon \left(\frac{x'(1-x')}{(x'-z')(1-z'-x')} \right) \\
&= \left| \frac{(z'-x')(1-z'-x')}{z'(1-z')} \right|^{-\frac{\epsilon}{2}} \\
&\quad \times \left\{ \theta_{1a} \theta_{2a} \tilde{F}_\epsilon \left(\frac{x'(1-x')}{(x'-z')(1-z'-x')} + i0 \right) \right. \\
&\quad + \theta_{1a} \theta_{2b} (-1+i0)^{-\frac{\epsilon}{2}} \tilde{F}_\epsilon \left(\frac{x'(1-x')}{(x'-z')(1-z'-x')} + i0 \right) \\
&\quad + \theta_{1b} \theta_{2b} \tilde{F}_\epsilon \left(\frac{x'(1-x')}{(x'-z')(1-z'-x')} - i0 \right) \\
&\quad \left. + \theta_{1b} \theta_{2a} (-1-i0)^{-\frac{\epsilon}{2}} \tilde{F}_\epsilon \left(\frac{x'(1-x')}{(x'-z')(1-z'-x')} - i0 \right) \right\},
\end{aligned} \tag{A.10}$$

where $\theta_{1a} = \theta(z'-x')$, $\theta_{1b} = \theta(x'-z')$, $\theta_{2a} = \theta(1-z'-x')$, $\theta_{2b} = \theta(z'+x'-1)$.

Appendix B

Plus Distribution Procedure

In this appendix, we describe the procedure used to extract endpoint singularities in terms of plus distributions. These singularities appear in the partonic coefficient functions when one or both of the scaling variables approach their threshold values, i.e. $x' \rightarrow 1$ and $z' \rightarrow 1$. The method is used repeatedly in the NLO and NNLO calculations to isolate the singular behaviour in the threshold limits as explicit poles in the dimensional regularization parameter, accompanied by plus distributions and delta functions.

The plus distribution is defined through its action on a test function. For a function $g(\xi)$ which is regular at $\xi = 1$, we define (see [8, 103, 104, 109, 429])

$$\int_0^1 d\xi g(\xi) [h(\xi)]_+ = \int_0^1 d\xi (g(\xi) - g(1)) h(\xi). \quad (\text{B.1})$$

Here $[h(\xi)]_+ = h(\xi)$ for $\xi \neq 1$. Like the Dirac delta function, the plus distribution action is defined only under an integral.

Equivalently, the plus distribution may be represented as

$$[h(\xi)]_+ = \lim_{\beta \rightarrow 0^+} \left[h(\xi) \theta(1 - \xi - \beta) - \delta(1 - \xi - \beta) \int_0^{1-\beta} dy h(y) \right]. \quad (\text{B.2})$$

This form makes explicit how the endpoint contribution is isolated into a delta function. For example, one obtains

$$\left[\frac{1}{1-\xi} \right]_+ = \lim_{\beta \rightarrow 0^+} \left[\frac{1}{1-\xi} \theta(1-\xi-\beta) + \log(\beta) \delta(1-\xi-\beta) \right], \quad (\text{B.3})$$

$$\left[\frac{\log(1-\xi)}{1-\xi} \right]_+ = \lim_{\beta \rightarrow 0^+} \left[\frac{\log(1-\xi)}{1-\xi} \theta(1-\xi-\beta) + \frac{1}{2} \log^2(\beta) \delta(1-\xi-\beta) \right]. \quad (\text{B.4})$$

In the coefficient functions of SIDIS, infrared singularities arise from soft and collinear configurations of massless partons. Near threshold, these singularities appear as factors of the form $(1-x')^{-1}$ and/or $(1-z')^{-1}$, which are divergent in the limits $x' \rightarrow 1$ and $z' \rightarrow 1$. Such terms can arise either from the master integrals themselves or from the coefficients multiplying them at the squared-amplitude level. In dimensional regularization, with $d = 4 + \epsilon$, these endpoint singularities are regulated by factors such as $(1-x')^{a\epsilon}$ and $(1-z')^{b\epsilon}$, which originate from the phase-space measure.

The double-virtual contribution is localized at Born kinematics and is therefore proportional to

$$\delta(1-x')\delta(1-z'). \quad (\text{B.5})$$

In contrast, the real-emission contributions contain non-trivial endpoint structures.

At NLO, the real-emission contribution contains singular factors of the form

$$\begin{aligned} & \frac{(1-x')^{\frac{\epsilon}{2}}(1-z')^{\frac{\epsilon}{2}}}{1-x'} f(x', z', \epsilon), \quad \frac{(1-x')^{\frac{\epsilon}{2}}(1-z')^{\frac{\epsilon}{2}}}{1-z'} f(x', z', \epsilon), \\ & \frac{(1-x')^{\frac{\epsilon}{2}}(1-z')^{\frac{\epsilon}{2}}}{(1-x')(1-z')} f(x', z', \epsilon), \end{aligned} \quad (\text{B.6})$$

where $f(x', z', \epsilon)$ is regular in the endpoint limits.

At NNLO, similar structures occur in the real-virtual contribution. In addition,

factors depending on combinations such as $z' - x'$ and $1 - z' - x'$ may appear. A representative structure is

$$\frac{(1-x')^{a\epsilon}(1-z')^{b\epsilon}|z'-x'|^{c\epsilon}|1-z'-x'|^{d\epsilon}}{(1-x')(1-z')(z'-x')(1-z'-x')}f_1(x', z', \epsilon). \quad (\text{B.7})$$

Here $f_1(x', z', \epsilon)$ is regular in its arguments. In the cases encountered in the calculation, a and b take values such as $1/2$ or 1 , while c and d can take values such as 0 or $-1/2$.

For the double-real contribution, one encounters terms of the form

$$\frac{(1-x')^\epsilon(1-z')^\epsilon}{(1-x')(1-z')(z'-x')((1+x')^2-4x'z')}f_2(x', z', \epsilon), \quad (\text{B.8})$$

where $f_2(x', z', \epsilon)$ is regular in the relevant endpoint limits. After partial fractioning, the singular factors can be organized into combinations such as

$$\frac{1}{(1-x')(1-z')}, \quad \frac{1}{(1-x')(z'-x')}, \quad \frac{1}{(1-x')((1+x')^2-4x'z')}, \quad (\text{B.9})$$

together with single endpoint factors such as

$$\frac{1}{1-x'}, \quad \frac{1}{1-z'}. \quad (\text{B.10})$$

Several public packages are available for performing partial fraction decomposition and related algebraic manipulations, see for e.g. [248, 520–524]. The extraction of the endpoint pole structure is then performed sequentially. One may first isolate the singularity at $x' \rightarrow 1$ and then at $z' \rightarrow 1$, or vice versa. The final result is independent of this order, provided the distributions are consistently interpreted under the corresponding integrals.

Let us first consider the one-variable case. We start from

$$\begin{aligned}
\int_0^1 d\xi g(\xi) \frac{(1-\xi)^{a\epsilon}}{1-\xi} &= \int_0^1 d\xi (g(\xi) - g(1)) \frac{(1-\xi)^{a\epsilon}}{1-\xi} + g(1) \int_0^1 d\xi \frac{(1-\xi)^{a\epsilon}}{1-\xi} \\
&= \int_0^1 d\xi (g(\xi) - g(1)) \sum_{i=0}^{\infty} \frac{(a\epsilon)^i}{i!} \frac{\log^i(1-\xi)}{1-\xi} + \frac{g(1)}{a\epsilon} \\
&= \int_0^1 d\xi g(\xi) \sum_{i=0}^{\infty} \frac{(a\epsilon)^i}{i!} \left[\frac{\log^i(1-\xi)}{1-\xi} \right]_+ + \frac{g(1)}{a\epsilon} \int_0^1 d\xi \delta(1-\xi).
\end{aligned} \tag{B.11}$$

Since this relation holds for an arbitrary regular test function $g(\xi)$, we obtain the distributional identity

$$\begin{aligned}
\frac{(1-\xi)^{a\epsilon}}{1-\xi} &= \left[\frac{(1-\xi)^{a\epsilon}}{1-\xi} \right]_P \\
&= \frac{1}{a\epsilon} \delta(1-\xi) + \left[\frac{(1-\xi)^{a\epsilon}}{1-\xi} \right]_+ \\
&= \frac{1}{a\epsilon} \delta(1-\xi) + \sum_{i=0}^{\infty} \frac{(a\epsilon)^i}{i!} \left[\frac{\log^i(1-\xi)}{1-\xi} \right]_+.
\end{aligned} \tag{B.12}$$

In practical calculations, this expansion is truncated at the sufficient order in ϵ required by the accompanying poles from the matrix elements, master integrals, renormalization constants, and mass-factorization kernels.

If the singular factor multiplies a regular function $f(\xi)$, it is useful to add and subtract the endpoint value $f(1)$:

$$\begin{aligned}
\frac{(1-\xi)^{a\epsilon}}{1-\xi} f(\xi) &= (f(\xi) - f(1)) \frac{(1-\xi)^{a\epsilon}}{1-\xi} + f(1) \frac{(1-\xi)^{a\epsilon}}{1-\xi} \\
&= (f(\xi) - f(1)) \sum_{i=0}^{\infty} \frac{(a\epsilon)^i}{i!} \frac{\log^i(1-\xi)}{1-\xi} + f(1) \left[\frac{(1-\xi)^{a\epsilon}}{1-\xi} \right]_P \\
&= (f(\xi) - f(1)) \frac{(1-\xi)^{a\epsilon}}{1-\xi} + f(1) \left[\frac{(1-\xi)^{a\epsilon}}{1-\xi} \right]_P.
\end{aligned} \tag{B.13}$$

The first term is regular at $\xi = 1$, because $f(\xi) - f(1)$ vanishes in this limit. Therefore it may be expanded as an ordinary function. The second term contains the

distributional contribution.

The same procedure can be applied to the case of two endpoint variables. For a function $f(x', z')$ which is regular in the endpoint limits, one obtains

$$\begin{aligned}
& \frac{(1-x')^{a\epsilon}}{1-x'} \frac{(1-z')^{b\epsilon}}{1-z'} f(x', z') \\
&= \frac{(1-x')^{a\epsilon}}{1-x'} \left(\left(f(x', z') - f(x', 1) \right) \frac{(1-z')_R^{b\epsilon}}{1-z'} + f(x', 1) \left[\frac{(1-z')_R^{b\epsilon}}{1-z'} \right]_P \right) \\
&= \left(f(x', z') - f(x', 1) - f(1, z') + f(1, 1) \right) \frac{(1-x')_R^{a\epsilon}}{1-x'} \frac{(1-z')_R^{b\epsilon}}{1-z'} \\
&\quad + \left(f(1, z') - f(1, 1) \right) \left[\frac{(1-x')^{a\epsilon}}{1-x'} \right]_P \frac{(1-z')_R^{b\epsilon}}{1-z'} \\
&\quad + \left(f(x', 1) - f(1, 1) \right) \frac{(1-x')_R^{a\epsilon}}{1-x'} \left[\frac{(1-z')^{b\epsilon}}{1-z'} \right]_P \\
&\quad + f(1, 1) \left[\frac{(1-x')^{a\epsilon}}{1-x'} \right]_P \left[\frac{(1-z')^{b\epsilon}}{1-z'} \right]_P. \tag{B.14}
\end{aligned}$$

Here the subscript R denotes the regular part, which can be expanded as an ordinary function in ϵ , while the subscript P denotes the distributional prescription, see Eq. (B.12). The last term contains the double-endpoint contribution, including the $\delta(1-x')\delta(1-z')$ term.

In some contributions, the endpoint singularities are multiplied by additional factors such as $|z' - x'|^{c\epsilon}$, , where $|z' - x'|$ denotes the modulus of $z' - x'$. In this case, the endpoint subtraction must also account for the limiting behaviour of this factor. For instance,

$$\left| z' - x' \right|^{c\epsilon} \Big|_{z'=1} = (1-x')^{c\epsilon}, \quad \left| z' - x' \right|^{c\epsilon} \Big|_{x'=1} = (1-z')^{c\epsilon}. \tag{B.15}$$

A useful decomposition is then

$$\frac{(1-x')^{a\epsilon}(1-z')^{b\epsilon}|z'-x'|^{c\epsilon}}{(1-x')(1-z')} f(x', z')$$

$$\begin{aligned}
&= \frac{(1-x')^{a\epsilon}}{(1-x')} \left(\left(f(x', z') |z' - x'|^{c\epsilon} - f(x', 1)(1-x')^{c\epsilon} \right) \frac{(1-z')_R^{b\epsilon}}{1-z'} \right. \\
&\quad \left. + f(x', 1)(1-x')^{c\epsilon} \left[\frac{(1-z')^{b\epsilon}}{1-z'} \right]_P \right) \\
&= \left(f(x', z') |z' - x'|_R^{c\epsilon} - f(1, z')(1-z')_R^{c\epsilon} \right) \frac{(1-x')_R^{a\epsilon}}{1-x'} \frac{(1-z')_R^{b\epsilon}}{1-z'} \\
&\quad + f(1, z') \left[\frac{(1-x')^{a\epsilon}}{1-x'} \right]_P \frac{(1-z')_R^{(b+c)\epsilon}}{1-z'} - \left(f(x', 1) - f(1, 1) \right) \frac{(1-x')_R^{(a+c)\epsilon}}{1-x'} \frac{(1-z')_R^{b\epsilon}}{1-z'} \\
&\quad - f(1, 1) \left[\frac{(1-x')^{(a+c)\epsilon}}{1-x'} \right]_P \frac{(1-z')_R^{b\epsilon}}{1-z'} \\
&\quad + \left(f(x', 1) - f(1, 1) \right) \frac{(1-x')_R^{(a+c)\epsilon}}{1-x'} \left[\frac{(1-z')^{b\epsilon}}{1-z'} \right]_P \\
&\quad + f(1, 1) \left[\frac{(1-x')^{(a+c)\epsilon}}{1-x'} \right]_P \left[\frac{(1-z')^{b\epsilon}}{1-z'} \right]_P. \tag{B.16}
\end{aligned}$$

This form separates the endpoint contributions while keeping the remaining terms regular in the appropriate limits.

Another useful case occurs when denominators of the form $1/(z' - x')$ appear together with an endpoint denominator. In the limit $x' \rightarrow 1$, one has

$$(z' - x') \Big|_{x'=1} = -(1 - z'). \tag{B.17}$$

Therefore, the subtraction at $x' = 1$ generates terms involving $1/(1 - z')$. A representative decomposition is

$$\begin{aligned}
&\frac{(1-x')^{a\epsilon}(1-z')^{b\epsilon}|z' - x'|^{c\epsilon}}{(1-x')(z' - x')} f(x', z') \\
&= (1-z')^{b\epsilon} \left(\left(\frac{|z' - x'|^{c\epsilon}}{z' - x'} f(x', z') + \frac{(1-z')^{c\epsilon}}{1-z'} f(1, z') \right) \frac{(1-x')_R^{a\epsilon}}{1-x'} \right. \\
&\quad \left. - \frac{(1-z')^{c\epsilon}}{1-z'} f(1, z') \left[\frac{(1-x')^{a\epsilon}}{1-x'} \right]_P \right) \\
&= f(x', z') \frac{(1-x')_R^{a\epsilon}}{1-x'} \frac{(1-z')_R^{b\epsilon}|z' - x'|_R^{c\epsilon}}{z' - x'} + (f(1, z') - f(1, 1)) \frac{(1-x')_R^{a\epsilon}}{1-x'} \frac{(1-z')_R^{(b+c)\epsilon}}{1-z'} \\
&\quad + f(1, 1) \frac{(1-x')_R^{a\epsilon}}{1-x'} \left[\frac{(1-z')^{(b+c)\epsilon}}{1-z'} \right]_P
\end{aligned}$$

$$\begin{aligned}
& - \left(f(1, z') - f(1, 1) \right) \left[\frac{(1 - x')^{a\epsilon}}{1 - x'} \right]_{\text{P}} \frac{(1 - z')_{\text{R}}^{(b+c)\epsilon}}{1 - z'} \\
& - f(1, 1) \left[\frac{(1 - x')^{a\epsilon}}{1 - x'} \right]_{\text{P}} \left[\frac{(1 - z')^{(b+c)\epsilon}}{1 - z'} \right]_{\text{P}} .
\end{aligned} \tag{B.18}$$

The procedure described above provides a systematic way to extract the endpoint pole structure from the real-emission contributions. After applying this decomposition to all singular terms, the coefficient functions can be written in terms of ordinary functions, plus distributions in x' and z' , and delta functions. These contributions are then combined with the virtual corrections, renormalization of coupling constant, and performing mass-factorization, to obtain the finite renormalized coefficient functions.

Appendix C

Useful Formulas

In this appendix, we collect some useful formulas for special functions that appear in the evaluation of master integrals and in the analytic expressions of the coefficient functions.

C.1 Hypergeometric Functions

An integral representation of the Gauss hypergeometric function ${}_2F_1$ is given by

$${}_2F_1(A_1, A_2; B_1; z) = \frac{\Gamma_{B_1}}{\Gamma_{A_2}\Gamma_{B_1-A_2}} \int_0^1 du \frac{u^{A_2-1}(1-u)^{B_1-A_2-1}}{(1-zu)^{A_1}}. \quad (\text{C.1})$$

This representation is valid for $\text{Re}(B_1) > \text{Re}(A_2) > 0$, for real values of z , the integral is well defined for $z < 1$.

Several transformation identities are useful in simplifying and analytically continuing hypergeometric functions. First, the function is symmetric under the interchange of the first two parameters,

$${}_2F_1(A_1, A_2; B_1; z) = {}_2F_1(A_2, A_1; B_1; z), \quad (\text{C.2})$$

Euler's transformation and Pfaff transformations are given by

$$\begin{aligned}
{}_2F_1(A_1, A_2; B_1; z) &= (1-z)^{B_1-A_1-A_2} {}_2F_1(B_1-A_1, B_1-A_2; B_1; z), \\
{}_2F_1(A_1, A_2; B_1; z) &= (1-z)^{-A_1} {}_2F_1\left(A_1, B_1-A_2; B_1; \frac{z}{z-1}\right), \\
{}_2F_1(A_1, A_2; B_1; z) &= (1-z)^{-A_2} {}_2F_1\left(B_1-A_1, A_2; B_1; \frac{z}{z-1}\right). \tag{C.3}
\end{aligned}$$

For further details on hypergeometric functions and their properties, see, for e.g. [294–296]. Some of the identities used in this thesis to manipulate the parameters of hypergeometric functions are

$$\begin{aligned}
&(A_2 - A_1)(1-z) {}_2F_1(A_1, A_2; B_1; z) - (B_1 - A_1) {}_2F_1(A_1 - 1, A_2; B_1; z) \\
&\quad + (B_1 - A_2) {}_2F_1(A_1, A_2 - 1; B_1; z) = 0, \tag{C.4}
\end{aligned}$$

$$\begin{aligned}
&B_1(1-z) {}_2F_1(A_1, A_2; B_1; z) - B_1 {}_2F_1(A_1, A_2 - 1; B_1; z) \\
&\quad + (B_1 - A_1) {}_2F_1(A_1, A_2; B_1 + 1; z) = 0, \tag{C.5}
\end{aligned}$$

Hypergeometric functions depending on the dimensional regularization parameter ϵ can be expanded in powers of ϵ and get polylogarithms. For example,

$$\begin{aligned}
{}_2F_1\left(\frac{\epsilon}{2}, \frac{\epsilon}{2}; 1 + \frac{\epsilon}{2}; z\right) &= 1 + \left(\frac{\epsilon}{2}\right)^2 \text{Li}_2(z) + \left(\frac{\epsilon}{2}\right)^3 \left[S_{1,2}(z) - \text{Li}_3(z)\right] \\
&\quad + \left(\frac{\epsilon}{2}\right)^4 \left[S_{1,3}(z) - S_{2,2}(z) + \text{Li}_4(z)\right] + \mathcal{O}(\epsilon^5). \tag{C.6}
\end{aligned}$$

This expansion is initially obtained in the region $|z| < 1$. It can then be analytically continued to other regions using the appropriate branch prescription. Several packages for expanding hypergeometric functions in ϵ have been discussed [328–331]. Here $\text{Li}_n(z)$ denotes the classical polylogarithm, while $S_{n,p}(z)$ denotes the Nielsen polylogarithm. We recall their definitions and some useful properties below.

