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The singular behavior of massive QCD amplitudes

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ABSTRACT: We discuss the structure of infrared singularities in on-shell QCD amplitudes with massive partons and present a general factorization formula in the limit of small parton masses. The factorization formula gives rise to an all-order exponentiation of both, the soft poles in dimensional regularization and the large collinear logarithms of the parton masses. Moreover, it provides a universal relation between any on-shell amplitude with massive external partons and its corresponding massless amplitude. For the form factor of a heavy quark we present explicit results including the fixed-order expansion up to three loops in the small mass limit. For general scattering processes we show how our constructive method applies to the computation of all singularities as well as the constant (mass-independent) terms of a generic massive n-parton QCD amplitude up to the next-to-next-to-leading order corrections.

KEYWORDS: NLO Computations, Hadronic Colliders, QCD.



Contents

1.	Introduction	1
2.	Factorization of QCD amplitudes	3
3.	The Sudakov form factor in QCD	7
4.	Fixed-order expansions and resummation coefficients 4.1 The factor $Z^{(m 0)}$	16 16
	4.2 The form factor \mathcal{F}	19
5.	Applications	25
6.	Summary	29
A.	The complete form factor \mathcal{F} at one loop	30

1. Introduction

Amplitudes for hard scattering processes in Quantum Chromodynamics (QCD) are of basic importance both for theory and phenomenology and predictions for these matrix elements have to include higher-order quantum corrections. They are mandatory for precision measurements of Standard Model parameters and critical to the determination of backgrounds for new physics phenomena. Many explicit computations of hard multi-parton processes do not only provide us with a wealth of information but have also helped significantly in understanding underlying principles such as factorization or the universal structure of collinear and infrared singularities.

These singularities are particularly prominent for at least two reasons. First of all, the independent knowledge of the universal limits when parton momenta become collinear or a gluon momentum tends to zero serves as a very strong check on any complete calculation. Secondly, the calculation of finite cross-sections in QCD beyond leading order has to combine consistently squared matrix elements with different numbers of partons in the final state. In any such formalism (see e.g. [1]) the individual contributions have to be suitably integrated over the available phase space and are usually infrared divergent. At next-to-leading order (NLO) in QCD the singular behavior of the corresponding amplitudes with both massive and massless partons in the final state has been extensively studied [2-4].

Research beyond NLO in the past years has been primarily focused on the calculation of massless amplitudes at next-to-next-to-leading order (NNLO), see for example [5-9]and numerous references therein. The progress at NNLO and investigations of the singular behavior of amplitudes at higher loops [10] have significantly contributed to our understanding of their general structure from the view point of all-order resummations [11]. This in turn leads to predictions for the soft and collinear behavior of massless amplitudes at any order based on a small number of perturbatively calculable anomalous dimensions.

For massive amplitudes however much less is known beyond NLO in QCD despite the fact that NNLO precision predictions with massive quarks are clearly needed in view of the data from present and the prospects of future high-energy colliders (see refs. [12-14] for related progress). Prominent examples of such measurements are for instance the forward-backward asymmetry $A_{\rm FB}$ for inclusive heavy quark production in e^+e^- -annihilation [15, 16], and cross-sections for heavy flavor production and decays at the Tevatron and the LHC (see e.g. ref. [17]).

The aim of this article is a first systematic investigation of the structure of massive QCD amplitudes in singular limits beyond NLO. To that end, we extend the studies of refs. [10, 11] to partonic scattering processes including the presence of massive particles. The masses of the latter screen the divergences of the massless amplitudes and give rise to large logarithmically enhanced contributions of Sudakov type [18], which dominate the high energy behavior of the scattering amplitudes. It is precisely the structure of these large logarithms together with soft singularities appearing as poles in (d - 4) in d dimensions, that we wish to address here for a general non-Abelian SU(N)-gauge theory such as QCD. Throughout the article we neglect power corrections in the parton masses m.

The outline of the paper is as follows. In section 2 we recall the general framework for the factorization of *n*-parton amplitudes in QCD and discuss its modifications to incorporate massive partons. As a result we derive an extremely simple universal multiplicative relation between a massive amplitude in the small mass limit and its massless version. This is one main result of this paper. The corresponding multiplicative factor (which we call Z) can be linked to the QCD form factor of massive and massless partons. Next in section 3, we specifically address the resummation and exponentiation of the QCD form factor for heavy quarks, which is our second main result. On this basis we provide in section 4 all resummation coefficients and new fixed-order expansions of the massive form factor up to three loops. For the resummation coefficients we observe striking relations between the massless and the massive case. In section 4 we also present explicit results for the universal multiplicative factor Z up to two loops and discuss its relation to the perturbative fragmentation function of a heavy quark [19]. We argue that our formalism represents the proper generalization of ref. [19] at the level of amplitudes. In section 5 we demonstrate the predictive power of the factorization ansatz for QCD amplitudes with examples from $2 \rightarrow n$ scattering processes, such as hadronic $t\bar{t}$ -production. There we discuss the complete structure of the soft and collinear singularities including the logarithmically enhanced terms to NNLO in perturbative QCD. We summarize in section 6 and present some technical details in the appendix A.

2. Factorization of QCD amplitudes

We are interested in a general $2 \rightarrow n$ scattering processes of partons p_i

p:
$$p_1(k_1, m_1, c_1) + p_2(k_2, m_2, c_2) \to p_3(k_3, m_3, c_3) + \ldots + p_{n+2}(k_{n+2}, m_{n+2}, c_{n+2}), \quad (2.1)$$

where $\{p_i\}$ denotes the set of partons (of specific flavors) with associated momenta $\{k_i\}$, masses $\{m_i\}$ and color quantum numbers $\{c_i\}$. The latter are in the range $1 \dots N^2 - 1$ for particles in the adjoint (gluons) and $1 \dots N$ for particles in the fundamental representation (quarks) of a SU(N)-gauge theory.

The scattering amplitude $\mathcal{M}^{[p]}$ for the process (2.1) is conveniently expressed in a basis of color tensors $(c_I)_{\{c_i\}}$. Following ref. [11] we write $\mathcal{M}^{[p]}$ as

$$\mathcal{M}_{\{c_i\}}^{[p]}\left(\{k_i\}, \frac{Q^2}{\mu^2}, \alpha_{\rm s}(\mu^2), \epsilon\right) = \mathcal{M}_I^{[p]}\left(\{k_i\}, \frac{Q^2}{\mu^2}, \alpha_{\rm s}(\mu^2), \epsilon\right) (c_I)_{\{c_i\}}$$
(2.2)
= $|\mathcal{M}_{\rm p}\rangle$,

where μ is the renormalization scale, Q the hard scale of the process typically related to the center-of-mass energy, e.g. $Q = \sqrt{s}$ with $s = (k_1 + k_2)^2$, and ϵ the parameter of dimensional regularization, $d = 4 - 2\epsilon$. The amplitude $|\mathcal{M}_p\rangle$ is a vector in the space of color tensors c_I with summation over I being understood. We consider $\mathcal{M}^{[p]}$ at fixed values of the external parton momenta k_i , thus $k_i^2 = m_i^2$ and especially $k_i^2 = 0$ for massless partons. Any additional explicit dependence on the parton masses m_i in eq. (2.2) is suppressed.

Let us start by recalling that on-shell amplitudes for massless partonic processes in $d = 4 - 2\epsilon$ dimensions can be factorized into products of functions $\mathcal{J}_0^{[p]}$, $\mathcal{S}_0^{[p]}$ and $\mathcal{H}^{[p]}$. These functions are called jet, soft and hard functions and are known to organize the contributions of various momentum regions relevant to the structure of the singularities in the scattering amplitude. Following refs. [10, 11] we can write

$$|\mathcal{M}_{\rm p}\rangle = \mathcal{J}_0^{[\rm p]} \left(\frac{Q^2}{\mu^2}, \alpha_{\rm s}(\mu^2), \epsilon\right) \mathcal{S}_0^{[\rm p]} \left(\{k_i\}, \frac{Q^2}{\mu^2}, \alpha_{\rm s}(\mu^2), \epsilon\right) |\mathcal{H}_{\rm p}\rangle.$$
(2.3)

The short-distance dynamics of the hard scattering is described by $\mathcal{H}_{\rm p}$, which is infrared finite. Analogous to the decomposition in eq. (2.2) $|\mathcal{H}_{\rm p}\rangle$ is a vector in the space of color tensors c_I . Coherent soft radiation arising from the overall color flow is summarized by $\mathcal{S}_0^{[p]}$, where we also use matrix notation suppressing the color indices. The function $\mathcal{J}_0^{[p]}$ depends only on the external partons and collects all collinearly sensitive contributions. It is otherwise independent of the color flow.

Given the factorization formula (2.3) one can then organize the singularity structure of any massless QCD amplitude. After the usual ultraviolet renormalization is performed, these singularities generally consist of two types, soft and collinear. Being of infrared origin, they are related to the emission of gluons with vanishing energy and to collinear parton radiation off massless hard partons, respectively. In this way all soft and collinear singularities in massless amplitudes are regularized and appear as explicit poles in ϵ as indicated in eq. (2.2). Typically two powers of $1/\epsilon$ are generated per loop. When masses are introduced the picture described above gets modified. In QCD, which has only massless gauge bosons, the soft singularities remain as single poles in ϵ while some of the collinear singularities are now screened by the mass m of the heavy fields. Nevertheless, in presence of masses, we speak of *quasi-collinear* singularities [2] that exhibit logarithmic dependence on m. To be specific, in the present paper we will consider the small mass limit of massive QCD amplitudes $\mathcal{M}^{[p]}$ such as in eq. (2.2). Naturally, in this limit we require that all masses in the amplitude are either zero or equal to a common value m and much smaller than the characteristic hard scale Q of the reaction. Thus, in the limit $Q^2 \gg m^2$ we aim at organizing all poles in ϵ and all powers of $\ln^k(m), k \ge 0$, (including mass independent terms) from the underlying factorization principles.

From an alternative point of view however, the differences between a massless and a massive amplitude for a given physical process can also be thought of as a mere change in the regularization scheme. Here, the limit of small masses for any given amplitude may simply be seen as an alternative to working in *d*-dimensions in order to regulate the soft and/or collinear singularities. Of course, gauge invariance has to be retained. In this interpretation parton masses act as formal regulators and massive amplitudes in the limit $m^2 \ll Q^2$ must share essential properties with the corresponding massless amplitudes. Such arguments have been previously used in refs. [20-22] in the context of QED corrections to the Bhabha process. Within QCD with n_l light quarks and one heavy flavor, this requires to properly account for the decoupling of the heavy quark. We will further elaborate on this point below, in particular on the relevant aspects of the decoupling theorem [23].