C.2 Classical Polylogarithms

The classical polylogarithm is given through the integral relation

$$\text{Li}_{n+1}(z) = \int_0^z \frac{dt}{t} \text{Li}_n(t), \quad n \geq 1, \quad (\text{C.7})$$

with $\text{Li}_1(z) = -\log(1-z)$. Some useful integral representations for $n = 2, 3$ are

$$\begin{aligned} \text{Li}_2(z) &= -\int_0^z dt \frac{\log(1-t)}{t} = -\int_0^1 dt \frac{\log(1-zt)}{t}, \\ \text{Li}_3(z) &= \int_0^1 dt \frac{\log(t) \log(1-zt)}{t} = \frac{z}{2} \int_0^1 dt \frac{\log^2(t)}{1-zt}. \end{aligned} \quad (\text{C.8})$$

For argument $z = 1$, Li reduces to Riemann zeta function i.e. $\text{Li}_n(1) = \zeta_n$ for $n \geq 2$.

A useful generalization of the classical polylogarithms is given by the Nielsen polylogarithms, defined as

$$S_{n,p}(x) = \frac{(-1)^{n+p-1}}{p!(n-1)!} \int_0^1 \frac{dt}{t} \log^{n-1}(t) \log^p(1-xt). \quad (\text{C.9})$$

With this convention, the classical polylogarithms are obtained as the special case

$$S_{n,1}(x) = \text{Li}_{n+1}(x).$$

For the case with $n = 1, p = 2$,

$$S_{1,2}(z) = \frac{1}{2} \int_0^1 \frac{dt}{t} \log^2(1-zt) = z \int_0^1 dt \frac{\log(t) \log(1-zt)}{1-zt}. \quad (\text{C.10})$$

These functions frequently appear in the ϵ -expansion of hypergeometric functions and in the analytic expressions of the master integrals. For more details on classical and Nielsen polylogarithms, see for e.g. [525–528].

For arguments outside the principal convergence region, the functions are defined

by analytic continuation. With the branch prescription, one has for $x > 0$,

$$\log(-x + i0) = \log(x) + i\pi. \quad (\text{C.11})$$

Some useful continuation identities are $x \leq 1$,

$$\begin{aligned} \text{Li}_2\left(\frac{1}{x} + i0\right) &= \log(x) \log(1-x) - \frac{1}{2} \log^2(x) + \text{Li}_2(1-x) + \zeta_2 - i\pi \log(x), \\ \text{Li}_2(1+x+i0) &= -\log(x) \log(1+x) - \text{Li}_2(-x) + \zeta_2 - i\pi \log(1+x), \\ \text{Li}_3\left(\frac{1}{x} + i0\right) &= -\frac{1}{2} \log^2(x) \log(1-x) + \frac{1}{6} \log^3(x) - S_{1,2}(1-x) \\ &\quad - \text{Li}_2(1-x) \log(x) + \zeta_3 - \zeta_2 \log(x) + \frac{i}{2} \pi \log^2(x), \\ \text{Li}_3(1+x+i0) &= -\frac{1}{2} \log(x) \log^2(1+x) - S_{1,2}(-x) - \text{Li}_2(-x) \log(1+x) \\ &\quad + \zeta_3 + \zeta_2 \log(1+x) - \frac{i}{2} \pi \log^2(1+x), \\ S_{1,2}\left(\frac{1}{x} + i0\right) &= -\frac{1}{2} \log(x) \log^2(1-x) + \frac{1}{2} \log^2(x) \log(1-x) - \frac{1}{6} \log^3(x) \\ &\quad - S_{1,2}(1-x) + \text{Li}_3(1-x) - \text{Li}_2(1-x) \log(1-x) + \zeta_3 \\ &\quad + 3\zeta_2 \log(x) + i\pi \log(x) \log(1-x) - \frac{i}{2} \pi \log^2(x) + i\pi \text{Li}_2(1-x), \\ S_{1,2}(1+x+i0) &= \frac{1}{2} \log^2(x) \log(1+x) - \text{Li}_3(-x) + \text{Li}_2(-x) \log(x) + \zeta_3 \\ &\quad - 3\zeta_2 \log(1+x) + i\pi \log(x) \log(1+x) + i\pi \text{Li}_2(-x). \end{aligned} \quad (\text{C.12})$$

where following identities are used,

$$\begin{aligned} \text{Li}_2(x) &= \zeta_2 - \log(x) \log(1-x) - \text{Li}_2(1-x), \\ \text{Li}_3(x) &= \zeta_3 - \frac{1}{2} \log^2(x) \log(1-x) - S_{1,2}(1-x) - \text{Li}_2(1-x) \log(x) + \zeta_2 \log(x), \\ S_{1,2}(x) &= \zeta_3 + \frac{1}{2} \log(x) \log^2(1-x) - \text{Li}_3(1-x) + \text{Li}_2(1-x) \log(1-x). \end{aligned} \quad (\text{C.13})$$

The precise imaginary parts depend on the branch prescription and must be chosen consistently with the kinematic region under consideration.

C.3 Generalized Polylogarithms

Generalized polylogarithms (GPLs) provide a convenient representation of the iterated integrals encountered in multi-loop and phase-space calculations [290, 397, 529–539], see also [393, 398, 539–544]. In the differential-equation method for solving Feynman integrals, they often appear in the solution of differential systems for master integrals. In this thesis, GPLs arise in the coefficients obtained after expanding the master integrals in powers of ϵ .

The generalized polylogarithm of weight n is defined recursively by

$$G(a_1, a_2, \dots, a_n; z) = \int_0^z \frac{dt}{t - a_1} G(a_2, \dots, a_n; t), \quad (\text{C.14})$$

here, a_i and z are complex variables and $G(; z) = 1$. The a_i are called the indices, or letters, of the GPL. The set of all such letters appearing in a given problem is called the alphabet. The number of indices is called the weight of the GPL. Thus, $G(a_1, \dots, a_n; z)$ has weight n . If all indices are zero, the definition is understood as

$$G(\underbrace{0, \dots, 0}_n; z) = \frac{1}{n!} \log^n z. \quad (\text{C.15})$$

The classical polylogarithms can be written as special cases of GPLs:

$$\begin{aligned} G(\underbrace{a, \dots, a}_n; z) &= \frac{1}{n!} \log^n \left(1 - \frac{z}{a} \right), \\ G(\underbrace{0, \dots, 0}_{n-1}, a; z) &= -\text{Li}_n \left(\frac{z}{a} \right), \\ G(\underbrace{0, \dots, 0}_{n-k}, \underbrace{a, \dots, a}_k; z) &= (-1)^k S_{n-k, k} \left(\frac{z}{a} \right) \end{aligned} \quad (\text{C.16})$$

In above equation $a \neq 0$. GPLs are therefore a direct generalization of logarithms and classical polylogarithms.

GPLs satisfy a shuffle algebra. The product of two GPLs with the same argument can be expressed as a sum over all shuffles of their indices. Let $\vec{a} = (a_1, a_2, \dots, a_n)$ denotes an ordered lists of indices. Then

$$G(\vec{a}; z)G(\vec{b}; z) = \sum_{\vec{c} \in \vec{a} \sqcup \vec{b}} G(\vec{c}; z), \quad (\text{C.17})$$

where $\vec{a} \sqcup \vec{b}$ denotes the set of all possible ways of merging the ordered lists $\vec{a}$ and $\vec{b}$ while preserving the relative order of the entries inside each list. For example,

$$\begin{aligned} G(a; z)G(b, c; z) &= G(a, b, c; z) + G(b, a, c; z) + G(b, c, a; z), \\ G(a, b; z)G(c, d; z) &= G(a, b, c, d; z) + G(a, c, b, d; z) + G(a, c, d, b; z) + G(c, a, b, d; z) \\ &\quad + G(c, a, d, b; z) + G(c, d, a, b; z). \end{aligned} \quad (\text{C.18})$$

Such relations are useful for simplifying products of GPLs for reducing expressions to a chosen functional basis.

There are a few special cases which require care. For $G(a_1, a_2, \dots, a_n; z)$, endpoint singularities may arise when $a_1 = z$; in particular, for argument $z = 1$, this corresponds to $a_1 = 1$. GPLs with trailing zeros i.e $a_n = 0$, are also treated separately using shuffle identities in order to express them in terms of GPLs without trailing zeros. For example, $G(a, 0; z)$ for $a \neq 0$,

$$G(a, 0; z) = G(a; z)G(0; z) - G(0, a; z). \quad (\text{C.19})$$

Another useful property is the rescaling relation, for $a_n \neq 0$ and $k \neq 0$,

$$G(ka_1, ka_2, \dots, ka_n; kz) = G(a_1, a_2, \dots, a_n; z). \quad (\text{C.20})$$

In practical calculations, GPLs may contain letters depending on kinematic vari-

ables. The fibration basis construction is a method for rewriting GPLs by exchanging the role of a variable appearing in the letters with the argument of the GPL. Let $\vec{w}(x)$ be an ordered list of letters depending on x and let z be independent of x . If the GPL is known at a reference point x_0 , one may write

$$G(\vec{w}(x); z) = G(\vec{w}(x_0); z) + \int_{x_0}^x dy \frac{d}{dy} G(\vec{w}(y); z). \quad (\text{C.21})$$

The derivative lowers the weight and gives lower-weight GPLs multiplied by rational functions of y . After partial fractioning and integration by parts, the expression is integrated back in y , yielding a representation in which the dependence on x is moved from the letters to the argument.

As a simple example, consider $G(1-x; z)$, where the variable x appears in the letter. We want to rewrite it in a form where x appears as the argument instead. Using the fibration-basis change, we write (choosing $x_0 = 0$),

$$\begin{aligned} G(1-x; z) &= G(1; z) + \int_0^x dy \frac{\partial}{\partial y} G(1-y; z) \\ &= G(1; z) + \int_0^x dy \frac{\partial}{\partial y} \int_0^z \frac{dw_1}{w_1 - (1-y)} \\ &= G(1; z) - \int_0^x dy \int_0^z \frac{dw_1}{(w_1 - (1-y))^2} \\ &= G(1; z) + \int_0^x dy \left[\frac{1}{z - (1-y)} - \frac{1}{y-1} \right] \\ &= G(1; z) + G(1-z; x) - G(1; x). \end{aligned} \quad (\text{C.22})$$

As a second example, consider $G(1, 1-x; z)$, using the fibration-basis change, we obtain

$$\begin{aligned} G(1, 1-x; z) &= G(1, 1; z) + \int_0^x dy \frac{\partial}{\partial y} G(1, 1-y; z) \\ &= G(1, 1; z) + \int_0^x dy \frac{\partial}{\partial y} \int_0^z \frac{dw_1}{w_1 - 1} \int_0^{w_1} \frac{dw_2}{w_2 - (1-y)} \end{aligned}$$

$$\begin{aligned}
&= G(1, 1; z) + \int_0^x dy \int_0^z \frac{dw_1}{w_1 - 1} \left[\frac{1}{w_1 - (1 - y)} - \frac{1}{y - 1} \right] \\
&= G(1, 1; z) + \int_0^x dy \int_0^z \frac{dw_1}{y} \left[\frac{1}{w_1 - 1} - \frac{1}{w_1 - (1 - y)} \right] \\
&\quad - G(1; z)G(1; x) \\
&= G(1, 1; z) + \int_0^x dy \frac{1}{y} [G(1; z) - G(1 - y; z)] - G(1; z)G(1; x) \\
&= G(1, 1; z) - \int_0^x dy \frac{1}{y} [G(1 - z; y) - G(1; y)] - G(1; z)G(1; x) \\
&= G(1, 1; z) - G(0, 1 - z; x) + G(0, 1; x) - G(1; z)G(1; x). \quad (\text{C.23})
\end{aligned}$$

The examples above illustrate how the fibration-basis change can be used to rewrite GPLs with variable-dependent letters into an equivalent form in which the chosen variable appears as the argument. This representation is often more convenient for analytic continuation and for simplifying the final expressions.

The formulae collected in this appendix form the basic toolkit used throughout the calculation, in particular for simplifying the master integrals, carrying out analytic continuation, and presenting the final results in a compact form.

Appendix D

Boundary Values of the RR Master Integrals

In this appendix, we present the explicit boundary values of the RR master integrals listed in Eq. (4.37), evaluated in the limit $x' \rightarrow 1$ and $z' \rightarrow 1$. These boundary values are obtained in closed form and serve as the boundary conditions required for solving the differential equations satisfied by the master integrals. They are evaluated in the $k_1 - k_2$ center-of-mass frame while keeping factors of the form $(1 - x')^{a\epsilon+b}$ and $(1 - z')^{c\epsilon+d}$. For convenience, we define,

$$\tilde{C}_\epsilon = \frac{1}{(4\pi)^{4+\epsilon}} \frac{\Gamma^2\left(1 + \frac{\epsilon}{2}\right)}{\Gamma^2(1 + \epsilon)} \quad (\text{D.1})$$

The boundary values of the master integrals are given by,

$$\begin{aligned} J(\mathcal{R}_1, 0, 0, 0) \Big|_{\{x', z'\} \rightarrow 1} &= \frac{2\pi\tilde{C}_\epsilon}{(1 + \epsilon)^2} (Q^2)^{\epsilon+1} (1 - x')^{\epsilon+1} (1 - z')^{\epsilon+1} , \\ J(\mathcal{R}_1, 0, 0, 1) \Big|_{\{x', z'\} \rightarrow 1} &= \frac{4\pi\tilde{C}_\epsilon}{\epsilon(1 + \epsilon)} (Q^2)^\epsilon (1 - x')^\epsilon (1 - z')^{1+\epsilon} , \\ J(\mathcal{R}_1, 1, 1, 1) \Big|_{\{x', z'\} \rightarrow 1} &= \frac{-16\pi\tilde{C}_\epsilon}{\epsilon^2} (Q^2)^{\epsilon-2} (1 - x')^{\epsilon-1} (1 - z')^\epsilon , \end{aligned}$$

$$\begin{aligned}
J(\mathcal{R}_2, 1, 1, 1) \Big|_{\{x', z'\} \rightarrow 1} &= \frac{-8\pi}{(4\pi)^{4+\epsilon}} \frac{1}{\epsilon} (Q^2)^{\epsilon-2} (1-x')^{\epsilon-1} (1-z')^{\epsilon-1} \\
&\quad \times \frac{{}_3F_2\left(\frac{\epsilon}{2}, \frac{\epsilon}{2}, \frac{\epsilon}{2}, 1+\frac{\epsilon}{2}, 1+\frac{3\epsilon}{2}, 1\right)}{\Gamma(1+\epsilon)}, \\
J(\mathcal{R}_3, 0, 0, 1) \Big|_{\{x', z'\} \rightarrow 1} &= \frac{-2\pi\tilde{C}_\epsilon}{(1+\epsilon)^2} (Q^2)^\epsilon (1-x')^{\epsilon+1} (1-z')^\epsilon, \\
J(\mathcal{R}_3, 1, 1, 1) \Big|_{\{x', z'\} \rightarrow 1} &= \frac{8\pi\tilde{C}_\epsilon}{\epsilon^2} (Q^2)^{\epsilon-2} (1-x')^\epsilon (1-z')^{\epsilon-1}, \\
J(\mathcal{R}_4, 1, 1, 1) \Big|_{\{x', z'\} \rightarrow 1} &= \frac{8\pi\tilde{C}_\epsilon}{\epsilon^2(1+\epsilon)^2} (Q^2)^{\epsilon-2} (1-x')^\epsilon (1-z')^{\epsilon-1}, \\
J(\mathcal{R}_5, 0, 0, 1) \Big|_{\{x', z'\} \rightarrow 1} &= \frac{-2\pi\tilde{C}_\epsilon}{(1+\epsilon)^2} (Q^2)^\epsilon (1-x')^{\epsilon+1} (1-z')^{\epsilon+1}, \\
J(\mathcal{R}_5, 0, 0, 2) \Big|_{\{x', z'\} \rightarrow 1} &= \frac{2\pi\tilde{C}_\epsilon}{(1+\epsilon)^2} (Q^2)^{\epsilon-1} (1-x')^{\epsilon+1} (1-z')^{\epsilon+1}, \\
J(\mathcal{R}_5, 0, 1, 1) \Big|_{\{x', z'\} \rightarrow 1} &= \frac{2\pi\tilde{C}_\epsilon}{(1+\epsilon)^2} (Q^2)^{\epsilon-1} (1-x')^{\epsilon+1} (1-z')^{\epsilon+1}, \\
J(\mathcal{R}_5, 1, 1, 1) \Big|_{\{x', z'\} \rightarrow 1} &= \frac{-4\pi\tilde{C}_\epsilon}{\epsilon(1+\epsilon)} (Q^2)^{\epsilon-2} (1-x')^{\epsilon+1} (1-z')^\epsilon, \\
J(\mathcal{R}_6, 0, 1, 1) \Big|_{\{x', z'\} \rightarrow 1} &= \frac{2\pi\tilde{C}_\epsilon}{(1+\epsilon)^2} (Q^2)^{\epsilon-1} (1-x')^{\epsilon+1} (1-z')^\epsilon, \\
J(\mathcal{R}_6, 1, 1, 1) \Big|_{\{x', z'\} \rightarrow 1} &= \frac{-4\pi\tilde{C}_\epsilon}{\epsilon(1+\epsilon)} (Q^2)^{\epsilon-2} (1-x')^{\epsilon+1} (1-z')^{\epsilon-1}, \\
J(\mathcal{R}_7, 0, 1, 1) \Big|_{\{x', z'\} \rightarrow 1} &= \frac{-4\pi\tilde{C}_\epsilon}{\epsilon(1+\epsilon)} (Q^2)^{\epsilon-1} (1-x')^\epsilon (1-z')^{\epsilon+1}, \\
J(\mathcal{R}_7, 1, 1, 1) \Big|_{\{x', z'\} \rightarrow 1} &= \frac{8\pi\tilde{C}_\epsilon}{\epsilon^2} (Q^2)^{\epsilon-2} (1-x')^\epsilon (1-z')^\epsilon, \\
J(\mathcal{R}_8, 1, 1, 1) \Big|_{\{x', z'\} \rightarrow 1} &= \frac{8\pi\tilde{C}_\epsilon}{\epsilon^2} (Q^2)^{\epsilon-2} (1-x')^\epsilon (1-z')^{\epsilon-1}, \\
J(\mathcal{R}_{10}, 1, 1, 1) \Big|_{\{x', z'\} \rightarrow 1} &= \frac{4\pi\tilde{C}_\epsilon}{\epsilon(1+\epsilon)} (Q^2)^{\epsilon-2} (1-x')^\epsilon (1-z')^{\epsilon+1}, \\
J(\mathcal{R}_{11}, 1, 1, 1) \Big|_{\{x', z'\} \rightarrow 1} &= \frac{-8\pi\tilde{C}_\epsilon}{\epsilon^2} (Q^2)^{\epsilon-2} (1-x')^{\epsilon-1} (1-z')^\epsilon, \\
J(\mathcal{R}_{12}, 1, 1, 1) \Big|_{\{x', z'\} \rightarrow 1} &= \frac{4\pi\tilde{C}_\epsilon}{\epsilon(1+\epsilon)} (Q^2)^{\epsilon-2} (1-x')^\epsilon (1-z')^\epsilon, \\
J(\mathcal{R}_{13}, 1, 1, 1) \Big|_{\{x', z'\} \rightarrow 1} &= \frac{-8\pi\tilde{C}_\epsilon}{\epsilon(1+\epsilon)} (Q^2)^{\epsilon-2} (1-x')^{\epsilon-1} (1-z')^{\epsilon+1}. \tag{D.2}
\end{aligned}$$

Appendix E

Results of the SV and NSV

Coefficient functions

In this appendix, we present the analytic results of the SV and NSV CFs, $(\Delta)\mathcal{C}_{J,cc}^{\text{SV}}$ and $(\Delta)\mathcal{C}_{J,cc}^{\text{NSV}}$ for $c = \{q, \bar{q}\}$ respectively. We present complete results at NLO and NNLO and partial results at N³LO in the threshold region for the CFs, expanded in a_s as $(\Delta)\mathcal{C}_{J,cc}^{(\text{N})\text{SV}} = \sum_{i=0}^{\infty} a_s^i(\mu_R^2)(\Delta)\mathcal{C}_{J,cc}^{(i),(\text{N})\text{SV}}$. For compactness, we do not present the expressions for the fourth order SV and NSV coefficient functions. These results are given in Eq. (66) and Eq. (70) respectively of [179]. Their normalization at LO reads $(\Delta)\mathcal{C}_{J,cc}^{(0),\text{SV}} = \delta(1-x')\delta(1-z')$ and $(\Delta)\mathcal{C}_{J,cc}^{(0),\text{NSV}} = 0$, and we have set $\mu_F^2 = \mu_R^2 = Q^2$ in the sequel.

E.1 SV Coefficient functions

For the perturbative expansion of the SV part of the CFs, we define in addition to C_A and C_F further group invariants of the color $SU(N_c)$ gauge group, namely We

also define

$$\begin{aligned}
\frac{d^{abc}d_{abc}}{N_F} &= \frac{(N_c^2 - 1)(N_c^2 - 4)}{16N_c^2}, & \frac{d_F^{abcd}d_F^{abcd}}{N_F} &= \frac{(N_c^2 - 1)(N_c^4 - 6N_c^2 + 18)}{96N_c^3}, \\
\frac{d_F^{abcd}d_A^{abcd}}{N_F} &= \frac{(N_c^2 - 1)(N_c^2 + 6)}{48}, & \frac{d_A^{abcd}d_A^{abcd}}{N_A} &= \frac{N_c^2(N_c^2 + 36)}{24}, \\
\frac{d_F^{abcd}d_A^{abcd}}{N_A} &= \frac{N_c(N_c^2 + 6)}{48}, & \frac{d_F^{abcd}d_F^{abcd}}{N_A} &= \frac{(N_c^4 - 6N_c^2 + 18)}{96N_c^2}, \\
N_F &= N_c, & N_A &= (N_c^2 - 1), & N_4 &= \frac{(N_c^2 - 4)}{N_c}.
\end{aligned} \tag{E.1}$$

Also, below we will use n_{fv} , which is defined as the charge weighted sum of quark flavors. At NLO, i.e. at $\mathcal{O}(a_s)$,

$$(\Delta)\mathcal{C}_{J,cc}^{(1),SV} = \delta_{\vec{x}'}\mathcal{D}_{\vec{z}'}^1 \left[C_F \left\{ 4 \right\} \right] - \delta_{\vec{x}'}\delta_{\vec{z}'} \left[C_F \left\{ 8 \right\} \right] + \mathcal{D}_{\vec{x}'}^0\mathcal{D}_{\vec{z}'}^0 \left[C_F \left\{ 2 \right\} \right] + (\mathbf{x}' \leftrightarrow \mathbf{z}'). \tag{E.2}$$

The NNLO CF at SV accuracy read

$$\begin{aligned}
(\Delta)\mathcal{C}_{J,cc}^{(2),SV} &= \delta_{\vec{x}'}\mathcal{D}_{\vec{z}'}^3 \left[C_F^2 \left\{ 8 \right\} \right] - \delta_{\vec{x}'}\mathcal{D}_{\vec{z}'}^2 \left[C_F C_A \left\{ \frac{22}{3} \right\} - C_F n_f \left\{ \frac{4}{3} \right\} \right] + \mathcal{D}_{\vec{x}'}^1\mathcal{D}_{\vec{z}'}^1 \left[C_F^2 \left\{ 24 \right\} \right] \\
&+ \mathcal{D}_{\vec{x}'}^0\mathcal{D}_{\vec{z}'}^2 \left[C_F^2 \left\{ 24 \right\} \right] - \mathcal{D}_{\vec{x}'}^0\mathcal{D}_{\vec{z}'}^1 \left[C_F C_A \left\{ \frac{44}{3} \right\} - C_F n_f \left\{ \frac{8}{3} \right\} \right] \\
&+ \delta_{\vec{x}'}\mathcal{D}_{\vec{z}'}^1 \left[C_F C_A \left\{ \frac{268}{9} - 8\zeta_2 \right\} - C_F n_f \left\{ \frac{40}{9} \right\} - C_F^2 \left\{ 64 + 32\zeta_2 \right\} \right] \\
&- \delta_{\vec{x}'}\delta_{\vec{z}'} \left[C_F C_A \left\{ \frac{1535}{24} - \frac{86}{3}\zeta_3 + \frac{269}{9}\zeta_2 - \frac{34}{5}\zeta_2^2 \right\} - C_F^2 \left\{ \frac{511}{8} - 30\zeta_3 + 29\zeta_2 - \frac{28}{5}\zeta_2^2 \right\} \right. \\
&- C_F n_f \left\{ \frac{127}{12} + \frac{4}{3}\zeta_3 + \frac{38}{9}\zeta_2 \right\} \left. \right] + \mathcal{D}_{\vec{x}'}^0\mathcal{D}_{\vec{z}'}^0 \left[C_F C_A \left\{ \frac{134}{9} - 4\zeta_2 \right\} - C_F n_f \left\{ \frac{20}{9} \right\} \right. \\
&- C_F^2 \left\{ 32 + 16\zeta_2 \right\} \left. \right] - \delta_{\vec{x}'}\mathcal{D}_{\vec{z}'}^0 \left[C_F C_A \left\{ \frac{808}{27} - 28\zeta_3 - \frac{44}{3}\zeta_2 \right\} - C_F n_f \left\{ \frac{112}{27} - \frac{8}{3}\zeta_2 \right\} \right. \\
&- C_F^2 \left\{ 32\zeta_3 \right\} \left. \right] + (\mathbf{x}' \leftrightarrow \mathbf{z}').
\end{aligned} \tag{E.3}$$

In the following we predict the CF at third order in a_s using the available information on the perturbative results.

- the knowledge of $\Psi_d^{q,(1)}$ and $\Psi_d^{q,(2)}$ can be used to predict the coefficients of $\{\delta_{\vec{x}'}\mathcal{D}_{\vec{z}'}^i, \delta_{\vec{z}'}\mathcal{D}_{\vec{x}'}^i\}$ for $i = 5, 4, 3, 2$ and $\{\mathcal{D}_{\vec{x}'}^i\mathcal{D}_{\vec{z}'}^j\}$ for $i + j = 4, 3, 2, 1$ in $(\Delta)\mathcal{C}_{J,cc}^{(3),SV}$.

- the results on the cusp and eikonal anomalous dimensions (A_3^q, f_3^q) can be used to obtain the coefficients of $\{\delta_{\bar{x}} \mathcal{D}_{\bar{z}'}^i, \delta_{\bar{z}'} \mathcal{D}_{\bar{x}'}^i\}$ for $i = 1, 0$ and $\{\mathcal{D}_{\bar{x}'}^0 \mathcal{D}_{\bar{z}'}^0\}$
- using $\mathcal{G}_{d,3}^{q,(1)}$ from the three-loop form factors and $\bar{\mathcal{G}}_{d,3}^{q,(1)}$ from the three-loop soft functions, we can obtain the coefficient of $\delta_{\bar{x}'} \delta_{\bar{z}'}$.

The results for the SV part of the CFs at third order obtained in this way read

$$\begin{aligned}
(\Delta) \mathcal{C}_{J,cc}^{(3),SV} = & \mathcal{D}_{\bar{x}'}^2 \mathcal{D}_{\bar{z}'}^2 \left[C_F^3 \left\{ 120 \right\} \right] + \delta_{\bar{x}'} \mathcal{D}_{\bar{z}'}^5 \left[C_F^3 \left\{ 8 \right\} \right] - \delta_{\bar{x}'} \mathcal{D}_{\bar{z}'}^4 \left[C_F^2 C_A \left\{ \frac{220}{9} \right\} - C_F^2 n_f \left\{ \frac{40}{9} \right\} \right] \\
& + \delta_{\bar{x}'} \mathcal{D}_{\bar{z}'}^3 \left[C_F C_A^2 \left\{ \frac{484}{27} \right\} - C_F n_f C_A \left\{ \frac{176}{27} \right\} + C_F n_f^2 \left\{ \frac{16}{27} \right\} + C_F^2 C_A \left\{ \frac{1072}{9} - 32\zeta_2 \right\} \right. \\
& - C_F^2 n_f \left\{ \frac{160}{9} \right\} - C_F^3 \left\{ 128 + 128\zeta_2 \right\} \left. \right] - \delta_{\bar{x}'} \mathcal{D}_{\bar{z}'}^2 \left[C_F C_A^2 \left\{ \frac{3560}{27} - \frac{88}{3}\zeta_2 \right\} + C_F n_f^2 \left\{ \frac{80}{27} \right\} \right. \\
& - C_F C_A n_f \left\{ \frac{1156}{27} - \frac{16}{3}\zeta_2 \right\} + C_F^2 C_A \left\{ \frac{560}{9} - 168\zeta_3 - 264\zeta_2 \right\} - C_F^2 n_f \left\{ \frac{68}{9} - 48\zeta_2 \right\} \\
& - C_F^3 \left\{ 320\zeta_3 \right\} \left. \right] + \mathcal{D}_{\bar{x}'}^1 \mathcal{D}_{\bar{z}'}^3 \left[C_F^3 \left\{ 160 \right\} \right] - \mathcal{D}_{\bar{x}'}^1 \mathcal{D}_{\bar{z}'}^2 \left[C_F^2 C_A \left\{ \frac{880}{3} \right\} - C_F^2 n_f \left\{ \frac{160}{3} \right\} \right] \\
& + \delta_{\bar{x}'} \mathcal{D}_{\bar{z}'}^1 \left[C_F C_A^2 \left\{ \frac{31006}{81} - 176\zeta_3 - \frac{680}{3}\zeta_2 + \frac{176}{5}\zeta_2^2 \right\} - C_F C_A n_f \left\{ \frac{8204}{81} - \frac{512}{9}\zeta_2 \right\} \right. \\
& + C_F n_f^2 \left\{ \frac{400}{81} - \frac{32}{9}\zeta_2 \right\} - C_F^2 C_A \left\{ \frac{8893}{9} + \frac{368}{3}\zeta_3 + \frac{5288}{9}\zeta_2 - \frac{912}{5}\zeta_2^2 \right\} + C_F^3 \left\{ 511 \right. \\
& - 240\zeta_3 + 744\zeta_2 + \frac{288}{5}\zeta_2^2 \left. \right\} + C_F^2 n_f \left\{ \frac{1072}{9} + \frac{320}{3}\zeta_3 + \frac{944}{9}\zeta_2 \right\} \left. \right] + \mathcal{D}_{\bar{x}'}^0 \mathcal{D}_{\bar{z}'}^4 \left[C_F^3 \left\{ 40 \right\} \right] \\
& - \mathcal{D}_{\bar{x}'}^0 \mathcal{D}_{\bar{z}'}^3 \left[C_F^2 C_A \left\{ \frac{880}{9} \right\} - C_F^2 n_f \left\{ \frac{160}{9} \right\} \right] + \mathcal{D}_{\bar{x}'}^1 \mathcal{D}_{\bar{z}'}^1 \left[C_F C_A^2 \left\{ \frac{484}{9} \right\} - C_F C_A n_f \left\{ \frac{176}{9} \right\} \right. \\
& + C_F n_f^2 \left\{ \frac{16}{9} \right\} + C_F^2 C_A \left\{ \frac{1072}{3} - 96\zeta_2 \right\} - C_F^2 n_f \left\{ \frac{160}{3} \right\} - C_F^3 \left\{ 384 + 384\zeta_2 \right\} \left. \right] \\
& - \mathcal{D}_{\bar{x}'}^0 \mathcal{D}_{\bar{z}'}^1 \left[C_F C_A^2 \left\{ \frac{7120}{27} - \frac{176}{3}\zeta_2 \right\} - C_F C_A n_f \left\{ \frac{2312}{27} - \frac{32}{3}\zeta_2 \right\} + C_F n_f^2 \left\{ \frac{160}{27} \right\} \right. \\
& + C_F^2 C_A \left\{ \frac{1120}{9} - 336\zeta_3 - 528\zeta_2 \right\} - C_F^2 n_f \left\{ \frac{136}{9} - 96\zeta_2 \right\} - C_F^3 \left\{ 640\zeta_3 \right\} \left. \right] \\
& - \delta_{\bar{x}'} \mathcal{D}_{\bar{z}'}^0 \left[C_F n_f^2 \left\{ \frac{1856}{729} + \frac{32}{27}\zeta_3 - \frac{160}{27}\zeta_2 \right\} + C_F^2 n_f \left\{ 3 + \frac{944}{9}\zeta_3 - \frac{40}{27}\zeta_2 - \frac{224}{15}\zeta_2^2 \right\} \right. \\
& - C_F C_A n_f \left\{ \frac{62626}{729} - \frac{536}{9}\zeta_3 - \frac{7760}{81}\zeta_2 + \frac{208}{15}\zeta_2^2 \right\} - C_F^2 C_A \left\{ \frac{12928}{27} + \frac{256}{9}\zeta_3 + \frac{128}{27}\zeta_2 \right. \\
& - 352\zeta_2\zeta_3 - \frac{352}{3}\zeta_2^2 \left. \right\} + C_F C_A^2 \left\{ \frac{297029}{729} + 192\zeta_5 - \frac{14264}{27}\zeta_3 - \frac{27752}{81}\zeta_2 + \frac{176}{3}\zeta_2\zeta_3 \right. \\
& + \frac{616}{15}\zeta_2^2 \left. \right\} - C_F^3 \left\{ 384\zeta_5 - 512\zeta_3 - 512\zeta_2\zeta_3 \right\} \left. \right] + \delta_{\bar{x}'} \delta_{\bar{z}'} \left[C_F N_4 n_{fv} \left\{ 4 - \frac{80}{3}\zeta_5 + \frac{14}{3}\zeta_3 \right. \right.
\end{aligned}$$

$$\begin{aligned}
& + 10\zeta_2 - \frac{2}{5}\zeta_2^2 \Big\} - C_F n_f^2 \left\{ \frac{7081}{486} + \frac{152}{81}\zeta_3 + \frac{1028}{81}\zeta_2 + \frac{64}{135}\zeta_2^2 \right\} - C_F C_A^2 \left\{ \frac{1505881}{1944} + 102\zeta_5 \right. \\
& - \frac{125105}{162}\zeta_3 + \frac{200}{3}\zeta_3^2 + \frac{124895}{162}\zeta_2 - 234\zeta_2\zeta_3 - \frac{23539}{270}\zeta_2^2 + \frac{4456}{315}\zeta_2^3 \Big\} + C_F C_A n_f \left\{ \frac{110651}{486} \right. \\
& - 4\zeta_5 - \frac{9944}{81}\zeta_3 + \frac{5696}{27}\zeta_2 - \frac{8}{3}\zeta_2\zeta_3 - \frac{1054}{135}\zeta_2^2 \Big\} + C_F^2 C_A \left\{ \frac{74321}{72} - \frac{3812}{9}\zeta_5 - \frac{2986}{3}\zeta_3 \right. \\
& + \frac{632}{3}\zeta_3^2 + \frac{33451}{27}\zeta_2 - \frac{2480}{9}\zeta_2\zeta_3 + \frac{1304}{135}\zeta_2^2 - \frac{3896}{63}\zeta_2^3 \Big\} - C_F^2 n_f \left\{ \frac{421}{6} + \frac{112}{9}\zeta_5 - 180\zeta_3 \right. \\
& + \frac{3844}{27}\zeta_2 + \frac{448}{9}\zeta_2\zeta_3 + \frac{2504}{135}\zeta_2^2 \Big\} - C_F^3 \left\{ \frac{5599}{12} - 664\zeta_5 + 230\zeta_3 - \frac{368}{3}\zeta_3^2 + \frac{1598}{3}\zeta_2 \right. \\
& - 280\zeta_2\zeta_3 + \frac{442}{5}\zeta_2^2 - \frac{20816}{315}\zeta_2^3 \Big\} \Big] + \mathcal{D}_{\vec{x}}^0 \mathcal{D}_{\vec{z}'}^2 \left[C_F C_A^2 \left\{ \frac{484}{9} \right\} - C_F C_A n_f \left\{ \frac{176}{9} \right\} \right. \\
& + C_F n_f^2 \left\{ \frac{16}{9} \right\} + C_F^2 C_A \left\{ \frac{1072}{3} - 96\zeta_2 \right\} - C_F^2 n_f \left\{ \frac{160}{3} \right\} - C_F^3 \left\{ 384 + 384\zeta_2 \right\} \Big] \\
& + \mathcal{D}_{\vec{x}}^0 \mathcal{D}_{\vec{z}'}^0 \left[C_F C_A^2 \left\{ \frac{15503}{81} - 88\zeta_3 - \frac{340}{3}\zeta_2 + \frac{88}{5}\zeta_2^2 \right\} - C_F C_A n_f \left\{ \frac{4102}{81} - \frac{256}{9}\zeta_2 \right\} \right. \\
& + C_F n_f^2 \left\{ \frac{200}{81} - \frac{16}{9}\zeta_2 \right\} - C_F^2 C_A \left\{ \frac{8893}{18} + \frac{184}{3}\zeta_3 + \frac{2644}{9}\zeta_2 - \frac{456}{5}\zeta_2^2 \right\} + C_F^2 n_f \left\{ \frac{536}{9} \right. \\
& + \frac{160}{3}\zeta_3 + \frac{472}{9}\zeta_2 \Big\} + C_F^3 \left\{ \frac{511}{2} - 120\zeta_3 + 372\zeta_2 + \frac{144}{5}\zeta_2^2 \right\} \Big] + (\mathbf{x}' \leftrightarrow \mathbf{z}'). \quad (\text{E.4})
\end{aligned}$$

Similarly at fourth order we can predict various terms as follows:

- using $\Psi_d^{q,(1)}$, $\Psi_d^{q,(2)}$, and the three-loop cusp and eikonal anomalous dimensions (A_3^q, f_3^q) , we can obtain the coefficients of $\{\delta_{\vec{x}'} \mathcal{D}_{\vec{z}'}^i, \delta_{\vec{z}'} \mathcal{D}_{\vec{x}'}^i\}$ for $i = 7, 6, 5, 4, 3, 2$ and $\{\mathcal{D}_{\vec{x}'}^i \mathcal{D}_{\vec{z}'}^j\}$ for $i + j = 6, 5, 4, 3, 2, 1$, in $(\Delta) \mathcal{C}_{J,cc}^{(4),\text{SV}}$.
- using $\overline{\mathcal{G}}_{d,3}^{q,(1)}$ from the three-loop soft functions as given in Eq. (5.41), along with higher order anomalous dimensions $(A_3^q, A_4^q, B_3^q, f_3^q)$, we obtain the coefficients of $\{\delta_{\vec{x}'} \mathcal{D}_{\vec{z}'}^1, \delta_{\vec{z}'} \mathcal{D}_{\vec{x}'}^1\}$ and $\{\mathcal{D}_{\vec{x}'}^0 \mathcal{D}_{\vec{z}'}^0\}$.
- finally, thanks to the recent computation [495], on four-loop eikonal anomalous dimension (f_4) , see also [503], the coefficients of $\{\delta_{\vec{x}'} \mathcal{D}_{\vec{z}'}^0, \delta_{\vec{z}'} \mathcal{D}_{\vec{x}'}^0\}$ in $(\Delta) \mathcal{C}_{J,cc}^{(4),\text{SV}}$, can now be predicted.