Our goal is the generalization of the infrared factorization formula (2.3) of refs. [10, 11] to the case of *massive* partons. To that end, we perform a similar factorization for the amplitude $\mathcal{M}^{[p]}$ into products of functions $\mathcal{J}^{[p]}$, $\mathcal{S}^{[p]}$ and $\mathcal{H}^{[p]}$. In the presence of a hard scale Q we can then write for the partonic process (2.1)

$$|\mathcal{M}_{\mathbf{p}}\rangle = \mathcal{J}^{[\mathbf{p}]}\left(\frac{Q^2}{\mu^2}, \frac{m_i^2}{\mu^2}, \alpha_{\mathbf{s}}(\mu^2), \epsilon\right) \mathcal{S}^{[\mathbf{p}]}\left(\{k_i\}, \frac{Q^2}{\mu^2}, \alpha_{\mathbf{s}}(\mu^2), \epsilon\right) |\mathcal{H}_{\mathbf{p}}\rangle, \qquad (2.4)$$

where all non-trivial mass dependence enters in the functions $\mathcal{J}^{[p]}$ and $\mathcal{S}^{[p]}$ and we neglect in $\mathcal{H}^{[p]}$ power suppressed terms in the parton masses m. The jet function now summarizes all *quasi-collinear* contributions from the external partons. It is therefore of the form

$$\mathcal{J}^{[p]}\left(\frac{Q^2}{\mu^2}, \frac{m_i^2}{\mu^2}, \alpha_{\rm s}(\mu^2), \epsilon\right) = \prod_{i=1}^{n+2} \mathcal{J}^{[i]}\left(\frac{Q^2}{\mu^2}, \frac{m_i^2}{\mu^2}, \alpha_{\rm s}(\mu^2), \epsilon\right), \qquad (2.5)$$

where $\mathcal{J}^{[i]}$ denotes the jet function of each external parton p_i .

We stress that the above factorization formula (2.4) is designed to correctly reproduce the leading power in the hard scale Q. Moreover, as the similarity between eqs. (2.3) and (2.4) suggests, the factorization is otherwise independent of details such as the partons in reaction (2.1) being massless or massive. However, eq. (2.4) still contains ambiguities related to the separation of finite terms in $\mathcal{J}^{[p]}$, $\mathcal{S}^{[p]}$ and $\mathcal{H}^{[p]}$. It also contains ambiguities related to sub-leading soft terms in $\mathcal{J}^{[p]}$ and $\mathcal{S}^{[p]}$. Following ref. [11] we fix this remaining freedom completely by demanding that

$$\mathcal{J}^{[i]}\left(\frac{Q^2}{\mu^2}, \frac{m_i^2}{\mu^2}, \alpha_{\rm s}(\mu^2), \epsilon\right) = \left(\mathcal{F}^{[i]}\left(\frac{Q^2}{\mu^2}, \frac{m_i^2}{\mu^2}, \alpha_{\rm s}, \epsilon\right)\right)^{\frac{1}{2}}, \qquad i = q, g, \qquad (2.6)$$

where the scalar function $\mathcal{F}^{[i]}$ denotes the gauge invariant space-like form factor of a quark or gluon to be discussed in detail in section 3 below. For the moment, suffice it to say that the function $\mathcal{F}^{[q]}$ is associated to the vertex $\gamma^* q q$ (or $\gamma^* q \bar{q}$), of a photon γ^* with virtuality Q^2 , and q/\bar{q} an external quark / anti-quark of mass m_q . Likewise, for a colored parton in the adjoint SU(N)-representation, the function $\mathcal{F}^{[g]}$ is either obtained from the effective vertex ϕgg of a scalar Higgs and two massless gluons, or from the corresponding vertex with two gluinos \tilde{g} of mass $m_{\tilde{q}}$.

The motivation for the choice made in eq. (2.6) above comes from the following consideration. Firstly, it reproduces the collinear dynamics as desired and, moreover, provides a specific prescription for the pure soft terms contained in the jet function. Secondly, it guarantees that the jet factor $\mathcal{J}^{[p]}$ remains *process-independent*, while all process-dependent soft interference terms are entirely delegated to the soft function $\mathcal{S}^{[p]}$. We recall that the role of parton masses is to simplify screen the collinear singularities. Since the soft and hard functions $\mathcal{S}^{[p]}$ and $\mathcal{H}^{[p]}$ are insensitive to these collinear dynamics, being the same in the massless or the massive case (provided $Q^2 \gg m^2$), logarithmically enhanced contributions of the type $\ln^k(m)$ are contained solely within $\mathcal{J}^{[p]}$. In other words, we require the (massive) factorization formula (2.4) to be valid for any amplitude. Then it also holds for the form factors $\mathcal{F}^{[i]}$ in eq. (2.6) itself, since these are the simplest amplitudes to which eq. (2.4) can be applied with $\mathcal{S}^{[ii \to 1]} = 1$ and $\mathcal{H}^{[ii \to 1]} = 1$, and this choice for $\mathcal{J}^{[p]}$ is also consistent with the corresponding massless case.

We also want to comment briefly on evolution and exponentiation. In eqs. (2.3) and (2.4) we have suppressed any additional scale dependence, which together with the renormalization group properties gives rise to evolution equations for $\mathcal{J}_0^{[p]}$, $\mathcal{S}_0^{[p]}$ and $\mathcal{J}^{[p]}$, $\mathcal{S}_0^{[p]}$. The solution of those evolution equations leads to an all-order exponentiation in terms of the corresponding anomalous dimensions, which is well known for massless partons, see e.g. refs. [11, 24]. In the case of massive partons, the exponentiation of the jet function $\mathcal{J}^{[i]}$ (the form factor $\mathcal{F}^{[i]}$, respectively) is discussed in detail in section 3, while we postpone the soft function $\mathcal{S}^{[p]}$ and its solution as a path-ordered exponential until section 5.

Finally, the factorization formula (2.4) along with our choice (2.6) for the jet function lends itself to an even more suggestive form for practical applications, namely, as a direct relation between the massless and the massive amplitude, $\mathcal{M}^{[p],(m=0)}$ and $\mathcal{M}^{[p],(m)}$, for any given physical process. To that end, we exploit the full predictive power of eq. (2.4) and derive the remarkably simple and suggestive relation

$$\mathcal{M}^{[p],(m)}\left(\{k_i\}, \frac{Q^2}{\mu^2}, \alpha_{\rm s}(\mu^2), \epsilon\right) = \qquad (2.7)$$
$$\prod_{i \in \{\text{all legs}\}} \left(Z_{[i]}^{(m|0)}\left(\frac{m^2}{\mu^2}, \alpha_{\rm s}(\mu^2), \epsilon\right) \right)^{\frac{1}{2}} \times \mathcal{M}^{[p],(m=0)}\left(\{k_i\}, \frac{Q^2}{\mu^2}, \alpha_{\rm s}(\mu^2), \epsilon\right),$$



Figure 1: Feynman diagrams contributing to the vertex $\gamma^* qq$ as examples for the flavor classes ll, hl, lh and hh discussed in the text. Curly lines denote gluons, double straight lines quarks of mass m and single straight lines massless quarks.

which is the first main result of this paper.

We have suppressed the color indices in eq. (2.7). As we see, the massless amplitude $\mathcal{M}^{[p],(m=0)}$ and its massive analogue $\mathcal{M}^{[p],(m)}$ in the small mass limit $m^2 \ll Q^2$ are multiplicatively related by a universal function $Z^{(m|0)}$. This result is consistent with ref. [2] (see section 5 for the detailed comparison). The function $Z^{(m|0)}$ is process independent and can be viewed as a sort of renormalization constant (or rather a constant relating two different regularization schemes). This relation can be used to predict any massive amplitude from the known massless one, the latter being much easier to compute in practice. Moreover, eq. (2.7) includes not only the singular terms in the massive amplitude but extends even to the constant contributions (i.e. the mass-independent terms).

With eq. (2.6) defining the jet function, the function $Z^{(m|0)}$ is given in terms of the respective form factors,

$$Z_{[i]}^{(m|0)}\left(\frac{m^2}{\mu^2}, \alpha_{\rm s}, \epsilon\right) = \mathcal{F}^{[i]}\left(\frac{Q^2}{\mu^2}, \frac{m^2}{\mu^2}, \alpha_{\rm s}, \epsilon\right) \left(\mathcal{F}^{[i]}\left(\frac{Q^2}{\mu^2}, 0, \alpha_{\rm s}, \epsilon\right)\right)^{-1}, \qquad (2.8)$$

where the index *i* denotes the (massive) parton and α_s is evaluated at the scale μ^2 . Eq. (2.8) explicitly demonstrates the process-independence of the factor $Z^{(m|0)}$. While both the massive and the massless form factors are functions of the process-dependent scale Q, this dependence cancels in their ratio leaving in the factor $Z^{(m|0)}$ only the ratio of process-independent scales μ^2/m^2 .

Although eq. (2.8) is valid in a more general setting, and in particular through any perturbative order, we will restrict in the following our attention to QCD amplitudes and in particular to those with massive quarks. For this case we will present explicit results for $Z_{[q]}^{(m|0)}$ up to two loops in section 4. Applications of eq. (2.7) will be presented in section 5.

^[4] Eqs. (2.7) and (2.8) are in addition subject to the following clarifications and qualifications. First of all, the form factors entering in eq. (2.8) for $Z_{[q]}^{(m|0)}$ are to be understood as being the form factors in a theory with either $n_l + 1$ massless quark flavors or n_l massless flavors and one heavy quark, respectively. In both cases we have the same *total* number of flavors $n_f = n_l + 1$. Secondly, our approach of relating the large logarithms in m to quasi-collinear momentum regions requires external massive legs. More precisely, we may define flavor classes, according to the total number of heavy quark lines in an amplitude at a given order of perturbation theory. In addition, the flavor classes distinguish for a given number of massive lines whether the latter represent external legs or form closed internal loops. For the form factor up to two loops, we illustrate the various cases ll, hl, lh and hh in figure 1. At tree level and one loop, we only have the pair of classes ll and hl, while from two loops onwards we also have the pair lh and hh. Both these pairs give rise to separate relations in eq. (2.8). Beyond two loops, yet new flavor classes can appear, see e.g. ref. [25]. In fact a related discussion of this issue has already emerged in the literature during the calculation of the NLO QCD corrections to the three jet rate with massive quarks in electron-positron annihilation, $e^+e^- \rightarrow q\bar{q}X$, see e.g. refs. [26, 27]. It is also clear how to generalize the definition of flavor classes to other types of colored heavy particles such as gluinos.

Let us finish this section by pointing out another property of eq. (2.7). It is a standard textbook knowledge that the two infrared regularizations of any one-loop QCD amplitude, either with a quark mass or dimensionally, are related to each other as follows

$$\ln(m) \to \frac{1}{\epsilon} + \text{finite terms in } \epsilon \,.$$
 (2.9)

Based on eqs. (2.4) and (2.7), we conclude in this paper that the proper generalization of eq. (2.9) beyond one loop is in the sense of process independent factorization. The factor $Z^{(m|0)}$ in eq. (2.8) is invertible and defines the building block of proportionality to all orders in the strong coupling.

3. The Sudakov form factor in QCD

In the previous section we have presented a factorization that describes the singularity structure of QCD amplitudes both in the massless case and in the limit of small masses $m^2 \ll Q^2$. This factorization is valid through any perturbative order and we have emphasized the central role of the form factor $\mathcal{F}^{[i]}$, which specifically includes the QCD corrections. Therefore, in this section we want to focus on $\mathcal{F}^{[i]}$ and address the issue of its exponentiation.