However, the coefficient of $\delta_{\vec{x}'} \delta_{\vec{z}'}$ cannot be predicted with the available information.

E.2 NSV Coefficient functions

The NSV contributions to the CFs are next. At NLO, i.e at $\mathcal{O}(a_s)$, we have

$$(\Delta)\mathcal{C}_{J,cc}^{(1),\text{NSV}} = \delta_{\bar{z}'}\mathcal{L}_{\bar{x}'}^0 \left[C_F \left\{ 4 \right\} \right] - \delta_{\bar{x}'}\mathcal{L}_{\bar{z}'}^0 \left[C_F \left\{ 4 \right\} \right] - \mathcal{D}_{\bar{x}'}^0\mathcal{L}_{\bar{z}'}^0 \left[C_F \left\{ 4 \right\} \right] \\ - \mathcal{D}_{\bar{z}'}^0\mathcal{L}_{\bar{x}'}^0 \left[C_F \left\{ 4 \right\} \right] - \delta_{\bar{x}'}\mathcal{L}_{\bar{z}'}^1 \left[C_F \left\{ 4 \right\} \right] - \delta_{\bar{z}'}\mathcal{L}_{\bar{x}'}^1 \left[C_F \left\{ 4 \right\} \right]. \quad (\text{E.5})$$

The NSV terms of the CFs at NNLO are given by

$$(\Delta)\mathcal{C}_{J,cc}^{(2),\text{NSV}} = \delta_{\bar{x}'}\mathcal{L}_{\bar{z}'}^0 \left[C_F C_A \left\{ \frac{1108}{27} - 28\zeta_3 - \frac{44}{3}\zeta_2 \right\} - C_F n_f \left\{ \frac{52}{27} - \frac{8}{3}\zeta_2 \right\} + C_F^2 \left\{ 64 \right. \right. \\ \left. \left. - 32\zeta_3 - 24\zeta_2 \right\} \right] + \delta_{\bar{z}'}\mathcal{L}_{\bar{x}'}^0 \left[C_F C_A \left\{ \frac{1492}{27} - 28\zeta_3 - \frac{68}{3}\zeta_2 \right\} - C_F n_f \left\{ \frac{364}{27} - \frac{8}{3}\zeta_2 \right\} \right. \\ \left. - C_F^2 \left\{ 64 + 32\zeta_3 + 32\zeta_2 \right\} \right] - \mathcal{D}_{\bar{x}'}^0\mathcal{L}_{\bar{z}'}^0 \left[C_F C_A \left\{ \frac{268}{9} - 8\zeta_2 \right\} - C_F n_f \left\{ \frac{40}{9} \right\} \right. \\ \left. - C_F^2 \left\{ 52 + 32\zeta_2 \right\} \right] - \mathcal{D}_{\bar{z}'}^0\mathcal{L}_{\bar{x}'}^0 \left[C_F C_A \left\{ \frac{532}{9} - 8\zeta_2 \right\} - C_F n_f \left\{ \frac{88}{9} \right\} - C_F^2 \left\{ 76 + 32\zeta_2 \right\} \right] \\ + \mathcal{D}_{\bar{x}'}^0\mathcal{L}_{\bar{z}'}^1 \left[C_F C_A \left\{ \frac{44}{3} \right\} - C_F n_f \left\{ \frac{8}{3} \right\} - C_F^2 \left\{ 16 \right\} \right] + \mathcal{D}_{\bar{z}'}^0\mathcal{L}_{\bar{x}'}^1 \left[C_F C_A \left\{ \frac{44}{3} \right\} \right. \\ \left. - C_F n_f \left\{ \frac{8}{3} \right\} + C_F^2 \left\{ 48 \right\} \right] - \mathcal{D}_{\bar{x}'}^0\mathcal{L}_{\bar{z}'}^2 \left[C_F^2 \left\{ 24 \right\} \right] - \mathcal{D}_{\bar{z}'}^0\mathcal{L}_{\bar{x}'}^2 \left[C_F^2 \left\{ 24 \right\} \right] \\ - \mathcal{D}_{\bar{x}'}^1\mathcal{L}_{\bar{z}'}^1 \left[C_F^2 \left\{ 48 \right\} \right] - \mathcal{D}_{\bar{z}'}^1\mathcal{L}_{\bar{x}'}^1 \left[C_F^2 \left\{ 48 \right\} \right] + \mathcal{D}_{\bar{x}'}^1\mathcal{L}_{\bar{z}'}^0 \left[C_F C_A \left\{ \frac{44}{3} \right\} - C_F n_f \left\{ \frac{8}{3} \right\} \right] \\ + \mathcal{D}_{\bar{z}'}^1\mathcal{L}_{\bar{x}'}^0 \left[C_F C_A \left\{ \frac{44}{3} \right\} - C_F n_f \left\{ \frac{8}{3} \right\} + C_F^2 \left\{ 32 \right\} \right] - \delta_{\bar{x}'}\mathcal{L}_{\bar{z}'}^1 \left[C_F C_A \left\{ \frac{358}{9} - 8\zeta_2 \right\} \right. \\ \left. - C_F n_f \left\{ \frac{40}{9} \right\} - C_F^2 \left\{ 62 + 32\zeta_2 \right\} \right] - \delta_{\bar{z}'}\mathcal{L}_{\bar{x}'}^1 \left[C_F C_A \left\{ \frac{442}{9} - 8\zeta_2 \right\} - C_F n_f \left\{ \frac{88}{9} \right\} \right. \\ \left. - C_F^2 \left\{ 66 + 32\zeta_2 \right\} \right] + \delta_{\bar{x}'}\mathcal{L}_{\bar{z}'}^2 \left[C_F C_A \left\{ \frac{22}{3} \right\} - C_F n_f \left\{ \frac{4}{3} \right\} - C_F^2 \left\{ 12 \right\} \right] \\ + \delta_{\bar{z}'}\mathcal{L}_{\bar{x}'}^2 \left[C_F C_A \left\{ \frac{22}{3} \right\} - C_F n_f \left\{ \frac{4}{3} \right\} + C_F^2 \left\{ 28 \right\} \right] - \mathcal{D}_{\bar{x}'}^2\mathcal{L}_{\bar{z}'}^0 \left[C_F^2 \left\{ 24 \right\} \right] \\ - \mathcal{D}_{\bar{z}'}^2\mathcal{L}_{\bar{x}'}^0 \left[C_F^2 \left\{ 24 \right\} \right] - \delta_{\bar{x}'}\mathcal{L}_{\bar{z}'}^3 \left[C_F^2 \left\{ 8 \right\} \right] - \delta_{\bar{z}'}\mathcal{L}_{\bar{x}'}^3 \left[C_F^2 \left\{ 8 \right\} \right]. \quad (\text{E.6})$$

At third order, only partial result for NSV contributions can be obtained with the the presently known ingredients, unlike the SV case. Using the complete second order results for $\Psi_d^{q,(1)}$ and $\Psi_d^{q,(2)}$ along with third order results ($A_3^q, C_3^q, \tilde{C}_3^q, D_3^q, \tilde{D}_3^q$)

and an intriguing relation $\overline{\varphi}_{q,z',3}^{(3)} = -\overline{\varphi}_{q,x',3}^{(3)} = -16/9\beta_0 C_F^2$, see [545], we can predict the coefficients of $\{\delta_{\overline{x}'}\mathcal{L}_{\overline{z}'}^i, \delta_{\overline{z}'}\mathcal{L}_{\overline{x}'}^i\}$ for $i = 5, 4, 3$ and of $\{\mathcal{D}_{\overline{x}'}^i\mathcal{L}_{\overline{z}'}^j, \mathcal{D}_{\overline{z}'}^i\mathcal{L}_{\overline{x}'}^j\}$ for $i + j = 4, 3, 2, 1, 0$. The coefficients of $\{\delta_{\overline{x}'}\mathcal{L}_{\overline{z}'}^i, \delta_{\overline{z}'}\mathcal{L}_{\overline{x}'}^i\}$ for $i = 2, 1, 0$ cannot be predicted at third order, as they require explicit information at that order, namely $\overline{\varphi}_{q,\xi,3}^{(i)}$ for $i = 0, 1, 2$ and $\xi = x', z'$. Thus, the available partial NSV results at $\mathcal{O}(a_s^3)$ are

$$\begin{aligned}
(\Delta)\mathcal{C}_{J,cc}^{(3),\text{NSV}} = & \mathcal{D}_{\overline{x}'}^0\mathcal{L}_{\overline{z}'}^0 \left[C_F n_f C_A \left\{ \frac{11012}{81} - \frac{560}{9}\zeta_2 \right\} - C_F n_f^2 \left\{ \frac{400}{81} - \frac{32}{9}\zeta_2 \right\} - C_F^2 n_f \left\{ \frac{940}{9} + \frac{320}{3}\zeta_3 \right. \right. \\
& + \left. \frac{1136}{9}\zeta_2 \right\} - C_F C_A^2 \left\{ \frac{46450}{81} - 176\zeta_3 - 256\zeta_2 + \frac{176}{5}\zeta_2^2 \right\} + C_F^2 C_A \left\{ \frac{7987}{9} + \frac{512}{3}\zeta_3 \right. \\
& + \left. \frac{6920}{9}\zeta_2 - \frac{912}{5}\zeta_2^2 \right\} - C_F^3 \left\{ 325 - 112\zeta_3 + 640\zeta_2 + \frac{288}{5}\zeta_2^2 \right\} \Big] \\
& + \mathcal{D}_{\overline{z}'}^0\mathcal{L}_{\overline{x}'}^0 \left[C_F^2 C_A \left\{ \frac{35605}{27} + \frac{896}{3}\zeta_3 + \frac{10520}{9}\zeta_2 - \frac{912}{5}\zeta_2^2 \right\} + C_F n_f C_A \left\{ \frac{21572}{81} - \frac{656}{9}\zeta_2 \right\} \right. \\
& - C_F n_f^2 \left\{ \frac{1648}{81} - \frac{32}{9}\zeta_2 \right\} - C_F^2 n_f \left\{ \frac{4588}{27} + \frac{320}{3}\zeta_3 + \frac{2000}{9}\zeta_2 \right\} - C_F C_A^2 \left\{ \frac{62242}{81} - 176\zeta_3 \right. \\
& - \left. \frac{944}{3}\zeta_2 + \frac{176}{5}\zeta_2^2 \right\} - C_F^3 \left\{ 697 - 880\zeta_3 + 848\zeta_2 + \frac{288}{5}\zeta_2^2 \right\} \Big] + \mathcal{D}_{\overline{x}'}^0\mathcal{L}_{\overline{z}'}^1 \left[C_F n_f^2 \left\{ \frac{160}{27} \right\} \right. \\
& + C_F C_A^2 \left\{ \frac{9100}{27} - \frac{176}{3}\zeta_2 \right\} - C_F n_f C_A \left\{ \frac{2672}{27} - \frac{32}{3}\zeta_2 \right\} + C_F^2 C_A \left\{ \frac{580}{9} - 336\zeta_3 - 496\zeta_2 \right\} \\
& + C_F^2 n_f \left\{ \frac{80}{9} + 96\zeta_2 \right\} + C_F^3 \left\{ 256 - 640\zeta_3 \right\} \Big] + \mathcal{D}_{\overline{z}'}^0\mathcal{L}_{\overline{x}'}^1 \left[C_F C_A^2 \left\{ \frac{10948}{27} - \frac{176}{3}\zeta_2 \right\} \right. \\
& - C_F n_f C_A \left\{ \frac{4064}{27} - \frac{32}{3}\zeta_2 \right\} + C_F^2 C_A \left\{ \frac{2420}{3} - 336\zeta_3 - 720\zeta_2 \right\} - C_F^2 n_f \left\{ \frac{416}{3} - 96\zeta_2 \right\} \\
& - C_F^3 \left\{ 768 + 640\zeta_3 + 736\zeta_2 \right\} + C_F n_f^2 \left\{ \frac{352}{27} \right\} \Big] + \mathcal{D}_{\overline{x}'}^0\mathcal{L}_{\overline{z}'}^2 \left[C_F^3 \left\{ 352 + 384\zeta_2 \right\} \right. \\
& + C_F n_f C_A \left\{ \frac{176}{9} \right\} - C_F C_A^2 \left\{ \frac{484}{9} \right\} - C_F n_f^2 \left\{ \frac{16}{9} \right\} - C_F^2 C_A \left\{ 368 - 96\zeta_2 \right\} + C_F^2 n_f \left\{ 48 \right\} \Big] \\
& + \mathcal{D}_{\overline{z}'}^0\mathcal{L}_{\overline{x}'}^2 \left[C_F n_f C_A \left\{ \frac{176}{9} \right\} - C_F n_f^2 \left\{ \frac{16}{9} \right\} - C_F C_A^2 \left\{ \frac{484}{9} \right\} - C_F^2 C_A \left\{ \frac{2096}{3} - 96\zeta_2 \right\} \right. \\
& + C_F^2 n_f \left\{ \frac{368}{3} \right\} + C_F^3 \left\{ 416 + 384\zeta_2 \right\} \Big] + \mathcal{D}_{\overline{x}'}^0\mathcal{L}_{\overline{z}'}^3 \left[C_F^2 C_A \left\{ \frac{880}{9} \right\} - C_F^2 n_f \left\{ \frac{160}{9} \right\} \right. \\
& - C_F^3 \left\{ 48 \right\} \Big] + \mathcal{D}_{\overline{z}'}^0\mathcal{L}_{\overline{x}'}^3 \left[C_F^2 C_A \left\{ \frac{880}{9} \right\} - C_F^2 n_f \left\{ \frac{160}{9} \right\} + C_F^3 \left\{ 176 \right\} \right] \\
& - \mathcal{D}_{\overline{x}'}^0\mathcal{L}_{\overline{z}'}^4 \left[C_F^3 \left\{ 40 \right\} \right] - \mathcal{D}_{\overline{z}'}^0\mathcal{L}_{\overline{x}'}^4 \left[C_F^3 \left\{ 40 \right\} \right] + \mathcal{D}_{\overline{x}'}^1\mathcal{L}_{\overline{z}'}^0 \left[C_F C_A^2 \left\{ \frac{7120}{27} - \frac{176}{3}\zeta_2 \right\} \right. \\
& + C_F n_f^2 \left\{ \frac{160}{27} \right\} - C_F n_f C_A \left\{ \frac{2312}{27} - \frac{32}{3}\zeta_2 \right\} + C_F^2 C_A \left\{ 376 - 336\zeta_3 - 560\zeta_2 \right\} \\
& - C_F^3 \left\{ 640\zeta_3 + 96\zeta_2 \right\} - C_F^2 n_f \left\{ 40 - 96\zeta_2 \right\} \Big] + \mathcal{D}_{\overline{z}'}^1\mathcal{L}_{\overline{x}'}^0 \left[C_F C_A^2 \left\{ \frac{12928}{27} - \frac{176}{3}\zeta_2 \right\} \right.
\end{aligned}$$

$$\begin{aligned}
& + C_F n_f^2 \left\{ \frac{352}{27} \right\} - C_F n_f C_A \left\{ \frac{4424}{27} - \frac{32}{3} \zeta_2 \right\} + C_F^2 C_A \left\{ \frac{4456}{9} - 336 \zeta_3 - 656 \zeta_2 \right\} \\
& - C_F^2 n_f \left\{ \frac{808}{9} - 96 \zeta_2 \right\} - C_F^3 \left\{ 512 + 640 \zeta_3 + 640 \zeta_2 \right\} \Big] + \mathcal{D}_{\bar{x}'}^1 \mathcal{L}_{\bar{z}'}^1 \left[C_F^3 \left\{ 664 + 768 \zeta_2 \right\} \right. \\
& + C_F n_f C_A \left\{ \frac{352}{9} \right\} - C_F C_A^2 \left\{ \frac{968}{9} \right\} - C_F n_f^2 \left\{ \frac{32}{9} \right\} - C_F^2 C_A \left\{ \frac{2264}{3} - 192 \zeta_2 \right\} \\
& + C_F^2 n_f \left\{ \frac{320}{3} \right\} \Big] + \mathcal{D}_{\bar{z}'}^1 \mathcal{L}_{\bar{x}'}^1 \left[C_F n_f C_A \left\{ \frac{352}{9} \right\} - C_F C_A^2 \left\{ \frac{968}{9} \right\} - C_F n_f^2 \left\{ \frac{32}{9} \right\} \right. \\
& + C_F^2 n_f \left\{ \frac{704}{3} \right\} - C_F^2 C_A \left\{ \frac{4136}{3} - 192 \zeta_2 \right\} + C_F^3 \left\{ 872 + 768 \zeta_2 \right\} \Big] \\
& + \mathcal{D}_{\bar{x}'}^1 \mathcal{L}_{\bar{z}'}^2 \left[C_F^2 C_A \left\{ \frac{880}{3} \right\} - C_F^2 n_f \left\{ \frac{160}{3} \right\} - C_F^3 \left\{ 80 \right\} \right] + \mathcal{D}_{\bar{z}'}^1 \mathcal{L}_{\bar{x}'}^2 \left[C_F^2 C_A \left\{ \frac{880}{3} \right\} \right. \\
& - C_F^2 n_f \left\{ \frac{160}{3} \right\} + C_F^3 \left\{ 464 \right\} \Big] - \mathcal{D}_{\bar{x}'}^1 \mathcal{L}_{\bar{z}'}^3 \left[C_F^3 \left\{ 160 \right\} \right] - \mathcal{D}_{\bar{z}'}^1 \mathcal{L}_{\bar{x}'}^3 \left[C_F^3 \left\{ 160 \right\} \right] \\
& + \mathcal{D}_{\bar{x}'}^2 \mathcal{L}_{\bar{z}'}^0 \left[C_F n_f C_A \left\{ \frac{176}{9} \right\} - C_F C_A^2 \left\{ \frac{484}{9} \right\} - C_F n_f^2 \left\{ \frac{16}{9} \right\} - C_F^2 C_A \left\{ 416 - 96 \zeta_2 \right\} \right. \\
& + C_F^2 n_f \left\{ 64 \right\} + C_F^3 \left\{ 312 + 384 \zeta_2 \right\} \Big] + \mathcal{D}_{\bar{z}'}^2 \mathcal{L}_{\bar{x}'}^0 \left[C_F n_f C_A \left\{ \frac{176}{9} \right\} - C_F C_A^2 \left\{ \frac{484}{9} \right\} \right. \\
& - C_F n_f^2 \left\{ \frac{16}{9} \right\} + C_F^2 n_f \left\{ \frac{320}{3} \right\} - C_F^2 C_A \left\{ \frac{1952}{3} - 96 \zeta_2 \right\} + C_F^3 \left\{ 456 + 384 \zeta_2 \right\} \Big] \\
& + \mathcal{D}_{\bar{x}'}^2 \mathcal{L}_{\bar{z}'}^1 \left[C_F^2 C_A \left\{ \frac{880}{3} \right\} - C_F^2 n_f \left\{ \frac{160}{3} \right\} \right] + \mathcal{D}_{\bar{z}'}^2 \mathcal{L}_{\bar{x}'}^1 \left[C_F^2 C_A \left\{ \frac{880}{3} \right\} - C_F^2 n_f \left\{ \frac{160}{3} \right\} \right. \\
& + C_F^3 \left\{ 384 \right\} \Big] - \mathcal{D}_{\bar{x}'}^2 \mathcal{L}_{\bar{z}'}^2 \left[C_F^3 \left\{ 240 \right\} \right] - \mathcal{D}_{\bar{z}'}^2 \mathcal{L}_{\bar{x}'}^2 \left[C_F^3 \left\{ 240 \right\} \right] \\
& + \delta_{\bar{x}'} \mathcal{L}_{\bar{z}'}^3 \left[C_F n_f C_A \left\{ \frac{176}{27} \right\} - C_F C_A^2 \left\{ \frac{484}{27} \right\} - C_F n_f^2 \left\{ \frac{16}{27} \right\} - C_F^2 C_A \left\{ \frac{3316}{27} - 32 \zeta_2 \right\} \right. \\
& + C_F^2 n_f \left\{ \frac{400}{27} \right\} + C_F^3 \left\{ 124 + 128 \zeta_2 \right\} \Big] + \delta_{\bar{z}'} \mathcal{L}_{\bar{x}'}^3 \left[C_F n_f C_A \left\{ \frac{176}{27} \right\} - C_F C_A^2 \left\{ \frac{484}{27} \right\} \right. \\
& - C_F n_f^2 \left\{ \frac{16}{27} \right\} + C_F^2 n_f \left\{ \frac{1136}{27} \right\} - C_F^2 C_A \left\{ \frac{6284}{27} - 32 \zeta_2 \right\} + C_F^3 \left\{ 132 + 128 \zeta_2 \right\} \Big] \\
& + \mathcal{D}_{\bar{x}'}^3 \mathcal{L}_{\bar{z}'}^0 \left[C_F^2 C_A \left\{ \frac{880}{9} \right\} - C_F^2 n_f \left\{ \frac{160}{9} \right\} + C_F^3 \left\{ 32 \right\} \right] + \mathcal{D}_{\bar{z}'}^3 \mathcal{L}_{\bar{x}'}^0 \left[C_F^2 C_A \left\{ \frac{880}{9} \right\} \right. \\
& - C_F^2 n_f \left\{ \frac{160}{9} \right\} + C_F^3 \left\{ 96 \right\} \Big] - \mathcal{D}_{\bar{x}'}^3 \mathcal{L}_{\bar{z}'}^1 \left[C_F^3 \left\{ 160 \right\} \right] - \mathcal{D}_{\bar{z}'}^3 \mathcal{L}_{\bar{x}'}^1 \left[C_F^3 \left\{ 160 \right\} \right] \\
& + \delta_{\bar{x}'} \mathcal{L}_{\bar{z}'}^4 \left[C_F^2 C_A \left\{ \frac{220}{9} \right\} - C_F^2 n_f \left\{ \frac{40}{9} \right\} - C_F^3 \left\{ 16 \right\} \right] + \delta_{\bar{z}'} \mathcal{L}_{\bar{x}'}^4 \left[C_F^2 C_A \left\{ \frac{220}{9} \right\} \right. \\
& - C_F^2 n_f \left\{ \frac{40}{9} \right\} + C_F^3 \left\{ 48 \right\} \Big] - \mathcal{D}_{\bar{x}'}^4 \mathcal{L}_{\bar{z}'}^0 \left[C_F^3 \left\{ 40 \right\} \right] - \mathcal{D}_{\bar{z}'}^4 \mathcal{L}_{\bar{x}'}^0 \left[C_F^3 \left\{ 40 \right\} \right] \\
& - \delta_{\bar{x}'} \mathcal{L}_{\bar{z}'}^5 \left[C_F^3 \left\{ 8 \right\} \right] - \delta_{\bar{z}'} \mathcal{L}_{\bar{x}'}^5 \left[C_F^3 \left\{ 8 \right\} \right]. \tag{E.7}
\end{aligned}$$

In analogy to the third order, many terms at the fourth order can be predicted from the knowledge of $\Psi_d^{q,(1)}$, $\Psi_d^{q,(2)}$ and other higher order results ($A_3^q, C_3^q, \tilde{C}_3^q, D_3^q, \tilde{D}_3^q$) and the relation $\bar{\varphi}_{q,z',3}^{(3)} = -\bar{\varphi}_{q,x',3}^{(3)} = -16/9\beta_0 C_F^2$. For example, we can predict the coefficients of $\{\delta_{\bar{x}'}\mathcal{L}_{\bar{z}'}^i, \delta_{\bar{z}'}\mathcal{L}_{\bar{x}'}^i\}$ for $i = 7, 6, 5$ and $\{\mathcal{D}_{\bar{x}'}^i\mathcal{L}_{\bar{z}'}^j, \mathcal{D}_{\bar{z}'}^i\mathcal{L}_{\bar{x}'}^j\}$ for $i+j = 6, 5, 4$ and in addition the following terms: $\{\mathcal{D}_{\bar{x}'}^i\mathcal{L}_{\bar{z}'}^j, \mathcal{D}_{\bar{z}'}^i\mathcal{L}_{\bar{x}'}^j\}$ for $i+j = 3$ with constraint $i \geq 2$. However, with the present information available we cannot predict $\{\delta_{\bar{x}'}\mathcal{L}_{\bar{z}'}^i, \delta_{\bar{z}'}\mathcal{L}_{\bar{x}'}^i\}$ for $i = 4, 3, 2, 1, 0$ and $\{\mathcal{D}_{\bar{x}'}^i\mathcal{L}_{\bar{z}'}^j, \mathcal{D}_{\bar{z}'}^i\mathcal{L}_{\bar{x}'}^j\}$ for $i = 1, 0$ and $j = 2, 1, 0$. They require explicit third and fourth order results for $\bar{\varphi}_{q,\xi,3}^{(i)}$ for $i = 0, 1, 2$ and $\bar{\varphi}_{q,\xi,4}^{(i)}$ for $i = 0, 1, 2, 3, 4$ where $\xi = x', z'$.

Since the explicit expressions for the SV and NSV part of the fourth-order coefficient functions are rather lengthy, we do not present them here, the complete results can be found in Eq. (66) and Eq. (70) of [179].

Appendix F

Ingredients for Threshold Resummation

F.1 Coefficients in $\Gamma_{\hat{F}_q} : K_d^q$ and G_d^q

The coefficients K_d^q used in Eq. (5.23) up to fourth order in $\hat{a}_s$ are given below:

$$K_d^q(\mu_R^2, \varepsilon) = \sum_{i=0}^{\infty} \hat{a}_s^i \left(\frac{\mu_R^2}{\mu^2} \right)^{i \frac{\varepsilon}{2}} S_\varepsilon^i K_d^{q(i)}(\varepsilon), \quad (\text{F.1})$$

where

$$\begin{aligned} K_d^{q(1)}(\varepsilon) &= \frac{1}{\varepsilon} \left\{ -2A_1^q \right\}, \\ K_d^{q(2)}(\varepsilon) &= \frac{1}{\varepsilon^2} \left\{ 2\beta_0 A_1^q \right\} + \frac{1}{\varepsilon} \left\{ -A_2^q \right\}, \\ K_d^{q(3)}(\varepsilon) &= \frac{1}{\varepsilon^3} \left\{ -\frac{8}{3}\beta_0^2 A_1^q \right\} + \frac{1}{\varepsilon^2} \left\{ \frac{2}{3}\beta_1 A_1^q + \frac{8}{3}\beta_0 A_2^q \right\} + \frac{1}{\varepsilon} \left\{ -\frac{2}{3}A_3^q \right\}, \\ K_d^{q(4)}(\varepsilon) &= \frac{1}{\varepsilon^4} \left\{ 4\beta_0^3 A_1^q \right\} - \frac{1}{\varepsilon^3} \left\{ \frac{8}{3}\beta_0\beta_1 A_1^q + 6\beta_0^2 A_2^q \right\} + \frac{1}{\varepsilon^2} \left\{ \frac{1}{3}\beta_2 A_1^q + \beta_1 A_2^q + 3\beta_0 A_3^q \right\} \end{aligned}$$

$$+ \frac{1}{\varepsilon} \left\{ -\frac{1}{2} A_4^q \right\}. \quad (\text{F.2})$$

The constants A_i^q are the a_s^i coefficients of the cusp anomalous dimension A^q :

$$A^q(a_s(\mu_R^2)) = \sum_i a_s^i(\mu_R^2) A_i^q. \quad (\text{F.3})$$

The finite terms G_d^q in Eq. (5.23) can be written as

$$G_d^q(\hat{a}_s, Q^2, \mu_R^2, \varepsilon) = G_d^q(a_s(Q^2), \varepsilon) + \sum_{i=1}^{\infty} \hat{a}_s^i \left(\frac{Q^2}{\mu^2} \right)^{i \frac{\varepsilon}{2}} S_\varepsilon^i K_d^{q,(i)}(\varepsilon) - K_d^q(\mu_R^2, \varepsilon). \quad (\text{F.4})$$

The first terms is expanded as: $G_d^q(a_s(Q^2), \varepsilon) = \sum_{i=1}^{\infty} a_s^i(Q^2) G_{d,i}^q(\varepsilon)$, where

$$G_{d,i}^q(\varepsilon) = 2B_i^q + f_i^q + \chi_{d,i}^q + \sum_{j=1}^{\infty} \varepsilon^j \mathcal{G}_{d,i}^{q,(j)}, \quad (\text{F.5})$$

with

$$\begin{aligned} \chi_{d,1}^q &= 0, \chi_{d,2}^q = -2\beta_0 \mathcal{G}_{d,1}^{q,(1)}, \chi_{d,3}^q = -2\beta_1 \mathcal{G}_{d,1}^{q,(1)} - 2\beta_0 \left(\mathcal{G}_{d,2}^{q,(1)} + 2\beta_0 \mathcal{G}_{d,1}^{q,(2)} \right), \\ \chi_{d,4}^q &= -2\beta_2 \mathcal{G}_{d,1}^{q,(1)} - 2\beta_1 \left(\mathcal{G}_{d,2}^{q,(1)} + 4\beta_0 \mathcal{G}_{d,1}^{q,(2)} \right) - 2\beta_0 \left(\mathcal{G}_{d,3}^{q,(1)} + 2\beta_0 \mathcal{G}_{d,2}^{q,(2)} + 4\beta_0^2 \mathcal{G}_{d,1}^{q,(3)} \right). \end{aligned} \quad (\text{F.6})$$

Next, the results for $\mathcal{G}_{d,i}^{q,(j)}$ are given below

$$\begin{aligned} \mathcal{G}_{d,1}^{q,(1)} &= C_F \left\{ -8 + \zeta_2 \right\}, \quad \mathcal{G}_{d,1}^{q,(2)} = C_F \left\{ 8 - \frac{7}{3} \zeta_3 - \frac{3}{4} \zeta_2 \right\}, \\ \mathcal{G}_{d,1}^{q,(3)} &= C_F \left\{ -8 + \frac{7}{4} \zeta_3 + \zeta_2 + \frac{47}{80} \zeta_2^2 \right\}, \\ \mathcal{G}_{d,1}^{q,(4)} &= C_F \left\{ 8 - \frac{31}{20} \zeta_5 - \frac{7}{3} \zeta_3 - \zeta_2 + \frac{7}{24} \zeta_2 \zeta_3 - \frac{141}{320} \zeta_2^2 \right\}, \\ \mathcal{G}_{d,1}^{q,(5)} &= C_F \left\{ -8 + \frac{93}{80} \zeta_5 + \frac{7}{3} \zeta_3 - \frac{49}{144} \zeta_3^2 + \zeta_2 - \frac{7}{32} \zeta_2 \zeta_3 + \frac{47}{80} \zeta_2^2 + \frac{949}{4480} \zeta_2^3 \right\}, \end{aligned}$$

$$\begin{aligned}
\mathcal{G}_{d,2}^{q,(1)} = & C_F n_f \left\{ \frac{5813}{162} - \frac{8}{3} \zeta_3 + \frac{37}{9} \zeta_2 \right\} - C_F C_A \left\{ \frac{70165}{324} - \frac{260}{3} \zeta_3 + \frac{575}{18} \zeta_2 - \frac{88}{5} \zeta_2^2 \right\} \\
& - C_F^2 \left\{ \frac{1}{4} + 60 \zeta_3 - 58 \zeta_2 + \frac{88}{5} \zeta_2^2 \right\}, \\
\mathcal{G}_{d,2}^{q,(2)} = & C_F n_f \left\{ -\frac{129389}{1944} + \frac{301}{27} \zeta_3 - \frac{425}{54} \zeta_2 + \frac{7}{12} \zeta_2^2 \right\} - C_F^2 \left\{ \frac{109}{16} - 12 \zeta_5 - 184 \zeta_3 \right. \\
& + \frac{437}{4} \zeta_2 + 28 \zeta_2 \zeta_3 - \frac{108}{5} \zeta_2^2 \left. \right\} + C_F C_A \left\{ \frac{1547797}{3888} - 51 \zeta_5 - \frac{12479}{54} \zeta_3 + \frac{7297}{108} \zeta_2 \right. \\
& + \frac{89}{3} \zeta_2 \zeta_3 - \frac{653}{24} \zeta_2^2 \left. \right\}, \\
\mathcal{G}_{d,2}^{q,(3)} = & C_F n_f \left\{ \frac{2628821}{23328} - 6 \zeta_5 - \frac{4085}{162} \zeta_3 + \frac{8405}{648} \zeta_2 - \frac{11}{6} \zeta_2 \zeta_3 - \frac{1873}{720} \zeta_2^2 \right\} \\
& - C_F C_A \left\{ \frac{31174909}{46656} - 105 \zeta_5 - \frac{154405}{324} \zeta_3 + \frac{569}{6} \zeta_3^2 + \frac{155701}{1296} \zeta_2 + \frac{239}{12} \zeta_2 \zeta_3 \right. \\
& - \frac{100907}{1440} \zeta_2^2 + \frac{809}{140} \zeta_2^3 \left. \right\} + C_F^2 \left\{ \frac{1287}{64} - 9 \zeta_5 - \frac{1807}{4} \zeta_3 + 134 \zeta_3^2 + \frac{2991}{16} \zeta_2 \right. \\
& + 13 \zeta_2 \zeta_3 - \frac{127}{2} \zeta_2^2 + \frac{858}{35} \zeta_2^3 \left. \right\}, \\
\mathcal{G}_{d,2}^{q,(4)} = & C_F n_f \left\{ -\frac{50947325}{279936} + \frac{3109}{180} \zeta_5 + \frac{91985}{1944} \zeta_3 - \frac{289}{108} \zeta_3^2 - \frac{160493}{7776} \zeta_2 + \frac{791}{216} \zeta_2 \zeta_3 \right. \\
& + \frac{12781}{2160} \zeta_2^2 + \frac{953}{480} \zeta_2^3 \left. \right\} + C_F C_A \left\{ \frac{599567077}{559872} + 93 \zeta_7 - \frac{96503}{360} \zeta_5 - \frac{3643249}{3888} \zeta_3 \right. \\
& + \frac{32339}{216} \zeta_3^2 + \frac{3110773}{15552} \zeta_2 + \frac{497}{20} \zeta_2 \zeta_5 + \frac{16739}{432} \zeta_2 \zeta_3 - \frac{619829}{4320} \zeta_2^2 + \frac{7103}{120} \zeta_2^2 \zeta_3 \\
& - \frac{7073}{1344} \zeta_2^3 \left. \right\} - C_F^2 \left\{ \frac{10901}{256} + \frac{675}{2} \zeta_7 - 99 \zeta_5 - \frac{50219}{48} \zeta_3 + \frac{373}{2} \zeta_3^2 + \frac{19405}{64} \zeta_2 \right. \\
& + 3 \zeta_2 \zeta_5 + \frac{235}{6} \zeta_2 \zeta_3 - \frac{24453}{160} \zeta_2^2 + \frac{2597}{30} \zeta_2^2 \zeta_3 + \frac{123}{4} \zeta_2^3 \left. \right\}, \\
\mathcal{G}_{d,3}^{q,(1)} = & C_F N_4 n_{fv} \left\{ 12 - 80 \zeta_5 + 14 \zeta_3 + 30 \zeta_2 - \frac{6}{5} \zeta_2^2 \right\} - C_F C_A^2 \left\{ \frac{48902713}{8748} - \frac{688}{3} \zeta_5 \right. \\
& - \frac{85883}{18} \zeta_3 + \frac{1136}{3} \zeta_3^2 + \frac{1083305}{486} \zeta_2 - \frac{1786}{9} \zeta_2 \zeta_3 - \frac{37271}{90} \zeta_2^2 + \frac{6152}{63} \zeta_2^3 \left. \right\} \\
& - C_F n_f^2 \left\{ \frac{258445}{2187} - \frac{536}{81} \zeta_3 + \frac{3466}{81} \zeta_2 + \frac{40}{9} \zeta_2^2 \right\} + C_F^2 C_A \left\{ \frac{230}{3} - \frac{3020}{3} \zeta_5 \right.
\end{aligned}$$

$$\begin{aligned}
& -\frac{23402}{9}\zeta_3 + 296\zeta_3^2 + \frac{55499}{18}\zeta_2 - \frac{3448}{3}\zeta_2\zeta_3 + \frac{2432}{45}\zeta_2^2 - \frac{15448}{105}\zeta_2^3 \Big\} \\
& - C_F^3 \left\{ \frac{1527}{4} - 1992\zeta_5 + 2130\zeta_3 - 48\zeta_3^2 + 206\zeta_2 - 840\zeta_2\zeta_3 + 534\zeta_2^2 \right. \\
& \left. - \frac{21584}{105}\zeta_2^3 \right\} + C_F C_A n_f \left\{ \frac{3702974}{2187} - 72\zeta_5 - \frac{68660}{81}\zeta_3 + \frac{155008}{243}\zeta_2 \right. \\
& \left. + \frac{392}{9}\zeta_2\zeta_3 - \frac{1298}{45}\zeta_2^2 \right\} + C_F^2 n_f \left\{ \frac{73271}{162} - \frac{368}{3}\zeta_5 + \frac{19700}{27}\zeta_3 - \frac{7541}{18}\zeta_2 \right. \\
& \left. - \frac{152}{3}\zeta_2\zeta_3 - \frac{704}{45}\zeta_2^2 \right\}. \tag{F.7}
\end{aligned}$$