To be precise we restrict the discussion here to $\mathcal{F}^{[q]}$ for the vertex $\gamma^* q \bar{q}$ of a photon and an external quark-anti-quark pair, i.e. to massive partons in the fundamental representation of the SU(N)-gauge group. Furthermore we confine ourselves to the case of one (heavy) external quark line and no internal massive loops, which means we consider the flavor classes *ll* and *hl* (see figure 1). We briefly comment on classes *lh* and *hh* at the end of this section. The gluon form factor $\mathcal{F}^{[g]}$ for all-massless partons in the adjoint representation on the other hand, which describes the vertex ϕgg of a scalar Higgs and two gluons is well known, see e.g. ref. [28]. Also the necessary modifications to account for massive partons in the adjoint representation such as gluinos in supersymmetric QCD have been worked out to one loop in ref. [2]. Given a photon of virtuality Q^2 (we take space-like $q^2 = -Q^2 < 0$ throughout this section) the general expression for the vertex function Γ_{μ} reads

$$\Gamma_{\mu}(k_{1},k_{2}) = ie_{q} \bar{u}(k_{1}) \left(\gamma_{\mu} \mathcal{F}_{1}^{[q]}(Q^{2},m^{2},\alpha_{s}) + \frac{1}{2m} \sigma_{\mu\nu} q^{\nu} \mathcal{F}_{2}^{[q]}(Q^{2},m^{2},\alpha_{s}) \right) u(k_{2}). \quad (3.1)$$

Here the external quark (anti-quark) of momentum k_1 (k_2) is on-shell with m denoting its mass and e_q its charge, thus $k_1^2 = m^2$ (and $k_2^2 = m^2$). The scalar functions $\mathcal{F}_1^{[q]}$ and $\mathcal{F}_2^{[q]}$ on the right-hand side are the space-like quark form factors, which can be calculated order by order in the strong coupling constant α_s . Results for the perturbative QCD corrections to $\mathcal{F}_1^{[q]}$ in eq. (3.1) are known through three loops in the massless on-shell case [29–31, 28], while the case of on-shell heavy quarks through two loops has been considered in series of papers [32–34]. $\mathcal{F}_1^{[q]}$ and $\mathcal{F}_2^{[q]}$ are gauge invariant, but divergent and in dimensional regularization with $d = 4 - 2\epsilon$ these divergences show up as poles ϵ^{-k} . As we are concerned with the small mass limit $m^2 \ll Q^2$, we will in the following mainly consider the pure vector-like form factor $\mathcal{F}_1^{[q]}$, since $\mathcal{F}_2^{[q]}$ vanishes for massless quarks. In the remainder we drop all indices and define $\mathcal{F} \equiv \mathcal{F}_1^{[q]}$.

The universality of soft and collinear radiation leads on quite general grounds to an exponentiation of the respective singular terms in the form factor, be it poles in ϵ or large logarithms $\ln(m)$ of Sudakov type. This has been well studied in the literature in various approaches [35-39]. Moreover, in the massless case explicit formulae have been given up to the next-to-next-to-leading contributions [30, 40, 41]. However, to the best of our knowledge, an equally valid exponentiated representation for the massive form factor in dimensional regularization, which holds beyond the leading contributions has still been lacking. In this paper we present it for the first time. In doing so we use two complementary derivations based on evolution equations [35] and on inclusive partonic cross-sections [39].

Let us start with the former method and recall the evolution equations for the form factor [35]

$$- \mu^2 \frac{\partial}{\partial \mu^2} \ln \mathcal{F}\left(\frac{Q^2}{\mu^2}, \frac{m^2}{\mu^2}, \alpha_{\rm s}, \epsilon\right) = \frac{1}{2} K\left(\frac{m^2}{\mu^2}, \alpha_{\rm s}, \epsilon\right) + \frac{1}{2} G\left(\frac{Q^2}{\mu^2}, \alpha_{\rm s}, \epsilon\right) .$$
(3.2)

The key input [42] from QCD factorization are the dependence on the hard scale Q which rests entirely in the function G and, to logarithmic accuracy, the separation of the mass dependence in the function K. Both functions, G and K, are subject to renormalization group equations [35, 42],

$$\mu^2 \frac{d}{d\mu^2} G\left(\frac{Q^2}{\mu^2}, \alpha_{\rm s}, \epsilon\right) = -\lim_{m \to 0} \mu^2 \frac{d}{d\mu^2} K\left(\frac{m^2}{\mu^2}, \alpha_{\rm s}, \epsilon\right) = A(\alpha_{\rm s}), \qquad (3.3)$$

where we assume $\alpha_s = \alpha_s(\mu^2)$. Under renormalization group flow both G and K are governed by the same anomalous dimension A, because their sum is an invariant of the renormalization group. The anomalous dimension A is well known for instance as the coefficient of the $1/(1-x)_+$ -contribution to the diagonal splitting functions or alternatively as the anomalous dimension of a Wilson line with a cusp [43]. Its power expansion in the strong coupling is currently known up to three loops [44, 45] and we use the convention (also employed for all other expansions in α_s throughout this article)

$$A(\alpha_{\rm s}) = \sum_{i=1}^{\infty} \left(\frac{\alpha_{\rm s}}{4\pi}\right)^i A_i \equiv \sum_{i=1}^{\infty} (a_{\rm s})^i A_i, \qquad (3.4)$$

where we have introduced the shorthand notation $a_{\rm s}(\mu^2) \equiv \alpha_s(\mu^2)/(4\pi)$ and similarly for the *d*-dimensional coupling to be defined below. For later reference, we also mention that we choose the $\overline{\rm MS}$ -scheme for the coupling constant renormalization. The heavy mass *m* on the other hand is always taken to be the pole mass, thus the renormalization of *m* imposes the on-shell condition. We explicitly relate the bare (unrenormalized) coupling $\alpha_{\rm s}^{\rm b}$ to the renormalized coupling $\alpha_{\rm s}$ by

$$\alpha_{\rm s}^{\rm b} S_{\epsilon} = Z_{\alpha_{\rm s}} \,\alpha_{\rm s} \,, \tag{3.5}$$

where the renormalization constant Z_{α_s} in the $\overline{\text{MS}}$ -scheme is given by

$$Z_{\alpha_{\rm s}} = 1 - \frac{\beta_0}{\epsilon} a_{\rm s} + \left(\frac{\beta_0^2}{\epsilon^2} - \frac{1}{2}\frac{\beta_1}{\epsilon}\right) a_{\rm s}^2 - \left(\frac{\beta_0^3}{\epsilon^3} - \frac{7}{6}\frac{\beta_1\beta_0}{\epsilon^2} + \frac{1}{3}\frac{\beta_2}{\epsilon}\right) a_{\rm s}^3 + \dots, \qquad (3.6)$$

and the bare expansion parameter is normalized as $a_s^b = \alpha_s^b/(4\pi)$. For simplicity, we always set the ubiquitous factor $S_{\epsilon} = (4\pi)^{\epsilon} \exp(-\epsilon \gamma_{\rm E}) = 1$.

In eq. (3.3) all dependence on the infrared sector of the theory, i.e. the structure of the singularities is described by the function K. The function G, on the other hand, includes all dependence on the hard scale Q^2 and is finite for $\epsilon \to 0$. It is straight forward to solve the evolution equation (3.3) for G. Integration gives

$$G\left(\frac{Q^2}{\mu^2}, \alpha_{\rm s}, \epsilon\right) = -G\left(\bar{a}\left(Q^2, \epsilon\right)\right) - \int_{0}^{Q^2/\mu^2} \frac{d\lambda}{\lambda} A(\bar{a}(\lambda\mu^2, \epsilon)), \qquad (3.7)$$

with the boundary condition $G(\bar{a})$ to be derived by matching to fixed-order results for the form factor.

Working in *d*-dimensions the solution for *G* in eq. (3.7) naturally depends on the *d*dimensional running coupling $\bar{a}(Q^2, \epsilon)$. The latter can be expressed as a power series in the usual strong coupling constant $\alpha_s(\mu^2)$ evaluated at a scale μ^2 . This relation is now known through NNLO accuracy [30],

$$\begin{pmatrix} \frac{k^2}{\mu^2} \end{pmatrix}^{\epsilon} \bar{a}(k^2, \epsilon) =$$

$$\frac{a_{\rm s}}{X} \left\{ 1 - \epsilon \frac{\beta_1}{\beta_0^2} \frac{\ln X}{X} \right\} - \frac{a_{\rm s}^2}{X^2} \left\{ \frac{\beta_1}{\beta_0} (\ln X + Y) \right\} + \frac{a_{\rm s}^3}{X^3} \left\{ \frac{\beta_1^2}{\beta_0^2} \frac{3}{2} \ln^2 X \left(1 + Y + \frac{1}{4} Y^2 \right) \right. \\ \left. + \frac{\beta_2}{\beta_0} \ln X \left(\frac{1}{6} (3 + Y)(1 - X) - 1 - Y - \frac{1}{3} Y^2 \right) \right\} + \mathcal{O} \left(a_{\rm s}^4 \right) ,$$

$$(3.8)$$

which is consistent with the β -function in *d*-dimensions [41, 46]. Here we have used $a_s = a_s(\mu^2)$, the obvious boundary condition $\bar{a}(\mu^2, \epsilon) = a_s(\mu^2)$ and the abbreviations

$$X = 1 - a_{\rm s} \frac{\beta_0}{\epsilon} \left(\left(\frac{k^2}{\mu^2} \right)^{-\epsilon} - 1 \right) , \qquad Y = \frac{\epsilon(1 - X)}{a_{\rm s}\beta_0} . \tag{3.9}$$

The differential equation for K in eq. (3.3) is similar to the one for the function G with the obvious difference that the scale Q is replaced by the mass m. The solution reads:

$$K\left(\frac{m^2}{\mu^2}, \alpha_{\rm s}, \epsilon\right) = -K\left(\bar{a}\left(m^2, \epsilon\right)\right) + \int_{0}^{m^2/\mu^2} \frac{d\lambda}{\lambda} A(\bar{a}(\lambda\mu^2, \epsilon)).$$
(3.10)

Combining the above results we obtain the solution of the evolution equation (3.2) for the form factor \mathcal{F} ,

$$\ln \mathcal{F}\left(\frac{Q^2}{\mu^2}, \frac{m^2}{\mu^2}, \alpha_{\rm s}, \epsilon\right) = \frac{1}{2} \int_{0}^{Q^2/\mu^2} \frac{d\xi}{\xi} \left\{ G(\bar{a}(\xi\mu^2, \epsilon)) + \int_{0}^{\xi} \frac{d\lambda}{\lambda} A(\bar{a}(\lambda\mu^2, \epsilon)) \right\} - \frac{1}{2} \int_{0}^{m^2/\mu^2} \frac{d\xi}{\xi} \left\{ K(\bar{a}(\xi\mu^2, \epsilon)) - \int_{0}^{\xi} \frac{d\lambda}{\lambda} A(\bar{a}(\lambda\mu^2, \epsilon)) \right\} ,$$

which satisfies the boundary condition $\mathcal{F}(0, 0, \alpha_s, \epsilon) = 1$ and eq. (3.2). Finally, we rearrange the above result as,

$$\ln \mathcal{F}\left(\frac{Q^{2}}{\mu^{2}}, \frac{m^{2}}{\mu^{2}}, \alpha_{s}, \epsilon\right) =$$

$$-\frac{1}{2} \int_{0}^{Q^{2}/\mu^{2}} \frac{d\xi}{\xi} \left\{ G(\bar{a}(\xi\mu^{2}, \epsilon)) + K(\bar{a}(\xi\mu^{2}m^{2}/Q^{2}, \epsilon)) + \int_{\xi m^{2}/Q^{2}}^{\xi} \frac{d\lambda}{\lambda} A(\bar{a}(\lambda\mu^{2}, \epsilon)) \right\}.$$
(3.11)

Upon expansion of the *d*-dimensional coupling according to eq. (3.8), $\ln \mathcal{F}$ develops per power of a_s double logarithms of Q^2/m^2 and single poles in ϵ , which are generated by the two integrations. To be specific, the single poles are governed by the function Kin eq. (3.11) and are generated only by the outer ξ -integration. On the other hand, the inner λ -integration over A gives only rise to logarithms (as long as the infrared cutoff is set by the heavy quark mass). All quantities in eq. (3.11) are expressed in terms of the d-dimensional coupling \bar{a} . In this way all integrations are regulated and no singularities other than poles in ϵ arise.