F.2 Coefficients in $\Phi_{d,q}^{\text{SV}}$: $\overline{K}_d^q$ and $\overline{G}_d^q$

Here we present the SV coefficients in $\Phi_{d,q}$ in Eq. (5.35). We expand $\overline{K}_d^q(\mu_R^2, x', z', \varepsilon) = \delta(1-x')\delta(1-z') \sum_{i=0}^{\infty} \hat{a}_s^i \left(\frac{\mu_R^2}{\mu^2} \right)^{i \frac{\varepsilon}{2}} S_\varepsilon^i \overline{K}_d^{q(i)}(\varepsilon)$ to fourth order in a_s , where

$$\begin{aligned}
\overline{K}_d^{q(1)}(\varepsilon) &= \frac{1}{\varepsilon} \left\{ 2A_1^q \right\}, \\
\overline{K}_d^{q(2)}(\varepsilon) &= \frac{1}{\varepsilon^2} \left\{ -2\beta_0 A_1^q \right\} + \frac{1}{\varepsilon} \left\{ A_2^q \right\}, \\
\overline{K}_d^{q(3)}(\varepsilon) &= \frac{1}{\varepsilon^3} \left\{ \frac{8}{3}\beta_0^2 A_1^q \right\} + \frac{1}{\varepsilon^2} \left\{ -\frac{2}{3}\beta_1 A_1^q - \frac{8}{3}\beta_0 A_2^q \right\} + \frac{1}{\varepsilon} \left\{ \frac{2}{3}A_3^q \right\}, \\
\overline{K}_d^{q(4)}(\varepsilon) &= \frac{1}{\varepsilon^4} \left\{ -4\beta_0^3 A_1^q \right\} + \frac{1}{\varepsilon^3} \left\{ \frac{8}{3}\beta_0\beta_1 A_1^q + 6\beta_0^2 A_2^q \right\} + \frac{1}{\varepsilon^2} \left\{ -\frac{1}{3}\beta_2 A_1^q - \beta_1 A_2^q \right. \\
& \quad \left. - 3\beta_0 A_3^q \right\} + \frac{1}{\varepsilon} \left\{ \frac{1}{2}A_4^q \right\}. \tag{F.8}
\end{aligned}$$

The finite terms $\overline{G}_{d,\text{SV}}^{q(i)}(\varepsilon)$ are related to its renormalised counter parts $\overline{\mathcal{G}}_{d,i}^q(\varepsilon)$ in the following way:

$$\sum_{i=1}^{\infty} \hat{a}_s^i \left(\frac{Q^2(1-x')(1-z')}{\mu^2} \right)^{i \frac{\varepsilon}{2}} S_{\varepsilon}^i \overline{G}_{d,\text{SV}}^{q(i)}(\varepsilon) = \sum_{i=1}^{\infty} a_s^i (Q^2(1-x')(1-z')) \overline{\mathcal{G}}_{d,i}^q(\varepsilon). \quad (\text{F.9})$$

we find,

$$\begin{aligned} \overline{G}_{d,\text{SV}}^{q(1)}(\varepsilon) &= \overline{\mathcal{G}}_{d,1}^q(\varepsilon), \\ \overline{G}_{d,\text{SV}}^{q(2)}(\varepsilon) &= \frac{1}{\varepsilon} \left(-2\beta_0 \overline{\mathcal{G}}_{d,1}^q(\varepsilon) \right) + \overline{\mathcal{G}}_{d,2}^q(\varepsilon), \\ \overline{G}_{d,\text{SV}}^{q(3)}(\varepsilon) &= \frac{1}{\varepsilon^2} \left(4\beta_0^2 \overline{\mathcal{G}}_{d,1}^q(\varepsilon) \right) + \frac{1}{\varepsilon} \left(-\beta_1 \overline{\mathcal{G}}_{d,1}^q(\varepsilon) - 4\beta_0 \overline{\mathcal{G}}_{d,2}^q(\varepsilon) \right) + \overline{\mathcal{G}}_{d,3}^q(\varepsilon), \\ \overline{G}_{d,\text{SV}}^{q(4)}(\varepsilon) &= \frac{1}{\varepsilon^3} \left(-8\beta_0^3 \overline{\mathcal{G}}_{d,1}^q(\varepsilon) \right) + \frac{1}{\varepsilon^2} \left(\frac{16}{3} \beta_0 \beta_1 \overline{\mathcal{G}}_{d,1}^q(\varepsilon) + 12\beta_0^2 \overline{\mathcal{G}}_{d,2}^q(\varepsilon) \right), \\ &\quad + \frac{1}{\varepsilon} \left(-\frac{2}{3} \beta_2 \overline{\mathcal{G}}_{d,1}^q(\varepsilon) - 2\beta_1 \overline{\mathcal{G}}_{d,2}^q(\varepsilon) - 6\beta_0 \overline{\mathcal{G}}_{d,3}^q(\varepsilon) \right) + \overline{\mathcal{G}}_{d,4}^q(\varepsilon). \end{aligned} \quad (\text{F.10})$$

F.3 QCD β -functions

The QCD β -function is expanded as,

$$\beta(a_s) = - \sum_{i=0}^{\infty} a_s^{i+2} \beta_i, \quad (\text{F.11})$$

and known to five loops [26–29]. Here results up to four loops are presented,

$$\begin{aligned} \beta_0 &= \frac{11}{3} C_A - \frac{2}{3} n_f, \\ \beta_1 &= \frac{34}{3} C_A^2 - 2n_f C_F - \frac{10}{3} n_f C_A, \\ \beta_2 &= \frac{2857}{54} C_A^3 - \frac{1415}{54} C_A^2 n_f + \frac{79}{54} C_A n_f^2 + \frac{11}{9} C_F n_f^2 - \frac{205}{18} C_F C_A n_f + C_F^2 n_f, \end{aligned}$$

$$\begin{aligned}
\beta_3 = & n_f \frac{d_F^{abcd} d_A^{abcd}}{N_A} \left\{ \frac{512}{9} - \frac{1664}{3} \zeta_3 \right\} - \frac{d_A^{abcd} d_A^{abcd}}{N_A} \left\{ \frac{80}{9} - \frac{704}{3} \zeta_3 \right\} + C_A n_f^3 \left\{ \frac{53}{243} \right\} \\
& - n_f^2 \frac{d_F^{abcd} d_F^{abcd}}{N_A} \left\{ \frac{704}{9} - \frac{512}{3} \zeta_3 \right\} + C_A^2 n_f^2 \left\{ \frac{3965}{162} + \frac{56}{9} \zeta_3 \right\} + C_F n_f^3 \left\{ \frac{154}{243} \right\} \\
& - C_A^3 n_f \left\{ \frac{39143}{162} - \frac{68}{3} \zeta_3 \right\} + C_A^4 \left\{ \frac{150653}{486} - \frac{44}{9} \zeta_3 \right\} + C_F^2 n_f^2 \left\{ \frac{338}{27} - \frac{176}{9} \zeta_3 \right\} \\
& + C_F C_A n_f^2 \left\{ \frac{4288}{243} + \frac{112}{9} \zeta_3 \right\} + C_F C_A^2 n_f \left\{ \frac{7073}{486} - \frac{328}{9} \zeta_3 \right\} + C_F^3 n_f \left\{ 23 \right\} \\
& - C_F^2 C_A n_f \left\{ \frac{2102}{27} - \frac{176}{9} \zeta_3 \right\}. \tag{F.12}
\end{aligned}$$

F.4 Anomalous dimensions

In the SV+NSV limit, the diagonal Altarelli-Parisi splitting function $\mathbb{P}_{qq}$ takes the simple form

$$\mathbb{P}_{qq}(\mu_F^2, z) = \frac{2A^q(\mu_F^2)}{(1-z)_+} + 2B^q(\mu_F^2)\delta(1-z) + 2C^q(\mu_F^2)\ln(1-z) + 2\mathbb{D}^q(\mu_F^2). \tag{F.13}$$

Here, the cusp anomalous dimension A^q , which governs the behavior of soft-collinear emissions, is known up to four loops in QCD [488, 489, 492], see also [265, 266, 407, 546, 547] for the lower-order results.

The collinear anomalous dimension B^q which encodes the contribution from purely collinear emissions [265, 266], whereas the eikonal anomalous dimension f^q describes wide-angle soft-gluon emissions [266, 548]. Both quantities are known up to three loops in QCD. The first four-loop results for B^q and f^q were obtained in refs. [490, 491] and were subsequently refined in refs. [494, 549, 550]. More recently, analytic expressions have become available [495], determining B^q and f^q up to a single constant, denoted by $b_{4,FA}$. This constant was previously known numerically to high precision [494], and has recently also been expressed in terms of Riemann-

zeta values [503]. The coefficients C^q and D^q govern the NSV contribution. They can be expressed in terms of the perturbative coefficients of A^q , B^q , and the QCD β -function at lower orders, see Eqs. (5.46)–(5.49) and also [494, 500–502]. These relations have recently been confirmed up to fourth order [503]. In the following, we present the corresponding results through fourth order in a_s .

Soft anomalous dimensions:

$$\begin{aligned}
f_1^q &= 0, \\
f_2^q &= C_F C_A \left\{ \frac{808}{27} - 28\zeta_3 - \frac{22}{3}\zeta_2 \right\} - C_F n_f \left\{ \frac{112}{27} - \frac{4}{3}\zeta_2 \right\}, \\
f_3^q &= -C_F^2 n_f \left\{ \frac{1711}{27} - \frac{304}{9}\zeta_3 - 4\zeta_2 - \frac{32}{5}\zeta_2^2 \right\} + C_F C_A^2 \left\{ \frac{136781}{729} + 192\zeta_5 - \frac{1316}{3}\zeta_3 \right. \\
&\quad \left. - \frac{12650}{81}\zeta_2 + \frac{176}{3}\zeta_2\zeta_3 + \frac{352}{5}\zeta_2^2 \right\} - C_F C_A n_f \left\{ \frac{11842}{729} - \frac{728}{27}\zeta_3 - \frac{2828}{81}\zeta_2 + \frac{96}{5}\zeta_2^2 \right\} \\
&\quad - C_F n_f^2 \left\{ \frac{2080}{729} - \frac{112}{27}\zeta_3 + \frac{40}{27}\zeta_2 \right\}, \\
f_4^q &= \frac{d_F^{abcd} d_A^{abcd}}{N_F} \left\{ 192 - 2b_{4,FA} + 3484\zeta_7 - \frac{1840}{9}\zeta_5 - \frac{7808}{9}\zeta_3 - \frac{3344}{3}\zeta_3^2 - \frac{2176}{3}\zeta_2 \right. \\
&\quad \left. + 1024\zeta_2\zeta_5 - 1792\zeta_2\zeta_3 + \frac{224}{15}\zeta_2^2 - \frac{736}{5}\zeta_2^2\zeta_3 + \frac{27808}{315}\zeta_2^3 \right\} \\
&\quad + C_F C_A n_f^2 \left\{ \frac{27875}{17496} - 112\zeta_5 + \frac{32152}{243}\zeta_3 - \frac{15481}{729}\zeta_2 - \frac{224}{9}\zeta_2\zeta_3 + \frac{776}{45}\zeta_2^2 \right\} \\
&\quad - n_f \frac{d_F^{abcd} d_F^{abcd}}{N_F} \left\{ \frac{1600}{9}\zeta_5 - \frac{640}{9}\zeta_3 + \frac{320}{3}\zeta_3^2 - 256\zeta_2 + \frac{64}{5}\zeta_2^2 + \frac{1280}{21}\zeta_2^3 \right\} \\
&\quad - C_F n_f^3 \left\{ \frac{16160}{6561} + \frac{400}{243}\zeta_3 + \frac{16}{81}\zeta_2 - \frac{256}{135}\zeta_2^2 \right\} - C_F C_A^2 n_f \left\{ \frac{394109}{1944} + \frac{692}{27}\zeta_5 \right. \\
&\quad \left. + \frac{31340}{243}\zeta_3 - \frac{4420}{9}\zeta_3^2 - \frac{294539}{729}\zeta_2 + \frac{104}{9}\zeta_2\zeta_3 + \frac{4420}{9}\zeta_2^2 - \frac{27032}{189}\zeta_2^3 \right\} \\
&\quad + C_F C_A^3 \left\{ \frac{9311591}{6561} + \frac{1}{12}b_{4,FA} - \frac{11071}{6}\zeta_7 + \frac{106934}{27}\zeta_5 - \frac{829204}{243}\zeta_3 - \frac{4378}{9}\zeta_3^2 \right\}
\end{aligned}$$

$$\begin{aligned}
& -\frac{1164703}{729}\zeta_2 - \frac{1376}{3}\zeta_2\zeta_5 + \frac{12568}{9}\zeta_2\zeta_3 + \frac{231518}{135}\zeta_2^2 - \frac{4228}{15}\zeta_2^2\zeta_3 - \frac{173888}{315}\zeta_2^3 \Big\} \\
& + C_F^2 n_f^2 \left\{ \frac{16733}{486} + \frac{304}{9}\zeta_5 - \frac{4568}{81}\zeta_3 - \frac{172}{9}\zeta_2 + \frac{32}{3}\zeta_2\zeta_3 + \frac{128}{45}\zeta_2^2 \right\} \\
& - C_F^2 C_A n_f \left\{ \frac{813475}{972} - \frac{1448}{9}\zeta_5 - \frac{68882}{81}\zeta_3 + 312\zeta_3^2 - \frac{2819}{9}\zeta_2 + 160\zeta_2\zeta_3 \right. \\
& + \left. \frac{1976}{45}\zeta_2^2 - \frac{128}{35}\zeta_2^3 \right\} + C_F^3 n_f \left\{ \frac{21037}{108} - \frac{1600}{3}\zeta_5 + \frac{4424}{9}\zeta_3 - 80\zeta_3^2 - 2\zeta_2 + \frac{148}{5}\zeta_2^2 \right. \\
& - \left. \frac{320}{7}\zeta_2^3 \right\}. \tag{F.14}
\end{aligned}$$

Cusp anomalous dimensions:

$$\begin{aligned}
A_1^q &= 4C_F, \\
A_2^q &= C_A C_F \left\{ \frac{268}{9} - 8\zeta_2 \right\} - C_F n_f \left\{ \frac{40}{9} \right\}, \\
A_3^q &= C_F C_A^2 \left\{ \frac{490}{3} + \frac{88}{3}\zeta_3 - \frac{1072}{9}\zeta_2 + \frac{176}{5}\zeta_2^2 \right\} \\
& - C_F^2 n_f \left\{ \frac{110}{3} - 32\zeta_3 \right\} - C_F C_A n_f \left\{ \frac{836}{27} + \frac{112}{3}\zeta_3 - \frac{160}{9}\zeta_2 \right\} - C_F n_f^2 \left\{ \frac{16}{27} \right\}, \\
A_4^q &= \frac{d_F^{abcd} d_A^{abcd}}{N_c} \left\{ \frac{3520}{3}\zeta_5 + \frac{128}{3}\zeta_3 - 384\zeta_3^2 - 128\zeta_2 - \frac{7936}{35}\zeta_2^3 \right\} - C_F n_f^3 \left\{ \frac{32}{81} - \frac{64}{27}\zeta_3 \right\} \\
& - n_f \frac{d_F^{abcd} d_F^{abcd}}{N_c} \left\{ \frac{1280}{3}\zeta_5 + \frac{256}{3}\zeta_3 - 256\zeta_2 \right\} - C_F C_A^2 n_f \left\{ \frac{24137}{81} - \frac{2096}{9}\zeta_5 \right. \\
& + \left. \frac{23104}{27}\zeta_3 - \frac{20320}{81}\zeta_2 - \frac{448}{3}\zeta_2\zeta_3 + \frac{352}{15}\zeta_2^2 \right\} + C_F C_A^3 \left\{ \frac{84278}{81} - \frac{3608}{9}\zeta_5 \right. \\
& + \left. \frac{20944}{27}\zeta_3 - 16\zeta_3^2 - \frac{88400}{81}\zeta_2 - \frac{352}{3}\zeta_2\zeta_3 + \frac{3608}{5}\zeta_2^2 - \frac{20032}{105}\zeta_2^3 \right\} \\
& + C_F C_A n_f^2 \left\{ \frac{923}{81} + \frac{2240}{27}\zeta_3 - \frac{608}{81}\zeta_2 - \frac{224}{15}\zeta_2^2 \right\} + C_F^2 n_f^2 \left\{ \frac{2392}{81} - \frac{640}{9}\zeta_3 + \frac{64}{5}\zeta_2^2 \right\} \\
& - C_F^2 C_A n_f \left\{ \frac{34066}{81} - 160\zeta_5 - \frac{3712}{9}\zeta_3 - \frac{440}{3}\zeta_2 + 128\zeta_2\zeta_3 + \frac{352}{5}\zeta_2^2 \right\}
\end{aligned}$$

$$+ C_F^3 n_f \left\{ \frac{572}{9} - 320\zeta_5 + \frac{592}{3}\zeta_3 \right\}. \quad (\text{F.15})$$