Finally, after multiplying with a hard function C, we are in a position to write down the exponential for the complete massive form factor, which is our second main result,

$$\mathcal{F}\left(\frac{Q^{2}}{\mu^{2}}, \frac{m^{2}}{\mu^{2}}, a_{s}(\mu^{2}), \epsilon\right) = C(\bar{a}(\mu^{2}, \epsilon), \epsilon) \times$$

$$\exp\left[-\frac{1}{2} \int_{0}^{Q^{2}/\mu^{2}} \frac{d\xi}{\xi} \left\{ G(\bar{a}(\xi\mu^{2}, \epsilon)) + K(\bar{a}(\xi\mu^{2}m^{2}/Q^{2}, \epsilon)) + \int_{\xi m^{2}/Q^{2}}^{\xi} \frac{d\lambda}{\lambda} A(\bar{a}(\lambda\mu^{2}, \epsilon)) \right\} \right],$$
(3.12)

with all quantities on the right hand side being functions of \bar{a} in *d*-dimensions. Besides the known anomalous dimension A [44, 45] all other functions G, K and C can be determined in

a finite-order expansion. This will be accomplished in section 4. Before doing so however, there is one more feature of eq. (3.12) which deserves some comment.

As is well known, for renormalization schemes used in QCD based on dimensional regularization in the $\overline{\text{MS}}$ -scheme, the Appelquist-Carazzone decoupling theorem [23] does not hold true in its naive sense. In a theory with n_l light and n_h heavy flavors (thus $n_f = n_l + n_h$ for the total number of flavors) the contributions of a heavy quark of mass m to the Green functions of gluons and light quarks expressed in terms of the renormalized parameters of the full theory do not exhibit the expected 1/m suppression. The reason here is that the β -function governing the running of the strong coupling constant α_s does not depend on any masses. Neither do the anomalous dimensions describing the renormalization scale dependence of all other parameters of the theory. Rather, they exhibit discontinuities at the flavor thresholds, which are controlled by so-called decoupling constants.

In the exponential expression eq. (3.12) for the form factor we have used the standard $\overline{\text{MS}}$ coupling running with n_l light flavors. In order to compare eq. (3.12) or rather its expanded version to the fixed-order calculations [32] of the massive form factor, which also employ the $\overline{\text{MS}}$ -scheme, but a running coupling with a total number of flavors $n_f = n_l + 1$, one has to apply the decoupling relations. The necessary decoupling constant for α_s at flavor thresholds is known to $\mathcal{O}(\alpha_s^3)$ [47–49] (see also ref. [50]). To relate the two results, that is the expansion of eq. (3.12) on the one hand and the perturbative QCD corrections for the form factor through two-loops [32] on the other, we use the following relation for a_s ,

$$a_{s}^{(n_{f})} = a_{s}^{(n_{f})} - \frac{2}{3}L_{\mu,\epsilon} \left(a_{s}^{(n_{f})}\right)^{2} + \left\{ \left(\frac{4}{9} - \frac{\epsilon}{3}(5C_{A} + 3C_{F})\right)L_{\mu,\epsilon}^{2} - \frac{2}{3}(5C_{A} + 3C_{F})L_{\mu,\epsilon} + \frac{16}{9}C_{A} - \frac{15}{2}C_{F}\right\} \left(a_{s}^{(n_{f})}\right)^{3} + \mathcal{O}\left(\left(a_{s}^{(n_{f})}\right)^{4}\right),$$

$$(3.13)$$

where $a_s^{(n_l)}$ is the standard $\overline{\text{MS}}$ coupling for n_l quark flavors expanded in terms of $a_s^{(n_f)}$ for $n_f = n_l + 1$ flavors, both evaluated at the scale μ^2 . Eq. (3.13) uses the pole-mass m. The abbreviation $L_{\mu,\epsilon}$ denotes

$$L_{\mu,\epsilon} = \frac{1}{\epsilon} \left(\left(\frac{m^2}{\mu^2} \right)^{-\epsilon} - 1 \right) . \tag{3.14}$$

Eq. (3.13) is correct to NNLO and consistent with the standard β -function in *d*-dimensions for all terms proportional to $L_{\mu,\epsilon}$. For the constant terms at a_s^3 (i.e. those independent of $L_{\mu,\epsilon}$) it is accurate up to terms of order ϵ . Eq. (3.13) is to be inserted on the right hand side of eq. (3.8) to decouple the heavy quark in the *d*-dimensional coupling. Beyond one loop this generates in particular the correct scale dependence to the accuracy required in section 4.

Before moving on, we would like to discuss the exponentiation of the massive form factor in eq. (3.11) from a different perspective. As announced above, our starting point here is the observation that in sufficiently inclusive cross-sections, infrared singularities cancel between real and virtual diagrams. A suitable example for our purpose is the partonic cross-section of inclusive deep-inelastic scattering (DIS) of a massive quark. The purely virtual contributions to this partonic observable coincide with the squared massive space-like form factor.

To extract the form factor, we first derive the all-order exponentiation of the soft singularities of the cross-section for the scattering of a massive quark q off a virtual boson V^* , i.e. $q+V^* \rightarrow q+X$. To that end we follow the by-now standard methods for exponentiating inclusive partonic cross-sections in Mellin N-space, see e.g. refs. [37, 39, 51–53]. Working in the eikonal approximation we obtain

$$\ln(\sigma(N,\alpha_{\rm s})) = \int_{0}^{1} dx \left(\frac{x^{N-1}-1}{1-x}\right) g(1-x,\alpha_{\rm s}), \qquad (3.15)$$

where the function g contains the powers of logarithms $\ln(1-x)$ at higher orders of α_s and x is a kinematical variable related to the Bjorken variable x_B , and to be specified below.

Secondly, we use the fact that the purely virtual diagrams exhibit a simple xdependence proportional to $\delta(1-x)$, i.e. in N-space they contribute an N-independent factor. Thus, working in the eikonal approximation one can identify the contribution from the squared form factor (to all orders in the strong coupling) with the term "-1" in the factor $(x^{N-1}-1)$ in eq. (3.15). The complementary, N-dependent factor is entirely related to real emission diagrams. This way one can identify the logarithm of the form factor with the function

$$-\frac{1}{2}\int_{0}^{1}\frac{dz}{z}g(z,\alpha_{\rm s})\,,\,\,(3.16)$$

where z = 1 - x.

As it stands eq. (3.16) is not well defined. The reason is that it contains unregulated soft singularities. Their appearance is not unexpected, since the factor $(x^{N-1} - 1)$ in eq. (3.15) is constructed such that it ensures the cancellation between the soft singularities from the real and virtual corrections. Moreover, it is precisely this cancellation that leads to the appearance of the large distributions $[\ln^k(1-x)/(1-x)]_+$ (or large logarithms $\ln(N)$ in Mellin space) in the function g. Therefore, if one removes the real emission contributions in eq. (3.15), one can no longer rely on the delicate balance between real and virtual contributions to regularize the soft singularities. Clearly an alternative regularization of the latter is needed to render eq. (3.16) meaningful.

Since in this paper we are interested in regularizing the soft divergences in the massive form factor (or in any other amplitude) dimensionally, and in line with our previous discussion, we modify eq. (3.16) by replacing the usual coupling α_s with the *d*-dimensional one \bar{a} as defined in eq. (3.8),

$$\ln(\mathcal{F}(\alpha_s)) = -\frac{1}{2} \int_0^1 \frac{dz}{z} g(z, \bar{a}) \,. \tag{3.17}$$

We stress that the function g in eq. (3.17) is the same one that appears in the cross-section in eq. (3.15). The effect of the d-dimensional coupling is rather transparent, as it supplies additional powers of the factor $z^{-\epsilon}$, see e.g. the left hand side of eq. (3.8), which allows to regulate the z-integration in eq. (3.17) in the limit $z \to 0$.

For the derivation of the required hard cross-section for the process $q + V^* \rightarrow q + X$ we directly build on previous work on the exponentiation of massive cross-sections at next-toleading logarithmic accuracy [54, 55], where the light quark initiated process $q_l+V^* \rightarrow q+X$ was studied. Since in this work we are interested in the corresponding process initiated by heavy quarks, $q + V^* \rightarrow q + X$, one has to modify the analysis of ref. [54]. One possible option is to repeat the considerations of that reference keeping a non-vanishing mass for the initial state quark. However, a much simpler alternative is to express the coefficient function for the q-initiated process as a convolution of a perturbative distribution function for the initial-state heavy quark q and the coefficient function for the process $q_l + V^* \rightarrow q + X$ both evaluated at a common factorization scale μ_F . Since we are interested only in contributions that are enhanced in the soft limit and suppress power corrections with the quark mass m, only the $q \rightarrow q$ component of this distribution function is required. Moreover in the soft limit this function with space-like kinematics coincides with its time-like counterpart (see e.g. ref. [56]). All components of the time-like perturbative fragmentation function D are known through two loops and can be found in refs. [57, 58].

The exponential structure in the soft limit of the perturbative fragmentation function D of a heavy quark [19] is well understood [56, 59, 60]. In Mellin-N space we have

$$\ln(D(N)) = \int_{0}^{1} dx \frac{x^{N-1} - 1}{1 - x} \left\{ H\left(\alpha_{\rm s}((1 - x)^{2}m^{2})\right) + \int_{(1 - x)^{2}m^{2}}^{\mu_{F}^{2}} \frac{dk^{2}}{k^{2}} A\left(\alpha_{\rm s}(k^{2})\right) \right\}, (3.18)$$

where the anomalous dimension A is the same as the one appearing in eq. (3.4) while H is a new function.