Collinear anomalous dimensions:

$$B_1^q = 3C_F,$$

$$B_2^q = C_F^2 \left\{ \frac{3}{2} + 24\zeta_3 - 12\zeta_2 \right\} + C_F C_A \left\{ \frac{17}{6} - 12\zeta_3 + \frac{44}{3}\zeta_2 \right\} - C_F n_f \left\{ \frac{1}{3} + \frac{8}{3}\zeta_2 \right\},$$

$$\begin{aligned} B_3^q = & C_F^3 \left\{ \frac{29}{2} - 240\zeta_5 + 68\zeta_3 + 18\zeta_2 - 32\zeta_2\zeta_3 + \frac{288}{5}\zeta_2^2 \right\} - C_F^2 n_f \left\{ 23 + \frac{136}{3}\zeta_3 \right. \\ & \left. - \frac{20}{3}\zeta_2 - \frac{232}{15}\zeta_2^2 \right\} + C_F^2 C_A \left\{ \frac{151}{4} + 120\zeta_5 + \frac{844}{3}\zeta_3 - \frac{410}{3}\zeta_2 + 16\zeta_2\zeta_3 - \frac{988}{15}\zeta_2^2 \right\} \\ & - C_F C_A^2 \left\{ \frac{1657}{36} - 40\zeta_5 + \frac{1552}{9}\zeta_3 - \frac{4496}{27}\zeta_2 + 2\zeta_2^2 \right\} - C_F n_f^2 \left\{ \frac{17}{9} + \frac{16}{9}\zeta_3 - \frac{80}{27}\zeta_2 \right\} \\ & + C_F C_A n_f \left\{ 20 + \frac{200}{9}\zeta_3 - \frac{1336}{27}\zeta_2 + \frac{4}{5}\zeta_2^2 \right\}, \end{aligned}$$

$$\begin{aligned} B_4^q = & \frac{d_F^{abcd} d_A^{abcd}}{N_F} \left\{ \textcolor{red}{b}_{4,FA} \right\} - n_f \frac{d_F^{abcd} d_F^{abcd}}{N_F} \left\{ 192 + 1120\zeta_5 + \frac{992}{3}\zeta_3 - 256\zeta_3^2 - \frac{1888}{3}\zeta_2 \right. \\ & \left. - 64\zeta_2\zeta_3 + \frac{704}{15}\zeta_2^2 - \frac{2048}{45}\zeta_2^3 \right\} - C_F n_f^3 \left\{ \frac{131}{81} - \frac{304}{81}\zeta_3 - \frac{32}{81}\zeta_2 + \frac{64}{135}\zeta_2^2 \right\} \\ & - C_F C_A n_f^2 \left\{ \frac{193}{54} + \frac{88}{9}\zeta_5 + \frac{320}{9}\zeta_3 - \frac{3170}{81}\zeta_2 - \frac{80}{3}\zeta_2\zeta_3 + \frac{32}{9}\zeta_2^2 \right\} \\ & + C_F C_A^2 n_f \left\{ \frac{20027}{108} + \frac{1130}{9}\zeta_5 + \frac{9554}{27}\zeta_3 + \frac{416}{3}\zeta_3^2 - \frac{41092}{81}\zeta_2 - \frac{580}{3}\zeta_2\zeta_3 \right. \\ & \left. + \frac{2468}{45}\zeta_2^2 - \frac{4472}{135}\zeta_2^3 \right\} - C_F C_A^3 \left\{ \frac{371201}{648} + \frac{1}{24}\textcolor{red}{b}_{4,FA} + 2870\zeta_7 - \frac{11372}{9}\zeta_5 \right. \\ & \left. + \frac{153670}{81}\zeta_3 - 528\zeta_3^2 - \frac{4582}{3}\zeta_2 - 504\zeta_2\zeta_5 - \frac{472}{3}\zeta_2\zeta_3 + \frac{22388}{135}\zeta_2^2 - \frac{16}{5}\zeta_2^2\zeta_3 \right. \\ & \left. - \frac{48368}{315}\zeta_2^3 \right\} - C_F^2 n_f^2 \left\{ \frac{188}{27} - \frac{368}{9}\zeta_5 - \frac{56}{27}\zeta_3 - \frac{1244}{27}\zeta_2 + \frac{160}{9}\zeta_2\zeta_3 + \frac{4208}{135}\zeta_2^2 \right\} \\ & - C_F^2 C_A n_f \left\{ \frac{7751}{54} + \frac{7432}{9}\zeta_5 + \frac{15400}{27}\zeta_3 + \frac{1232}{3}\zeta_3^2 + \frac{3892}{27}\zeta_2 - \frac{2672}{9}\zeta_2\zeta_3 \right. \\ & \left. - \frac{55708}{135}\zeta_2^2 - \frac{2808}{35}\zeta_2^3 \right\} + C_F^2 C_A^2 \left\{ \frac{29639}{36} + 8610\zeta_7 + \frac{5354}{9}\zeta_5 + \frac{129662}{27}\zeta_3 \right. \end{aligned}$$

$$\begin{aligned}
& -\frac{7102}{3}\zeta_3^2 - \frac{46771}{27}\zeta_2 - 2104\zeta_2\zeta_5 + \frac{2096}{9}\zeta_2\zeta_3 - \frac{24340}{27}\zeta_2^2 - \frac{64}{5}\zeta_2^2\zeta_3 - \frac{21988}{35}\zeta_2^3 \Big\} \\
& + C_F^3 n_f \Big\{ 32 + 912\zeta_5 - 308\zeta_3 + 224\zeta_3^2 + 162\zeta_2 - \frac{256}{3}\zeta_2\zeta_3 - \frac{408}{5}\zeta_2^2 - \frac{51472}{315}\zeta_2^3 \Big\} \\
& - C_F^3 C_A \Big\{ \frac{2085}{4} + 10920\zeta_7 + 976\zeta_5 + 3260\zeta_3 - 3220\zeta_3^2 - 1167\zeta_2 - 2064\zeta_2\zeta_5 \\
& + \frac{1988}{3}\zeta_2\zeta_3 - \frac{4334}{5}\zeta_2^2 - \frac{256}{5}\zeta_2^2\zeta_3 - \frac{317188}{315}\zeta_2^3 \Big\} + C_F^4 \Big\{ \frac{4873}{24} + 5880\zeta_7 \\
& - 2520\zeta_5 + 2004\zeta_3 - 1152\zeta_3^2 - 450\zeta_2 - 384\zeta_2\zeta_5 - 120\zeta_2\zeta_3 - \frac{684}{5}\zeta_2^2 + \frac{128}{5}\zeta_2^2\zeta_3 \\
& - \frac{16888}{35}\zeta_2^3 \Big\}. \tag{F.16}
\end{aligned}$$

and the constant $b_{4,FA}$ is,

$$\begin{aligned}
b_{4,FA} = & 96 + 2800\zeta_7 - 400\zeta_5 - \frac{1232}{3}\zeta_3 - 704\zeta_3^2 - \frac{944}{3}\zeta_2 + 320\zeta_2\zeta_5 - 896\zeta_2\zeta_3 + \frac{64}{15}\zeta_2^2 \\
& - \frac{128}{5}\zeta_2^2\zeta_3 - \frac{12496}{315}\zeta_2^3. \tag{F.17}
\end{aligned}$$

C^q for space-like splitting functions:

$$\begin{aligned}
C_1^q &= 0, \\
C_2^q &= 16C_F^2, \\
C_3^q &= C_F^2 C_A \Big\{ \frac{2144}{9} - 64\zeta_2 \Big\} - C_F^2 n_f \Big\{ \frac{320}{9} \Big\}, \\
C_4^q &= + C_F^2 n_f^2 \Big\{ \frac{1216}{81} \Big\} + C_F^2 C_A n_f \Big\{ -\frac{41504}{81} - \frac{896}{3}\zeta_3 + \frac{640}{3}\zeta_2 \Big\} \\
& + C_F^2 C_A^2 \Big\{ \frac{177664}{81} + \frac{704}{3}\zeta_3 - \frac{4288}{3}\zeta_2 + \frac{1728}{5}\zeta_2^2 \Big\} - C_F^3 n_f \Big\{ \frac{880}{3} - 256\zeta_3 \Big\}. \tag{F.18}
\end{aligned}$$

$\tilde{C}^q$ for time-like splitting functions:

$$\begin{aligned}
\tilde{C}_1^q &= 0, \\
\tilde{C}_2^q &= -16C_F^2, \\
\tilde{C}_3^q &= -C_F^2 C_A \left\{ \frac{2144}{9} - 64\zeta_2 \right\} + C_F^2 n_f \left\{ \frac{320}{9} \right\}, \\
\tilde{C}_4^q &= C_F^2 n_f^2 \left\{ -\frac{1216}{81} \right\} + C_F^2 C_A n_f \left\{ \frac{41504}{81} + \frac{896}{3}\zeta_3 - \frac{640}{3}\zeta_2 \right\} \\
&\quad - C_F^2 C_A^2 \left\{ \frac{177664}{81} + \frac{704}{3}\zeta_3 - \frac{4288}{3}\zeta_2 + \frac{1728}{5}\zeta_2^2 \right\} + C_F^3 n_f \left\{ \frac{880}{3} - 256\zeta_3 \right\}.
\end{aligned} \tag{F.19}$$

D^q for space-like splitting functions:

$$\begin{aligned}
D_1^q &= -4C_F, \\
D_2^q &= C_F^2 \left\{ 12 \right\} - C_F C_A \left\{ \frac{400}{9} - 8\zeta_2 \right\} + C_F n_f \left\{ \frac{64}{9} \right\}, \\
D_3^q &= C_F^3 \left\{ 6 + 96\zeta_3 - 48\zeta_2 \right\} + C_F^2 C_A \left\{ \frac{302}{3} - 48\zeta_3 + \frac{104}{3}\zeta_2 \right\} - C_F n_f^2 \left\{ \frac{64}{27} \right\} \\
&\quad + C_F^2 n_f \left\{ 30 - 32\zeta_3 - \frac{32}{3}\zeta_2 \right\} - C_F C_A^2 \left\{ \frac{8582}{27} + \frac{88}{3}\zeta_3 - \frac{1336}{9}\zeta_2 + \frac{176}{5}\zeta_2^2 \right\} \\
&\quad + C_F C_A n_f \left\{ \frac{724}{9} + \frac{112}{3}\zeta_3 - \frac{208}{9}\zeta_2 \right\}, \\
D_4^q &= n_f \frac{d_F^{abcd} d_F^{abcd}}{N_F} \left\{ \frac{1280}{3}\zeta_5 + \frac{256}{3}\zeta_3 - 256\zeta_2 \right\} - \frac{d_F^{abcd} d_A^{abcd}}{N_F} \left\{ \frac{3520}{3}\zeta_5 + \frac{128}{3}\zeta_3 - 384\zeta_3^2 \right. \\
&\quad \left. - 128\zeta_2 - \frac{7936}{35}\zeta_2^3 \right\} - C_F n_f^3 \left\{ \frac{64}{27}\zeta_3 \right\} - C_F C_A n_f^2 \left\{ \frac{4093}{81} + \frac{2912}{27}\zeta_3 - \frac{1568}{81}\zeta_2 \right. \\
&\quad \left. - \frac{224}{15}\zeta_2^2 \right\} + C_F C_A^2 n_f \left\{ \frac{20921}{27} - \frac{2096}{9}\zeta_5 + \frac{27328}{27}\zeta_3 - \frac{34192}{81}\zeta_2 - \frac{448}{3}\zeta_2\zeta_3 \right. \\
&\quad \left. + \frac{704}{15}\zeta_2^2 \right\} - C_F C_A^3 \left\{ \frac{177266}{81} - \frac{3608}{9}\zeta_5 + \frac{23848}{27}\zeta_3 - 16\zeta_3^2 - \frac{131120}{81}\zeta_2 \right.
\end{aligned}$$

$$\begin{aligned}
& -\frac{352}{3}\zeta_2\zeta_3 + \frac{2552}{3}\zeta_2^2 - \frac{20032}{105}\zeta_3^2 \Big\} - C_F^2 n_f^2 \Big\{ \frac{6124}{81} - \frac{256}{3}\zeta_3 - \frac{640}{27}\zeta_2 + \frac{64}{5}\zeta_2^2 \Big\} \\
& + C_F^2 C_A n_f \Big\{ \frac{50602}{81} - 160\zeta_5 - \frac{4496}{9}\zeta_3 - \frac{12128}{27}\zeta_2 + 128\zeta_2\zeta_3 + \frac{1424}{15}\zeta_2^2 \Big\} \\
& + C_F^2 C_A^2 \Big\{ \frac{10537}{27} + 160\zeta_5 - \frac{8632}{9}\zeta_3 + \frac{19516}{27}\zeta_2 + 96\zeta_2\zeta_3 - \frac{296}{15}\zeta_2^2 \Big\} \\
& - C_F^3 n_f \Big\{ \frac{2486}{9} - 320\zeta_5 + \frac{1168}{3}\zeta_3 - 80\zeta_2 - \frac{928}{15}\zeta_2^2 \Big\} + C_F^3 C_A \Big\{ \frac{587}{3} + 480\zeta_5 \\
& + 1840\zeta_3 - 916\zeta_2 - 128\zeta_2\zeta_3 - \frac{2512}{15}\zeta_2^2 \Big\} + C_F^4 \Big\{ 58 - 960\zeta_5 + 272\zeta_3 + 72\zeta_2 \\
& - 128\zeta_2\zeta_3 + \frac{1152}{5}\zeta_2^2 \Big\}. \tag{F.20}
\end{aligned}$$

$\tilde{D}^q$ for time-like splitting functions:

$$\begin{aligned}
\tilde{D}_1^q &= -4C_F, \\
\tilde{D}_2^q &= -C_F^2 \Big\{ 12 \Big\} - C_F C_A \Big\{ \frac{400}{9} - 8\zeta_2 \Big\} + C_F n_f \Big\{ \frac{64}{9} \Big\}, \\
\tilde{D}_3^q &= -C_F^3 \Big\{ 6 + 96\zeta_3 - 48\zeta_2 \Big\} - C_F^2 C_A \Big\{ \frac{302}{3} - 48\zeta_3 + \frac{104}{3}\zeta_2 \Big\} - C_F n_f^2 \Big\{ \frac{64}{27} \\
& + C_F^2 n_f \Big\{ \frac{178}{3} - 32\zeta_3 + \frac{32}{3}\zeta_2 \Big\} - C_F C_A^2 \Big\{ \frac{8582}{27} + \frac{88}{3}\zeta_3 - \frac{1336}{9}\zeta_2 + \frac{176}{5}\zeta_2^2 \Big\} \\
& + C_F C_A n_f \Big\{ \frac{724}{9} + \frac{112}{3}\zeta_3 - \frac{208}{9}\zeta_2 \Big\} \Big\} \\
\tilde{D}_4^q &= n_f \frac{d_F^{abcd} d_F^{abcd}}{N_F} \Big\{ \frac{1280}{3}\zeta_5 + \frac{256}{3}\zeta_3 - 256\zeta_2 \Big\} - \frac{d_F^{abcd} d_A^{abcd}}{N_F} \Big\{ \frac{3520}{3}\zeta_5 + \frac{128}{3}\zeta_3 - 384\zeta_3^2 \\
& - 128\zeta_2 - \frac{7936}{35}\zeta_2^3 \Big\} - C_F n_f^3 \Big\{ \frac{64}{27}\zeta_3 \Big\} - C_F^2 n_f^2 \Big\{ \frac{4852}{81} - \frac{896}{9}\zeta_3 + \frac{640}{27}\zeta_2 + \frac{64}{5}\zeta_2^2 \Big\} \\
& + C_F C_A^2 n_f \Big\{ \frac{20921}{27} - \frac{2096}{9}\zeta_5 + \frac{27328}{27}\zeta_3 - \frac{34192}{81}\zeta_2 - \frac{448}{3}\zeta_2\zeta_3 + \frac{704}{15}\zeta_2^2 \Big\} \\
& - C_F C_A^3 \Big\{ \frac{177266}{81} - \frac{3608}{9}\zeta_5 + \frac{23848}{27}\zeta_3 - 16\zeta_3^2 - \frac{131120}{81}\zeta_2 - \frac{352}{3}\zeta_2\zeta_3 \Big\}
\end{aligned}$$

$$\begin{aligned}
& + \frac{2552}{3}\zeta_2^2 - \frac{20032}{105}\zeta_2^3 \Big\} - C_F C_A n_f^2 \Big\{ \frac{4093}{81} + \frac{2912}{27}\zeta_3 - \frac{1568}{81}\zeta_2 - \frac{224}{15}\zeta_2^2 \Big\} \\
& + C_F^2 C_A n_f \Big\{ \frac{56338}{81} - 160\zeta_5 - 560\zeta_3 + \frac{3344}{27}\zeta_2 + 128\zeta_2\zeta_3 + \frac{688}{15}\zeta_2^2 \Big\} \\
& + C_F^2 C_A^2 \Big\{ -\frac{10537}{27} - 160\zeta_5 + \frac{8632}{9}\zeta_3 - \frac{19516}{27}\zeta_2 - 96\zeta_2\zeta_3 + \frac{296}{15}\zeta_2^2 \Big\} \\
& + C_F^3 n_f \Big\{ \frac{1270}{9} + 320\zeta_5 - \frac{16}{3}\zeta_3 - 80\zeta_2 - \frac{928}{15}\zeta_2^2 \Big\} - C_F^3 C_A \Big\{ \frac{587}{3} + 480\zeta_5 \\
& + 1840\zeta_3 - 916\zeta_2 - 128\zeta_2\zeta_3 - \frac{2512}{15}\zeta_2^2 \Big\} - C_F^4 \Big\{ 58 - 960\zeta_5 + 272\zeta_3 + 72\zeta_2 \\
& - 128\zeta_2\zeta_3 + \frac{1152}{5}\zeta_2^2 \Big\}. \tag{F.21}
\end{aligned}$$

Above the color factors are defined in Eq. (E.1).