The exponentiation of the coefficient function for the process $q_l + V^* \rightarrow q + X$ was clarified in ref. [54]. With the same anomalous dimension A and a new function S the result reads,

$$\ln(\sigma_{q_l \to q}(N)) = \int_{0}^{1} dx \frac{x^{N-1} - 1}{1 - x} \left\{ S\left(\alpha_{\rm s}((1 - x)^2 M^2)\right) + \int_{\mu_F^2}^{(1 - x)^2 M^2} \frac{dk^2}{k^2} A\left(\alpha_{\rm s}(k^2)\right) \right\}, (3.19)$$

where in the limit $m^2 \ll Q^2$ the scale M equals $M^2 = Q^4/m^2$.

Let us briefly recall a few basic facts [54] about the derivation of eq. (3.19). The variable x, $0 \le x \le 1$, is the rescaled Bjorken variable $x = (1 + m^2/Q^2)x_B$. The upper limit of the k^2 -integration follows from kinematics and in the center-of-mass frame it is determined from the light quark energy $E : k^2 \le 4E^2(1-x)^2$. Moreover one has

$$2E \simeq \frac{Q^2 + m^2}{\sqrt{(1-x)Q^2 + m^2}}.$$
(3.20)

Since we are working in the soft limit $(1 - x) \rightarrow 0$, it is obvious that in the massive case eq. (3.20) leads exactly to the scale M in eq. (3.19), while for m = 0 it reduces to the well known expression of the massless case [39].

Convoluting eqs. (3.18) and (3.19) we obtain the desired coefficient function for the sub-process $q + V^* \rightarrow q + X$ in the soft limit. One can see that the dependence on the factorization scale drops out as it should. Following the procedure outlined around eqs. (3.16), (3.17) above, we finally obtain the Sudakov exponent for the massive form factor:

$$\Delta_F = -\frac{1}{2} \int_0^1 \frac{dz}{z} \left\{ S\left(\bar{a}(z^2 M^2, \epsilon)\right) + H\left(\bar{a}(z^2 m^2, \epsilon)\right) + \int_{z^2 m^2}^{z^2 M^2} \frac{dk^2}{k^2} A\left(\bar{a}(k^2, \epsilon)\right) \right\}.$$
 (3.21)

The complete form factor is obtained by multiplying the above exponent with a hard function H_F :

$$\mathcal{F}\left(\frac{Q^2}{\mu^2}, \frac{m^2}{\mu^2}, \alpha_{\rm s}, \epsilon\right) = H_F(Q^2, m^2, \bar{a}(\mu^2, \epsilon), \epsilon) \exp\{\Delta_F\}.$$
(3.22)

Here all functions A, H, S and H_F have perturbative expansions analogous to eq. (3.4). They can be obtained to a given order in α_s by matching for instance to the full calculation for \mathcal{F} . In addition, independent information on H and S arises also with the help of eqs. (3.18) or (3.19) from the calculation of the perturbative fragmentation function D or the hard partonic light-to-heavy DIS cross-section $\sigma_{q_l \to q}$.

The hard function H_F has an expansion in ϵ but is finite in the limit $\epsilon \to 0$, since all soft poles are collected in the exponent Δ_F . To completely define the hard function H_F one has again to specify the definition of the coupling α_s appearing in eqs. (3.21) and (3.22). This is the usual $\overline{\text{MS}}$ coupling defined in eq. (3.5) but running *only* with the number of light flavors n_l . The same number of flavors appears also in the anomalous dimensions, see e.g. refs. [56, 57]. Thus, in order to compare eq. (3.22) to the fixed-order calculation available in, say ref. [32], with a coupling constant α_s for $n_f = n_l + 1$ flavors, we again have to apply the decoupling relations [23, 47-49] in the form of eq. (3.13).

A comparison to the exact two-loop calculation of the vector form factor [32] shows that eq. (3.22) correctly predicts all soft terms $\sim 1/\epsilon^k$, $k \geq 1$ including their logarithmic mass dependence, while it does not control the powers of $\sim \ln^k(m)$ at order ϵ^0 which are of collinear origin. From the viewpoint of the exponentiation of *soft* singularities these latter logarithms must be included in the hard function H_F .

However, at the same time one expects that all pure collinear logarithms exponentiate as well. This feature is unrelated to the soft-gluon exponentiation discussed above but rather to the standard parton evolution equations (DGLAP). Here we recall the analysis of ref. [39] where the effect of collinear radiation in the outgoing jet results in modifications of the naive eikonal exponentiation. The additional collinear contributions in the final-state are taken into account by constructing a DGLAP-like evolution equation for the corresponding jet function. The latter, in turn, contributes to the well known DIS anomalous dimension B [37, 39]. In the massive case the virtuality of the final state is of order $(1 - x)Q^2 + m^2$ and does not vanish in the soft limit which brings additional $\ln(m)$ terms. In this paper we will not elaborate on that point further, as all purely collinear logarithmic terms can be read off from the exponentiated expressions of the form factor given in eq. (3.12). This picture is consistent with fixed-order calculations of the perturbative fragmentation function.¹ Indeed, one can easily verify that the logarithmic contributions in the one-loop form factor \mathcal{F}_1 for ϵ^0 and ϵ coincide with the pure virtual contributions to the one-loop fragmentation function D_1 , see for instance eq. (45) of ref. [57]. Unfortunately, the two-loop virtual contributions cannot be extracted from ref. [57]. In the next section we will elaborate on this relation.

Before completing this section on the massive form factor, we would like to address the question of its massless limit. Reconsidering eq. (3.11), i.e. the exponent of eq. (3.12), it is obvious that the limit $m \to 0$ is smooth. The contribution from the infrared function K vanishes for $m \to 0$, while the contribution from the G function is similar to the one in the well known massless case [40, 41]. The counterterm K in refs. [40, 41] can be expressed as

$$K(0, \alpha_{\rm s}, \epsilon) = \int_{0}^{1} \frac{dx}{x} A(\bar{a}(x\mu^2, \epsilon)) \quad , \qquad (3.23)$$

which is consistent with eqs. (3.11) and (3.12) after changing the integration boundaries according to refs. [40, 41]. Moreover, the function G in the massive case should be related to the G function of the massless case up to possibly constant difference. As we will demonstrate to two loops in the next section, the two functions in fact do coincide to all known orders in ϵ , i.e. the massless limit of the massive result eq. (3.12) requires setting both m = 0 and C = 1.

Therefore, the resummed quark form factor reads in the massless case

$$\ln \mathcal{F}\left(\frac{Q^2}{\mu^2}, 0, \alpha_{\rm s}, \epsilon\right) = -\frac{1}{2} \int_{0}^{Q^2/\mu^2} \frac{d\xi}{\xi} \left\{ B(\bar{a}(\xi\mu^2, \epsilon)) + h(\bar{a}(\xi\mu^2, \epsilon)) + \int_{0}^{\xi} \frac{d\lambda}{\lambda} A(\bar{a}(\lambda\mu^2, \epsilon)) \right\},$$

with the boundary condition $\mathcal{F}(0, 0, \alpha_{s}, \epsilon) = 1$. Now $\ln \mathcal{F}$ develops double poles in ϵ per power of a_{s} from the λ - and the ξ -integration over the anomalous dimension A. In eq. (3.24) we have identified the initial condition $G(\bar{a})$ of eq. (3.7) with the sum of two functions B+h. The physical interpretation of the new functions B and h, which also have expansions in the d-dimensional coupling, follows nicely from the previous considerations of inclusive DIS scattering. Following ref. [39] one can identify the function B with the coefficient governing the evolution of those large logarithms $\ln(N)$ in inclusive DIS scattering associated with the final state jet function. This has recently also been pointed out in ref. [61]. The function Bis known to three-loop accuracy [53] from explicit DIS calculations [25, 44, 45, 62]. The new contribution h on the other hand can be thought of as the massless limit of the function H in eq. (3.21). To determine h in a perturbative expansion we match the above exponent to the known three-loop result for the massless form factor [30] and we have checked that the α_{s}^{4} prediction based on eq. (3.24) agrees with previous results in the literature [30]. It is interesting to note that unlike the standard expression for the massless form factor

¹We would like to thank S. Catani for an interesting discussion on this point.

as given e.g. in refs. [30, 40, 41], the result we propose in this paper is comprised of well defined integrals. Moreover, we can directly interpret the respective parts as the three-loop contributions of the form factor to the DIS coefficient functions and the splitting functions respectively.

Finally let us briefly comment again on the various flavor classes, since the previous discussion was entirely focused on the flavor classes ll and hl. Beyond one loop we have for instance the contributions to \mathcal{F} from the class hh. These contributions are finite after performing the ultraviolet renormalization, but they still do contain Sudakov logarithms of the type $\ln^k(Q^2/m^2)$. In fact, up to two loops all remaining large logarithms $\ln^k(Q^2/m^2)$ in the heavy quark form factor not accounted for by eq. (3.12) are entirely related to the self-energy contributions of a heavy quark, i.e. the diagram denoted with hh in figure 1. It is well known [63, 64] that these contributions obey Sudakov exponentiation similar to eq. (3.12), although with different integration boundaries and evaluated at the matching scale $\mu^2 = m^2$. Thus, we can introduce the function \mathcal{F}_{hh} which exponentiates the logarithms in the flavor class hh,

$$\ln \mathcal{F}_{hh}(Q^{2}, m^{2}, \bar{a}(\mu^{2}, \epsilon), \epsilon) =$$

$$-\frac{1}{2} \int_{m^{2}/\mu^{2}}^{Q^{2}/\mu^{2}} \frac{d\xi}{\xi} \left\{ G'(\bar{a}(\xi\mu^{2}, \epsilon)) + K(\bar{a}(\xi\mu^{2}m^{2}/Q^{2}, \epsilon)) + \int_{m^{2}/\mu^{2}}^{\xi} \frac{d\lambda}{\lambda} A(\bar{a}(\lambda\mu^{2}, \epsilon)) \right\} \bigg|_{n_{f}=n_{h}}.$$
(3.24)

Eq. (3.24) is to be evaluated at the scale $\mu^2 = m^2$ and to be restricted to the purely fermionic contributions with the heavy quark pair coupling to the external boson and one additional virtual heavy quark line. Eq. (3.24) contains the same functions A and K as eq. (3.12), but a different function G'. As a matter of fact, its structure follows directly from integrating eqs. (3.2) and (3.7) under the condition that the infrared region is cut off at the scale m^2 . See e.g. refs. [63, 64] for details on the finite-order expansion of exponentials like eq. (3.24). We address this issue in future work.

4. Fixed-order expansions and resummation coefficients

In this section we will give the finite-order expansions for the various quantities, in particular for the factor $Z^{(m|0)}$ of eq. (2.8) and the form factor \mathcal{F} of eq. (3.12). All formulae in this section use the $\overline{\text{MS}}$ -scheme for the coupling constant, while the heavy mass is always taken to be the pole mass (on-shell scheme). In addition, as in the previous sections, we limit ourselves to the contributions in the flavor classes ll and hl. Throughout this section n_f denotes the number of massless flavors.

4.1 The factor $Z^{(m|0)}$

Let us start with the perturbative QCD expansion of eq. (2.8) for the factor $Z^{(m|0)}$ which we defined as the ratio of the massive and the massless form factors for a given parton and which we write as an expansion in terms of the renormalized coupling $a_s(\mu^2) \equiv \alpha_s(\mu^2)/(4\pi)$:

$$Z_{[i]}^{(m|0)}\left(\frac{m^2}{\mu^2}, \alpha_{\rm s}, \epsilon\right) = 1 + \sum_{j=1}^{\infty} (a_{\rm s})^j \ Z_{[i]}^{(j)} \,. \tag{4.1}$$

The quark form factor in massless QCD is known to three loops [30, 28], while the form factor of a massive quark is known for arbitrary values of the quark mass through two loops [32]. The expansion coefficients (4.1) in the case of a (heavy) quark q read

$$Z_{[q]}^{(1)} = C_F \left\{ \frac{2}{\epsilon^2} + \frac{2L_{\mu} + 1}{\epsilon} + L_{\mu}^2 + L_{\mu} + 4 + \zeta_2 + \epsilon \left(\frac{L_{\mu}^3}{3} + \frac{L_{\mu}^2}{2} + (4 + \zeta_2)L_{\mu} + 8 + \frac{\zeta_2}{2} - \frac{2}{3}\zeta_3 \right) + \epsilon^2 \left(\frac{L_{\mu}^4}{12} + \frac{L_{\mu}^3}{6} + \left(2 + \frac{\zeta_2}{2} \right) L_{\mu}^2 + \left(8 + \frac{\zeta_2}{2} - \frac{2}{3}\zeta_3 \right) L_{\mu} + 16 + 2\zeta_2 - \frac{\zeta_3}{3} + \frac{9}{20}\zeta_2^2 \right) \right\} + \mathcal{O}(\epsilon^3),$$

$$(4.2)$$

$$Z_{[q]}^{(2)} = C_F^2 \frac{2}{\epsilon^4} + \frac{1}{\epsilon^3} \left\{ C_F^2 (4L_\mu + 2) - \frac{11}{2} C_F C_A + n_f C_F \right\}$$
(4.3)

$$\begin{split} &+ \frac{1}{\epsilon^2} \bigg\{ C_F^{\ 2} \bigg(4L_{\mu}^2 + 4L_{\mu} + \frac{17}{2} + 2\zeta_2 \bigg) + C_F C_A \bigg(-\frac{11}{3} L_{\mu} + \frac{17}{9} - \zeta_2 \bigg) + n_f C_F \bigg(\frac{2}{3} L_{\mu} - \frac{2}{9} \bigg) \bigg\} \\ &+ \frac{1}{\epsilon} \bigg\{ C_F^{\ 2} \bigg(\frac{8}{3} L_{\mu}^3 + 4L_{\mu}^2 + (17 + 4\zeta_2) L_{\mu} + \frac{83}{4} - 4\zeta_2 + \frac{32}{3} \zeta_3 \bigg) \\ &+ C_F C_A \bigg(\bigg(\frac{67}{9} - 2\zeta_2 \bigg) L_{\mu} + \frac{373}{108} + \frac{15}{2} \zeta_2 - 15\zeta_3 \bigg) + n_f C_F \bigg(-\frac{10}{9} L_{\mu} - \frac{5}{54} - \zeta_2 \bigg) \bigg\} \\ &+ C_F^{\ 2} \bigg(\frac{4}{3} L_{\mu}^4 + \frac{8}{3} L_{\mu}^3 + (17 + 4\zeta_2) L_{\mu}^2 + \bigg(\frac{83}{2} - 8\zeta_2 + \frac{64}{3} \zeta_3 \bigg) L_{\mu} + \frac{561}{8} + \frac{61}{2} \zeta_2 - \frac{22}{3} \zeta_3 \\ &- 48 \ln 2\zeta_2 - \frac{77}{5} \zeta_2^2 \bigg) + C_F C_A \bigg(\frac{11}{9} L_{\mu}^3 + \bigg(\frac{167}{18} - 2\zeta_2 \bigg) L_{\mu}^2 + \bigg(\frac{1165}{54} + \frac{56}{3} \zeta_2 - 30\zeta_3 \bigg) L_{\mu} \\ &+ \frac{12877}{648} + \frac{323}{18} \zeta_2 + \frac{89}{9} \zeta_3 + 24 \ln 2\zeta_2 - \frac{47}{5} \zeta_2^2 \bigg) \\ &+ n_f C_F \bigg(-\frac{2}{9} L_{\mu}^3 - \frac{13}{9} L_{\mu}^2 + \bigg(-\frac{77}{27} - \frac{8}{3} \zeta_2 \bigg) L_{\mu} - \frac{1541}{324} - \frac{37}{9} \zeta_2 - \frac{26}{9} \zeta_3 \bigg) + \mathcal{O}(\epsilon) \,, \end{split}$$

where two-loop contributions arising from virtual heavy flavor lines are omitted (see figure 1) and

$$L_{\mu} = \ln\left(\frac{\mu^2}{m^2}\right) \,. \tag{4.4}$$

In presence of heavy flavors the form factor of a massless quark gets mass-dependent contributions at two loops from the diagram *lh* in figure 1. We will not consider such two-loop contributions in this paper. Unlike the massless quark, however, the gluon form factor receives mass-dependent corrections starting from one loop. These have their origin in the one-loop heavy flavor insertion in the tree-level gluon form factor. It is clear that for the gluon form factor the classification of figure 1 has to be suitably adapted by counting the number of (internal) heavy lines. It is easy to work out the one-loop result for the gluon $Z^{(m|0)}$ -factor in eq. (4.1) (see the appendix for the all-orders in ϵ result) and it reads:

$$Z_{[g]}^{(1)} = n_h \left\{ -\frac{2}{3\epsilon} - \frac{2}{3}L_\mu + \epsilon \left(-\frac{1}{3}L_\mu^2 - \frac{\zeta_2}{3} \right) + \epsilon^2 \left(-\frac{1}{9}L_\mu^3 - \frac{\zeta_2}{3}L_\mu + \frac{2\zeta_3}{9} \right) \right\} + \mathcal{O}(\epsilon^3) \,. \tag{4.5}$$

In addition, the following comments on eqs. (4.2), (4.3) above are in order. First of all, we have to supply the ϵ -expansion of the massive form factor including terms of order ϵ^2 at one loop, because of the singularity structure with $1/\epsilon^2$ -poles in massless one-loop form factor. Since the $\mathcal{O}(\epsilon^2)$ term of the one-loop massive form factor is not available in the literature we have calculated it following the setup of ref. [32]. Details are given in appendix A. One can easily verify that this term produces a finite contribution at two loops for an amplitude with n_h external massive quarks, n_l external massless quarks and n_g external gluons, which would be proportional to $n_l C_F^2 + n_g C_F C_A$ times the Born term.

Secondly, there is one important detail about the scheme for definition of coupling constant and masses. We assume the pole-mass definition for the heavy quark mass m as well as the standard $\overline{\text{MS}}$ coupling defined in eq. (3.5). Note that this definition for the coupling differs from the one used in e.g. in ref. [32] (and other references on higher order corrections for massive processes) where the coupling renormalization includes also the factor $\Gamma(1+\epsilon) \exp(\epsilon \gamma_{\rm E})$. For consistency with the massless calculations, we have performed a finite renormalization of the result in ref. [32]. The necessary relation is given by

$$a_{\rm s}\Big|_{\rm ref. [32]} = a_{\rm s} \left\{ 1 + a_{\rm s} \frac{1}{\epsilon} \left(\beta_0 - \frac{2}{3} \right) \left(\frac{\Gamma(1+\epsilon)}{\exp(-\epsilon\gamma_{\rm E})} - 1 \right) + \mathcal{O}(a_{\rm s}^2) \right\} , \qquad (4.6)$$

where we put the factor $(4\pi)^{\epsilon} \exp(-\epsilon \gamma_{\rm E}) = 1$ for simplicity and $\beta_0 = 11/3C_A - 2/3n_f$. It is easy to see that through two loops this amounts to the following finite correction (see eq. (4.8) below for definitions of \mathcal{F}_i) to the results presented in ref. [32]

$$\mathcal{F}_2\Big|_{\overline{\mathrm{MS}}} = \mathcal{F}_2\Big|_{\mathrm{ref.}\ [32]} + a_{\mathrm{s}}^2 \frac{\beta_0}{\epsilon} \left(\frac{\zeta_2}{2}\epsilon^2 + \mathcal{O}(\epsilon^3)\right) \mathcal{F}_1\Big|_{\mathrm{ref.}\ [32]}.$$
(4.7)

Finally we would like to elaborate on the relation between the factor $Z_{[q]}^{(m|0)}$ and the heavy quark perturbative fragmentation function we discussed in section 3 preceding eq. (3.24). At one loop, the virtual contribution to the fragmentation function was explicitly calculated in ref. [57] to all orders in ϵ . We present this result in appendix A in a particular form prior to collinear factorization and one can easily verify by a direct comparison that its expansion through $\mathcal{O}(\epsilon^2)$ coincides with the factor $Z_{[q]}^{(1)}$. Moreover, ref. [57] also contains the purely virtual fermionic contributions (i.e. proportional to the number of light flavors) at two loops. In terms of the usual renormalized coupling we have found the former to be in agreement with the terms proportional to n_f in the function $Z_{[q]}^{(2)}$ to all powers in ϵ appearing in eq. (4.3). This observation indicates that the factor $Z_{[q]}^{(m|0)}$ of eq. (2.8) indeed coincides with the virtual corrections to the collinearly unfactorized perturbative fragmentation function and one may actually view the complete agreement between all known terms of the two functions as a check on the derivation of $Z_{[q]}^{(m|0)}$. Although the latter object is not known to the level we have presented here for the function $Z_{[q]}^{(m|0)}$ the apparent coincidence allows for an interesting alternative interpretation of that function by relating it to the field renormalization constant of a heavy quark in light cone gauge $n \cdot A = 0$. Indeed, in the approach of ref. [57] to calculate the fragmentation function, the purely virtual corrections are nothing but insertions of self-energy type in external on-shell legs in this particular gauge. Clearly, it will be very interesting to further develop this line of reasoning.

4.2 The form factor \mathcal{F}

Next, we want to perform the finite-order expansion and matching of eq. (3.12) for the heavy quark form factor \mathcal{F} . Subsequently, with all functions G, K and F determined we will then be using eq. (3.12) for predictions of perturbative results at higher orders and derive explicit results at three loops. To that end we perform the integrations in eq. (3.11) after inserting the perturbative expansions of all quantities and simply evaluated resulting integrals. Details on this procedure may be found in refs. [30, 41].