Appendix G

Results of Physical Evolution

Kernel in SV and NSV limit

In this appendix we present the $\vec{N}$ -space result of K_l for $l = 0, 1, 2$, in threshold limit.

$$\begin{aligned} K_0 &= \mathbf{L}_1^0 \mathbf{L}_2^0 \left[C_F \left\{ 6 - 8\gamma_E \right\} \right] - \frac{\mathbf{L}_1^0 \mathbf{L}_2^0}{\mathbf{N}_1} \left[C_F \left\{ 2 \right\} \right] - \frac{\mathbf{L}_1^0 \mathbf{L}_2^0}{\mathbf{N}_2} \left[C_F \left\{ 2 \right\} \right] - \mathbf{L}_1^0 \mathbf{L}_2^1 \left[C_F \left\{ 4 \right\} \right] \\ &\quad - \mathbf{L}_1^1 \mathbf{L}_2^0 \left[C_F \left\{ 4 \right\} \right] \\ K_1 &= \mathbf{L}_1^0 \mathbf{L}_2^0 \left[-C_F n_f \left\{ \frac{34}{3} + \frac{8}{3} \zeta_2 - \frac{80}{9} \gamma_E - \frac{16}{3} \gamma_E^2 \right\} + C_F C_A \left\{ \frac{193}{3} - 24\zeta_3 + \frac{44}{3} \zeta_2 - \frac{536}{9} \gamma_E \right. \right. \\ &\quad \left. \left. + 16\gamma_E \zeta_2 - \frac{88}{3} \gamma_E^2 \right\} + C_F^2 \left\{ 3 + 48\zeta_3 - 24\zeta_2 \right\} \right] + \frac{\mathbf{L}_1^0 \mathbf{L}_2^0}{\mathbf{N}_1} \left[C_F n_f \left\{ \frac{56}{9} + \frac{8}{3} \gamma_E \right\} - C_F C_A \left\{ \frac{332}{9} \right. \right. \\ &\quad \left. \left. - 4\zeta_2 + \frac{44}{3} \gamma_E \right\} + C_F^2 \left\{ 12 - 16\gamma_E \right\} \right] + \frac{\mathbf{L}_1^0 \mathbf{L}_2^0}{\mathbf{N}_2} \left[C_F n_f \left\{ \frac{8}{9} + \frac{8}{3} \gamma_E \right\} - C_F C_A \left\{ \frac{68}{9} - 4\zeta_2 + \frac{44}{3} \gamma_E \right\} \right. \\ &\quad \left. - C_F^2 \left\{ 12 - 16\gamma_E \right\} \right] + \mathbf{L}_1^0 \mathbf{L}_2^1 \left[C_F n_f \left\{ \frac{40}{9} + \frac{16}{3} \gamma_E \right\} + C_F C_A \left\{ -\frac{268}{9} + 8\zeta_2 - \frac{88}{3} \gamma_E \right\} \right] \\ &\quad + \frac{\mathbf{L}_1^0 \mathbf{L}_2^1}{\mathbf{N}_2} \left[C_F n_f \left\{ \frac{4}{3} \right\} - C_F C_A \left\{ \frac{22}{3} \right\} + C_F^2 \left\{ 16 \right\} \right] + \frac{\mathbf{L}_1^0 \mathbf{L}_2^1}{\mathbf{N}_1} \left[C_F n_f \left\{ \frac{4}{3} \right\} - C_F C_A \left\{ \frac{22}{3} \right\} \right] \\ &\quad + \mathbf{L}_1^0 \mathbf{L}_2^2 \left[C_F n_f \left\{ \frac{4}{3} \right\} - C_F C_A \left\{ \frac{22}{3} \right\} \right] + \mathbf{L}_1^2 \mathbf{L}_2^0 \left[C_F n_f \left\{ \frac{4}{3} \right\} - C_F C_A \left\{ \frac{22}{3} \right\} \right] \\ &\quad + \mathbf{L}_1^1 \mathbf{L}_2^0 \left[C_F n_f \left\{ \frac{40}{9} + \frac{16}{3} \gamma_E \right\} - C_F C_A \left\{ \frac{268}{9} - 8\zeta_2 + \frac{88}{3} \gamma_E \right\} \right] \end{aligned}$$

$$\begin{aligned}
& + \mathbf{L}_1^1 \mathbf{L}_2^1 \left[C_F n_f \left\{ \frac{8}{3} \right\} - C_F C_A \left\{ \frac{44}{3} \right\} \right] + \frac{\mathbf{L}_1^1 \mathbf{L}_2^0}{\mathbf{N}_1} \left[C_F n_f \left\{ \frac{4}{3} \right\} - C_F C_A \left\{ \frac{22}{3} \right\} - C_F^2 \left\{ 16 \right\} \right] \\
& + \frac{\mathbf{L}_1^1 \mathbf{L}_2^0}{\mathbf{N}_2} \left[C_F n_f \left\{ \frac{4}{3} \right\} - C_F C_A \left\{ \frac{22}{3} \right\} \right] \\
K_2 = & \mathbf{L}_1^0 \mathbf{L}_2^0 \left[C_F n_f^2 \left\{ \frac{220}{9} - \frac{64}{27} \zeta_3 + \frac{304}{27} \zeta_2 - \frac{800}{81} \gamma_E - \frac{320}{27} \gamma_E^2 - \frac{128}{27} \gamma_E^3 \right\} - C_F C_A n_f \left\{ \frac{3052}{9} \right. \right. \\
& - \frac{3440}{27} \zeta_3 + \frac{4184}{27} \zeta_2 - \frac{136}{15} \zeta_2^2 - \frac{16408}{81} \gamma_E + \frac{320}{9} \gamma_E \zeta_2 - \frac{4624}{27} \gamma_E^2 + \frac{64}{3} \gamma_E^2 \zeta_2 - \frac{1408}{27} \gamma_E^3 \left. \right\} \\
& + C_F C_A^2 \left\{ \frac{3082}{3} + 80 \zeta_5 - \frac{22600}{27} \zeta_3 + \frac{13708}{27} \zeta_2 - \frac{676}{15} \zeta_2^2 - \frac{62012}{81} \gamma_E + 352 \gamma_E \zeta_3 + \frac{2144}{9} \gamma_E \zeta_2 \right. \\
& - \frac{352}{5} \gamma_E \zeta_2^2 - \frac{14240}{27} \gamma_E^2 + \frac{352}{3} \gamma_E^2 \zeta_2 - \frac{3872}{27} \gamma_E^3 \left. \right\} - C_F^2 n_f \left\{ \frac{235}{3} + \frac{512}{3} \zeta_3 - \frac{296}{3} \zeta_2 - \frac{112}{15} \zeta_2^2 \right. \\
& - \frac{220}{3} \gamma_E + 64 \gamma_E \zeta_3 - 16 \gamma_E^2 \left. \right\} + C_F^2 C_A \left\{ \frac{232}{3} + 240 \zeta_5 + \frac{3008}{3} \zeta_3 - \frac{2096}{3} \zeta_2 + 32 \zeta_2 \zeta_3 - \frac{8}{3} \zeta_2^2 \right\} \\
& + C_F^3 \left\{ 29 - 480 \zeta_5 + 136 \zeta_3 + 36 \zeta_2 - 64 \zeta_2 \zeta_3 + \frac{576}{5} \zeta_2^2 \right\} \left. \right] + \frac{\mathbf{L}_1^0 \mathbf{L}_2^0}{\mathbf{N}_1} \left[C_F C_A n_f \left\{ \frac{14002}{81} - \frac{176}{9} \zeta_2 \right. \right. \\
& + \frac{5120}{27} \gamma_E - \frac{32}{3} \gamma_E \zeta_2 + \frac{352}{9} \gamma_E^2 \left. \right\} - C_F n_f^2 \left\{ \frac{1208}{81} + \frac{448}{27} \gamma_E + \frac{32}{9} \gamma_E^2 \right\} + C_F^3 \left\{ 6 + 96 \zeta_3 - 48 \zeta_2 \right\} \\
& - C_F C_A^2 \left\{ \frac{36059}{81} - 88 \zeta_3 - \frac{1064}{9} \zeta_2 + \frac{88}{5} \zeta_2^2 + \frac{13852}{27} \gamma_E - \frac{176}{3} \gamma_E \zeta_2 + \frac{968}{9} \gamma_E^2 \right\} \\
& + C_F^2 C_A \left\{ \frac{302}{3} - 48 \zeta_3 + 64 \zeta_2 - \frac{1220}{9} \gamma_E + 64 \gamma_E \zeta_2 - \frac{616}{3} \gamma_E^2 \right\} + C_F^2 n_f \left\{ \frac{47}{3} - 16 \zeta_3 - 16 \zeta_2 \right. \\
& + \frac{224}{9} \gamma_E + \frac{112}{3} \gamma_E^2 \left. \right\} \left. \right] + \frac{\mathbf{L}_1^0 \mathbf{L}_2^0}{\mathbf{N}_2} \left[C_F n_f^2 \left\{ \frac{40}{81} - \frac{64}{27} \gamma_E - \frac{32}{9} \gamma_E^2 \right\} + C_F C_A n_f \left\{ \frac{3442}{81} - \frac{80}{9} \zeta_2 \right. \right. \\
& + \frac{1616}{27} \gamma_E - \frac{32}{3} \gamma_E \zeta_2 + \frac{352}{9} \gamma_E^2 \left. \right\} - C_F C_A^2 \left\{ \frac{20267}{81} - 88 \zeta_3 - \frac{536}{9} \zeta_2 + \frac{88}{5} \zeta_2^2 + \frac{6196}{27} \gamma_E - \frac{176}{3} \gamma_E \zeta_2 \right. \\
& + \frac{968}{9} \gamma_E^2 \left. \right\} - C_F^3 \left\{ 6 + 96 \zeta_3 - 48 \zeta_2 \right\} - C_F^2 C_A \left\{ \frac{302}{3} - 48 \zeta_3 - 112 \zeta_2 - \frac{1220}{9} \gamma_E + 64 \gamma_E \zeta_2 \right. \\
& - \frac{616}{3} \gamma_E^2 \left. \right\} + C_F^2 n_f \left\{ 29 - 16 \zeta_3 - 16 \zeta_2 - \frac{80}{9} \gamma_E - \frac{112}{3} \gamma_E^2 \right\} \left. \right] + \mathbf{L}_1^0 \mathbf{L}_2^1 \left[C_F C_A n_f \left\{ \frac{8204}{81} - \frac{160}{9} \zeta_2 \right. \right. \\
& + \frac{4624}{27} \gamma_E - \frac{64}{3} \gamma_E \zeta_2 + \frac{704}{9} \gamma_E^2 \left. \right\} - C_F n_f^2 \left\{ \frac{400}{81} + \frac{320}{27} \gamma_E + \frac{64}{9} \gamma_E^2 \right\} - C_F C_A^2 \left\{ \frac{31006}{81} - 176 \zeta_3 \right. \\
& - \frac{1072}{9} \zeta_2 + \frac{176}{5} \zeta_2^2 + \frac{14240}{27} \gamma_E - \frac{352}{3} \gamma_E \zeta_2 + \frac{1936}{9} \gamma_E^2 \left. \right\} + C_F^2 n_f \left\{ \frac{110}{3} - 32 \zeta_3 + 16 \gamma_E \right\} \left. \right] \\
& + \frac{\mathbf{L}_1^0 \mathbf{L}_2^1}{\mathbf{N}_1} \left[C_F C_A n_f \left\{ \frac{2740}{27} - \frac{16}{3} \zeta_2 + \frac{352}{9} \gamma_E \right\} - C_F n_f^2 \left\{ \frac{224}{27} + \frac{32}{9} \gamma_E \right\} - C_F C_A^2 \left\{ \frac{7916}{27} \right. \right. \\
& - \frac{88}{3} \zeta_2 + \frac{968}{9} \gamma_E \left. \right\} - C_F^2 n_f \left\{ 12 - \frac{64}{3} \gamma_E \right\} + C_F^2 C_A \left\{ 88 - \frac{352}{3} \gamma_E \right\} \left. \right] - \frac{\mathbf{L}_1^0 \mathbf{L}_2^1}{\mathbf{N}_2} \left[C_F n_f^2 \left\{ \frac{32}{27} \right. \right. \\
& + \frac{32}{9} \gamma_E \left. \right\} + C_F^2 n_f \left\{ \frac{260}{9} + \frac{160}{3} \gamma_E \right\} - C_F C_A n_f \left\{ \frac{988}{27} - \frac{16}{3} \zeta_2 + \frac{352}{9} \gamma_E \right\} + C_F C_A^2 \left\{ \frac{4088}{27} \right. \\
& - \frac{88}{3} \zeta_2 + \frac{968}{9} \gamma_E \left. \right\} - C_F^2 C_A \left\{ \frac{2012}{9} - 64 \zeta_2 + \frac{880}{3} \gamma_E \right\} \left. \right] + \mathbf{L}_1^0 \mathbf{L}_2^2 \left[C_F C_A n_f \left\{ \frac{1156}{27} - \frac{16}{3} \zeta_2 \right. \right. \\
& + \frac{352}{9} \gamma_E \left. \right\} - C_F n_f^2 \left\{ \frac{80}{27} + \frac{32}{9} \gamma_E \right\} - C_F C_A^2 \left\{ \frac{3560}{27} - \frac{88}{3} \zeta_2 + \frac{968}{9} \gamma_E \right\} + C_F^2 n_f \left\{ 4 \right\} \left. \right]
\end{aligned}$$

$$\begin{aligned}
& + \frac{\mathbf{L}_1^0 \mathbf{L}_2^2}{\mathbf{N}_1} \left[C_F C_A n_f \left\{ \frac{88}{9} \right\} - C_F n_f^2 \left\{ \frac{8}{9} \right\} - C_F C_A^2 \left\{ \frac{242}{9} \right\} \right] + \frac{\mathbf{L}_1^0 \mathbf{L}_2^2}{\mathbf{N}_2} \left[C_F C_A n_f \left\{ \frac{88}{9} \right\} - C_F n_f^2 \left\{ \frac{8}{9} \right\} \right. \\
& - C_F C_A^2 \left\{ \frac{242}{9} \right\} - C_F^2 n_f \left\{ 16 \right\} + C_F^2 C_A \left\{ 88 \right\} \left. \right] + \mathbf{L}_1^0 \mathbf{L}_2^3 \left[C_F C_A n_f \left\{ \frac{176}{27} \right\} - C_F n_f^2 \left\{ \frac{16}{27} \right\} \right. \\
& - C_F C_A^2 \left\{ \frac{484}{27} \right\} \left. \right] + \mathbf{L}_1^1 \mathbf{L}_2^0 \left[C_F C_A n_f \left\{ \frac{8204}{81} - \frac{160}{9} \zeta_2 + \frac{4624}{27} \gamma_E - \frac{64}{3} \gamma_E \zeta_2 + \frac{704}{9} \gamma_E^2 \right\} \right. \\
& - C_F n_f^2 \left\{ \frac{400}{81} + \frac{320}{27} \gamma_E + \frac{64}{9} \gamma_E^2 \right\} - C_F C_A^2 \left\{ \frac{31006}{81} - 176 \zeta_3 - \frac{1072}{9} \zeta_2 + \frac{176}{5} \zeta_2^2 + \frac{14240}{27} \gamma_E \right. \\
& - \frac{352}{3} \gamma_E \zeta_2 + \frac{1936}{9} \gamma_E^2 \left. \right\} + C_F^2 n_f \left\{ \frac{110}{3} - 32 \zeta_3 + 16 \gamma_E \right\} \left. \right] + \frac{\mathbf{L}_1^1 \mathbf{L}_2^0}{\mathbf{N}_1} \left[C_F C_A n_f \left\{ \frac{2380}{27} - \frac{16}{3} \zeta_2 \right. \right. \\
& + \frac{352}{9} \gamma_E \left. \right\} - C_F n_f^2 \left\{ \frac{224}{27} + \frac{32}{9} \gamma_E \right\} - C_F C_A^2 \left\{ \frac{5936}{27} - \frac{88}{3} \zeta_2 + \frac{968}{9} \gamma_E \right\} \\
& + C_F^2 n_f \left\{ \frac{332}{9} + \frac{160}{3} \gamma_E \right\} - C_F^2 C_A \left\{ \frac{2012}{9} - 64 \zeta_2 + \frac{880}{3} \gamma_E \right\} \left. \right] + \frac{\mathbf{L}_1^1 \mathbf{L}_2^0}{\mathbf{N}_2} \left[C_F C_A n_f \left\{ \frac{628}{27} - \frac{16}{3} \zeta_2 \right. \right. \\
& + \frac{352}{9} \gamma_E \left. \right\} - C_F n_f^2 \left\{ \frac{32}{27} + \frac{32}{9} \gamma_E \right\} - C_F C_A^2 \left\{ \frac{2108}{27} - \frac{88}{3} \zeta_2 + \frac{968}{9} \gamma_E \right\} + C_F^2 n_f \left\{ 20 - \frac{64}{3} \gamma_E \right\} \\
& - C_F^2 C_A \left\{ 88 - \frac{352}{3} \gamma_E \right\} \left. \right] + \mathbf{L}_1^1 \mathbf{L}_2^1 \left[C_F C_A n_f \left\{ \frac{2312}{27} - \frac{32}{3} \zeta_2 + \frac{704}{9} \gamma_E \right\} - C_F n_f^2 \left\{ \frac{160}{27} + \frac{64}{9} \gamma_E \right\} \right. \\
& - C_F C_A^2 \left\{ \frac{7120}{27} - \frac{176}{3} \zeta_2 + \frac{1936}{9} \gamma_E \right\} + C_F^2 n_f \left\{ 8 \right\} \left. \right] + \frac{\mathbf{L}_1^1 \mathbf{L}_2^1}{\mathbf{N}_1} \left[C_F C_A n_f \left\{ \frac{176}{9} \right\} - C_F n_f^2 \left\{ \frac{16}{9} \right\} \right. \\
& - C_F C_A^2 \left\{ \frac{484}{9} \right\} + C_F^2 n_f \left\{ \frac{64}{3} \right\} - C_F^2 C_A \left\{ \frac{352}{3} \right\} \left. \right] + \frac{\mathbf{L}_1^1 \mathbf{L}_2^1}{\mathbf{N}_2} \left[C_F C_A n_f \left\{ \frac{176}{9} \right\} - C_F n_f^2 \left\{ \frac{16}{9} \right\} \right. \\
& - C_F C_A^2 \left\{ \frac{484}{9} \right\} - C_F^2 n_f \left\{ \frac{64}{3} \right\} + C_F^2 C_A \left\{ \frac{352}{3} \right\} \left. \right] + \mathbf{L}_1^1 \mathbf{L}_2^2 \left[C_F C_A n_f \left\{ \frac{176}{9} \right\} - C_F n_f^2 \left\{ \frac{16}{9} \right\} \right. \\
& - C_F C_A^2 \left\{ \frac{484}{9} \right\} \left. \right] + \mathbf{L}_1^2 \mathbf{L}_2^0 \left[C_F C_A n_f \left\{ \frac{1156}{27} - \frac{16}{3} \zeta_2 + \frac{352}{9} \gamma_E \right\} - C_F n_f^2 \left\{ \frac{80}{27} + \frac{32}{9} \gamma_E \right\} \right. \\
& - C_F C_A^2 \left\{ \frac{3560}{27} - \frac{88}{3} \zeta_2 + \frac{968}{9} \gamma_E \right\} + C_F^2 n_f \left\{ 4 \right\} \left. \right] + \frac{\mathbf{L}_1^2 \mathbf{L}_2^0}{\mathbf{N}_1} \left[C_F C_A n_f \left\{ \frac{88}{9} \right\} - C_F n_f^2 \left\{ \frac{8}{9} \right\} \right. \\
& - C_F C_A^2 \left\{ \frac{242}{9} \right\} + C_F^2 n_f \left\{ 16 \right\} - C_F^2 C_A \left\{ 88 \right\} \left. \right] + \frac{\mathbf{L}_1^2 \mathbf{L}_2^0}{\mathbf{N}_2} \left[C_F C_A n_f \left\{ \frac{88}{9} \right\} - C_F n_f^2 \left\{ \frac{8}{9} \right\} \right. \\
& - C_F C_A^2 \left\{ \frac{242}{9} \right\} \left. \right] + \mathbf{L}_1^2 \mathbf{L}_2^1 \left[C_F C_A n_f \left\{ \frac{176}{9} \right\} - C_F n_f^2 \left\{ \frac{16}{9} \right\} - C_F C_A^2 \left\{ \frac{484}{9} \right\} \right. \\
& + \mathbf{L}_1^3 \mathbf{L}_2^0 \left[C_F C_A n_f \left\{ \frac{176}{27} \right\} - C_F n_f^2 \left\{ \frac{16}{27} \right\} - C_F C_A^2 \left\{ \frac{484}{27} \right\} \right], \tag{G.1}
\end{aligned}$$

where $L_j^i = \ln^i(N_j)$, for $j = 1, 2$.

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