For the (ultraviolet) renormalized massive form factor with space-like virtuality $q^2 = -Q^2 < 0$ and in terms of the renormalized coupling $\alpha_s(\mu^2)$ we have,

$$\mathcal{F}\left(\frac{Q^2}{\mu^2}, \frac{m^2}{\mu^2}, a_{\rm s}(\mu^2), \epsilon\right) = 1 + \sum_{i=1}^{\infty} (a_{\rm s})^i \mathcal{F}_i.$$
(4.8)

With the convention of eq. (3.4) for the expansion of A, G, K and C and setting the scale to $\mu^2 = m^2$, we find

$$\mathcal{F}_{1} = \frac{1}{\epsilon} \left\{ \frac{1}{2} A_{1}L + \frac{1}{2} (G_{1} + K_{1}) \right\} - \frac{1}{4} A_{1}L^{2} - \frac{1}{2} G_{1}L + C_{1} + \epsilon \left\{ \frac{1}{12} A_{1}L^{3} + \frac{1}{4} G_{1}L^{2} \right\}$$
(4.9)
$$-\epsilon^{2} \left\{ \frac{1}{48} A_{1}L^{4} + \frac{1}{12} G_{1}L^{3} \right\} + \mathcal{O}(\epsilon^{3}),$$

$$\begin{aligned} \mathcal{F}_{2} &= \frac{1}{\epsilon^{2}} \Biggl\{ \frac{1}{8} A_{1}^{2} L^{2} + \frac{1}{4} A_{1} (G_{1} + K_{1} - \beta_{0}) L + \frac{1}{8} (G_{1} + K_{1}) (G_{1} + K_{1} - 2\beta_{0}) \Biggr\} \tag{4.10} \\ &+ \frac{1}{\epsilon} \Biggl\{ -\frac{1}{8} A_{1}^{2} L^{3} - \frac{1}{8} A_{1} (3G_{1} + K_{1}) L^{2} + \frac{1}{4} (A_{2} - G_{1}^{2} - K_{1}G_{1} + 2A_{1}C_{1}) L + \frac{1}{4} (G_{2} + K_{2}) \\ &+ \frac{1}{2} C_{1} (G_{1} + K_{1}) \Biggr\} + \frac{7}{96} A_{1}^{2} L^{4} + \frac{1}{24} A_{1} (7G_{1} + K_{1} + 2\beta_{0}) L^{3} + \frac{1}{8} G_{1} (2G_{1} + K_{1} + 2\beta_{0}) L^{2} \\ &- \frac{1}{4} (A_{2} + A_{1}C_{1}) L^{2} - \frac{1}{2} (G_{2} + G_{1}C_{1}) L + C_{2} + \epsilon \Biggl\{ -\frac{1}{32} A_{1}^{2} L^{5} - \frac{1}{96} A_{1} (15G_{1} + K_{1} + 6\beta_{0}) L^{4} \\ &- \frac{1}{24} G_{1} (4G_{1} + K_{1} + 6\beta_{0}) L^{3} + \frac{1}{12} (2A_{2} + A_{1}C_{1}) L^{3} + \frac{1}{4} (2G_{2} + G_{1}C_{1}) L^{2} \Biggr\} + \mathcal{O}(\epsilon^{2}) \,, \end{aligned}$$

$$\mathcal{F}_{3} &= \frac{1}{\epsilon^{3}} \Biggl\{ \frac{1}{48} A_{1}^{3} L^{3} + \frac{1}{16} A_{1}^{2} (G_{1} + K_{1} - 2\beta_{0}) L^{2} + \frac{1}{16} A_{1} (G_{1} + K_{1}) (G_{1} + K_{1} - 4\beta_{0}) L \Biggr\} + \mathcal{O}(\epsilon^{2}) \,, \end{aligned}$$

$$(4.11) \\ &+ \frac{1}{6} A_{1} \beta_{0}^{2} L + \frac{1}{48} (G_{1} + K_{1}) (G_{1} + K_{1} - 2\beta_{0}) (G_{1} + K_{1} - 4\beta_{0}) \Biggr\} + \frac{1}{\epsilon^{2}} \Biggl\{ -\frac{1}{32} A_{1}^{3} L^{4} \\ &- \frac{1}{16} A_{1}^{2} (2G_{1} + K_{1} - \beta_{0}) L^{3} + \frac{1}{8} A_{1} (A_{2} + A_{1}C_{1}) L^{2} + \frac{1}{16} A_{1} \beta_{0} (3G_{1} + K_{1}) L^{2} \Biggr\}$$

$$\begin{split} &-\frac{1}{32}A_1(G_1+K_1)(5G_1+K_1)L^2+\frac{1}{24}A_2(3G_1+3K_1-4\beta_0)L+\frac{1}{24}A_1(3G_2+3K_2-4\beta_1)L\\ &-\frac{1}{16}G_1(G_1+K_1)(G_1+K_1-2\beta_0)L+\frac{1}{4}A_1C_1(G_1+K_1-\beta_0)L+\frac{1}{8}C_1(G_1+K_1)^2\\ &+\frac{1}{24}(G_1+K_1)(3G_2+3K_2-6\beta_0C_1-4\beta_1)-\frac{1}{6}\beta_0(G_2+K_2)\bigg\}+\frac{1}{\epsilon}\bigg\{\frac{5}{192}A_1^3L^5\\ &+\frac{1}{192}A_1^2(25G_1+7K_1+4\beta_0)L^4+\frac{1}{96}A_1(19G_1^2+K_1^2+14K_1G_1)L^3\\ &+\frac{1}{48}A_1\beta_0(4G_1+K_1)L^3-\frac{1}{16}A_1(3A_2+2A_1C_1)L^3+\frac{1}{32}G_1(G_1+K_1)(3G_1+K_1+2\beta_0)L^2\\ &-\frac{1}{8}A_2(2G_1+K_1)L^2-\frac{1}{16}A_1(5G_2+K_2+6G_1C_1+2K_1C_1)L^2+\frac{1}{36}A_1(32C_A-135C_F)L\\ &+\frac{1}{12}(2A_3+3A_2C_1+6A_1C_2)L+\frac{1}{8}(-3G_1G_2-2K_1G_2-K_2G_1)L-\frac{1}{4}G_1C_1(G_1+K_1)L\\ &+\frac{1}{6}(G_3+K_3)+\frac{1}{4}C_1(G_2+K_2)+\frac{1}{36}(G_1+K_1)(18C_2+32C_A-135C_F)\bigg\}\\ &-\frac{1}{64}A_1^3L^6-\frac{1}{64}A_1^2(6G_1+K_1+3\beta_0)L^5+\frac{1}{96}A_1(16A_2+7A_1C_1)L^4-\frac{1}{384}A_1(65G_1^2\\ &+30K_1G_1+K_1^2+90\beta_0G_1+10\beta_0K_1+16\beta_0^2)L^4+\frac{1}{48}A_2(13G_1+4K_1+8\beta_0)L^3\\ &+\frac{1}{48}A_1(19G_2+K_2+4\beta_1)L^3+\frac{1}{24}A_1C_1(7G_1+K_1+2\beta_0)L^3-\frac{1}{96}G_1(9G_1^2+K_1^2\\ &+8K_1G_1+22\beta_0G_1+10\beta_0K_1+16\beta_0^2)L^3-\frac{1}{4}(A_3+A_2C_1)L^2+\frac{1}{16}G_1(K_2+4\beta_1)L^2\\ &-\frac{1}{72}A_1(18C_2+32C_A-135C_F)L^2+\frac{1}{16}G_2(9G_1+4K_1+8\beta_0)L^2\\ &+\frac{1}{8}G_1C_1(2G_1+K_1+2\beta_0)L^2-\frac{1}{2}(G_3+G_2C_1+G_1C_2)L+C_3+\mathcal{O}(\epsilon)\,, \end{split}$$

where again contributions arising from virtual heavy flavor lines are omitted (class hh) and

$$L = \ln\left(\frac{Q^2}{m^2}\right) \,. \tag{4.12}$$

In the quantities G_3 and C_3 in eq. (4.11) we have also absorbed all constant contributions from the decoupling relation (3.13) at order a_s^3 . All these terms are independent of $L_{\mu,\epsilon}$ and can potentially include contributions of order ϵ at a_s^3 which we did not write out explicitly in eq. (3.13). Results for \mathcal{F}_i at a general scale $\mu^2 \neq m^2$ can be derived from eqs. (4.9)–(4.11) by standard methods.² They will be presented elsewhere.

Explicit results for \mathcal{F}_i in eqs. (4.9)–(4.11) can be obtained with the help of the known coefficients of the cusp anomalous dimension $A(a_s)$ due to refs. [44, 45, 65],

$$A_1 = 4C_F, (4.13)$$

$$A_2 = C_F C_A \left(\frac{268}{9} - 8\zeta_2\right) + n_f C_F \left(-\frac{40}{9}\right), \tag{4.14}$$

²We take the opportunity to point out a typographical mistake in eq. (62) of ref. [32]. The following term $C_A C_F \frac{11}{6} \left(\frac{3}{2} - \frac{1}{2(1-x)} - \frac{1}{(1+x)} \right) H(0,x)$ should actually read $C_A C_F \frac{11}{6} \left(\frac{3}{2} - \frac{2}{(1-x)} - \frac{1}{(1+x)} \right) H(0,x)$.

$$A_3 = C_F C_A^{\ 2} \left(\frac{490}{3} - \frac{1072}{9} \zeta_2 + \frac{88}{3} \zeta_3 + \frac{176}{5} \zeta_2^{\ 2} \right)$$
(4.15)

$$+ n_f C_F C_A \left(-\frac{836}{27} + \frac{160}{9} \zeta_2 - \frac{112}{3} \zeta_3 \right) + n_f C_F^2 \left(-\frac{110}{3} + 32\zeta_3 \right) + n_f^2 C_F \left(-\frac{16}{27} \right).$$

The respective coefficients for $G(a_s)$ and $K(a_s)$ read,

$$G_1 = -6C_F + \epsilon C_F \left(-16 + 2\zeta_2\right) + \epsilon^2 C_F \left(-32 + 3\zeta_2 + \frac{28}{3}\zeta_3\right)$$
(4.16)

$$+\epsilon^{3}C_{F}\left(-64+8\zeta_{2}+14\zeta_{3}+\frac{47}{10}\zeta_{2}^{2}\right)+\mathcal{O}\left(\epsilon^{4}\right),$$
(4.17)

$$G_2 = C_F^{\ 2} \left(-3 + 24\zeta_2 - 48\zeta_3\right) + C_F C_A \left(-\frac{2545}{27} - \frac{44}{3}\zeta_2 + 52\zeta_3\right) \tag{4.18}$$

$$+n_f C_F \left(\frac{418}{27} + \frac{8}{3}\zeta_2\right) + \mathcal{O}(\epsilon) ,$$

 $K_1 = 2C_F ,$
(4.19)

$$K_{2} = C_{F}^{2} (3 - 24\zeta_{2} + 48\zeta_{3}) + C_{F} C_{A} \left(\frac{373}{27} + 30\zeta_{2} - 60\zeta_{3}\right) + n_{f} C_{F} \left(-\frac{10}{27} - 4\zeta_{2}\right). \quad (4.20)$$

Here we have included higher orders of ϵ in the anomalous dimensions, to ensure that all large logarithms in m are actually generated entirely by the integrations over ξ and λ in eq. (3.12). Although this is not a compelling choice it captures all structures in the exponential, which are universally related to parton dynamics. This is contrary to "minimal" versions proposed e.g. in ref. [24].

For the coefficients of the matching function $C(a_s)$ we find,

$$\begin{split} C_1 &= C_F(4+\zeta_2) + \epsilon C_F\left(8 + \frac{1}{2}\zeta_2 - \frac{2}{3}\zeta_3\right) + \epsilon^2 C_F\left(16 + 2\zeta_2 - \frac{1}{3}\zeta_3 + \frac{9}{20}\zeta_2^2\right) + \mathcal{O}\left(\epsilon^3\right) \,, (4.21) \\ C_2 &= C_F^2 \left(30 + 55\zeta_2 - 36\zeta_3 - 48\zeta_2 \ln 2 - \frac{251}{10}\zeta_2^2\right) \\ &+ C_A C_F \left(-\frac{2387}{27} + \frac{71}{36}\zeta_2 + \frac{479}{9}\zeta_3 + 24\zeta_2 \ln 2 - \frac{3}{5}\zeta_2^2\right) \\ &+ n_f C_F \left(\frac{356}{27} - \frac{37}{18}\zeta_2 - \frac{38}{9}\zeta_3\right) + \mathcal{O}\left(\epsilon\right) \,. \end{split}$$

Putting everything together, including the terms of order ϵ^2 at one loop (see appendix A) we arrive at the following results,

$$\mathcal{F}_{1} = C_{F} \left\{ \frac{1}{\epsilon} (2L-2) - L^{2} + 3L - 4 + 2\zeta_{2} + \epsilon \left(\frac{1}{3}L^{3} - \frac{3}{2}L^{2} + (8-\zeta_{2})L - 8 + 2\zeta_{2} + 4\zeta_{3} \right) + \epsilon^{2} \left(-\frac{1}{12}L^{4} + \frac{1}{2}L^{3} - \left(4 - \frac{1}{2}\zeta_{2} \right)L^{2} + \left(16 - \frac{3}{2}\zeta_{2} - \frac{14}{3}\zeta_{3} \right)L - 16 + 6\zeta_{2} + \frac{20}{3}\zeta_{3} + \frac{14}{5}\zeta_{2}^{2} \right) \right\} + \mathcal{O}(\epsilon^{3}),$$

$$(4.23)$$

$$\mathcal{F}_2 = C_F^2 \left\{ \frac{1}{\epsilon^2} (2L^2 - 4L + 2) + \frac{1}{\epsilon} (-2L^3 + 8L^2 - (14 - 4\zeta_2)L + 8 - 4\zeta_2) \right\}$$
(4.24)

$$\begin{split} &+ \frac{7}{6}L^4 - \frac{20}{3}L^3 + \left(\frac{55}{2} - 4\zeta_2\right)L^2 - \left(\frac{85}{2} - 32\zeta_3\right)L + 46 + 39\zeta_2 - 44\zeta_3 - 48\zeta_2 \ln 2 \\ &- \frac{118}{5}\zeta_2^2 + \epsilon \left(-\frac{1}{2}L^5 + \frac{11}{3}L^4 - \left(\frac{137}{6} - \frac{8}{3}\zeta_2\right)L^3 + \left(\frac{153}{2} - \frac{112}{3}\zeta_3\right)L^2\right)\right\} \\ &+ C_A C_F \left\{\frac{1}{\epsilon^2} \left(-\frac{11}{3}L + \frac{11}{3}\right) + \frac{1}{\epsilon} \left(\left(\frac{67}{9} - 2\zeta_2\right)L - \frac{49}{9} + 2\zeta_2 - 2\zeta_3\right) + \frac{11}{9}L^3 \\ &- \left(\frac{238}{18} - 2\zeta_2\right)L^2 + \left(\frac{2545}{54} + \frac{22}{3}\zeta_2 - 26\zeta_3\right)L - \frac{1595}{27} - \frac{7}{9}\zeta_2 + \frac{134}{3}\zeta_3 + 24\zeta_2 \ln 2 \\ &- \frac{3}{5}\zeta_2^2 + \epsilon \left(-\frac{11}{12}L^4 + \left(\frac{565}{54} - \frac{4}{3}\zeta_2\right)L^3 - \left(\frac{3337}{54} + \frac{11}{2}\zeta_2 - 26\zeta_3\right)L^2\right)\right\} \\ &+ C_F n_f \left\{\frac{1}{\epsilon^2} \left(\frac{2}{3}L - \frac{2}{3}\right) + \frac{1}{\epsilon} \left(-\frac{10}{9}L + \frac{10}{9}\right) - \frac{2}{9}L^3 + \frac{19}{9}L^2 - \left(\frac{209}{27} + \frac{4}{3}\zeta_2\right)L + \frac{212}{27} \\ &- \frac{14}{9}\zeta_2 - \frac{8}{3}\zeta_3 + \epsilon \left(\frac{1}{6}L^4 - \frac{47}{27}L^3 + \left(\frac{281}{27} + \zeta_2\right)L^2\right)\right\} + O(L\epsilon) + O(\epsilon^2), \end{split}$$

$$\mathcal{F}_3 = C_F^3 \left\{\frac{1}{\epsilon^3} \left(\frac{4}{3}L^3 - 4L^2 + 4L - \frac{4}{3}\right) + \frac{1}{\epsilon^2} \left(-2L^4 + 10L^3 - (22 - 4\zeta_2)L^2\right) \\ &+ (22 - 8\zeta_2)L - 8 + 4\zeta_2\right) + \frac{1}{\epsilon} \left(\frac{5}{3}L^5 - \frac{34}{3}L^4 + \left(\frac{137}{3} - 6\zeta_2\right)L^3 - \left(89 - 56\zeta_3\right)L^2 \\ &+ \left(129 + 88\zeta_2 - 136\zeta_3 - 96\zeta_3\ln 2 - \frac{236}{5}\zeta_2^2\right)L\right) - L^6 + \frac{17}{2}L^5 - \left(\frac{148}{3} - \frac{16}{3}\zeta_2\right)L^4 \\ &+ \left(\frac{494}{3} + \frac{17}{17}\zeta_2 - \frac{268}{3}\zeta_3\right)L^3\right\} + C_F^2C_A \left\{\frac{1}{\epsilon^3} \left(-\frac{22}{23}L^2 + \frac{44}{3}L - \frac{22}{3}\right) + \frac{1}{\epsilon^2} \left(\frac{11}{3}L^3 + \left(\frac{29}{9} - 4\zeta_2\right)L^2 - \left(\frac{1}{9} - \frac{2}{3}\zeta_2 + 4\zeta_3\right)L - \frac{34}{9} + \frac{10}{9}\zeta_2 + 4\zeta_3\right) + \frac{1}{\epsilon} \left(\frac{11}{9}L^4 - \left(\frac{526}{3} - \frac{36}{3}\zeta_3 - 48\zeta_2\ln 2\right) \right) \\ &+ \frac{26}{5}\zeta_2^2\right)L - \frac{11}{14}L^5 + \left(\frac{4289}{108} - \frac{16}{3}\zeta_2\right)L^4 - \left(\frac{6260}{27} + \frac{9}{15}\zeta_2 - \frac{23}{3}\zeta_3\right)L^3\right\} \\ &+ C_F C_A^2 \left\{\frac{1}{\epsilon^3} \left(\frac{242}{27}L - \frac{247}{27}\right) + \frac{1}{\epsilon^2} \left(-\left(\frac{2086}{81} - \frac{44}{9}\zeta_2\right)L + \frac{1600}{81} - \frac{44}{9}\zeta_2\right)L^3\right\} \\ &+ C_F C_A^2 \left\{\frac{1}{\epsilon^3} \left(\frac{242}{27}L - \frac{247}{27}\right) + \frac{1}{\epsilon^2} \left(-\left(\frac{2086}{81} - \frac{44}{9}\zeta_2\right)L + \frac{1609}{81} - \frac{4}{9}\zeta_2\right)L^3\right\} \\ &+ C_F C_A^2 \left\{\frac{1}{\epsilon^3} \left(\frac{242}{27}L - \frac{247}{27}\right) + \frac{1}{\epsilon^2} \left(-\left(\frac{2086}{81} - \frac{44}{9}\zeta_2\right)L + \frac{160}{81} - \frac{4}{9}\zeta_2\right)L^$$

+(22)

$$+C_F^2 \left\{ \frac{1}{\epsilon} \left(-15L \right) \right\} + C_F C_A \left\{ \frac{1}{\epsilon} \left(\frac{32}{9}L \right) \right\} + \mathcal{O}(L^0 \epsilon^{-1}) + \mathcal{O}(L^2 \epsilon^0) + \mathcal{O}(\epsilon) + \mathcal{O}($$

Further improvements on the accuracy of the three-loop prediction \mathcal{F}_3 require an extension of the two-loop result \mathcal{F}_2 to order ϵ . We will return to this issue in a future publication.

Let us close this section with a few comments. First of all, it is clear we can obtain a three-loop prediction, i.e. the coefficient $Z_{[q]}^{(3)}$ in eq. (4.1) for the factor $Z_{[q]}^{(m|0)}$ from the exponentiated massive form factor in eq. (3.12) with the help of eq. (4.25) and the known three-loop results in the massless case [28, 30]. Next, putting the discussion in a broader perspective, we note that exponentiations similar to eq. (3.12) have also been studied for electroweak interactions [63, 66] in massive gauge theories, where large logarithms in the mass of the gauge boson appear. There, the resummation has been used as a generating functional for Sudakov logarithms at higher orders. Of course, those details of the exponentials which depend on the infrared sector of the theory are modified in comparison to eq. (3.12). However, it is rather striking to observe that the coefficients for G_1 and G_2 from our determination in eqs. (4.16) and (4.18) agree precisely with the values for $\zeta^{(1)}$, $\zeta^{(2)}$ in ref. [66] (up to an overall factor 1/2 due to different normalizations). In both cases, the relevant coefficients control the single logarithm L at the respective order.

On top of this, it is even more striking, that the very same coefficients G_1 and G_2 from eqs. (4.16), (4.18) for the form factor of a massive quark also coincide with the corresponding results in massless case [28, 30] (up to an overall sign from different definitions). This observation, which calls for an explanation, suggests a universality of the function G which extends even to higher orders in ϵ , see e.g. eq. (4.16). It also offers the chance for a conjecture about the coefficient of the single logarithm L for \mathcal{F}_3 in eq. (4.11) purely on the basis of the corresponding massless result, provided, of course, that all necessary terms to higher order in ϵ up to two loops are known.

The potential consequences of such a universal nature of the function G would be rather interesting. For instance, in the massless case there exist additional relations between the functions $\mathcal{F}^{[q]}$ and $\mathcal{F}^{[g]}$, i.e. the form factors for the vertices $\gamma^* qq$ and ϕgg . These relations manifest themselves in underlying structures for the respective function $G^{[i]}$ (i = q, g) [28, 61, 67] such that one can decompose the resummation coefficients $G^{[i]}$ in the massless case according to

$$G_1^{[i]} = 2\left(B_1^{[i]} - \delta_{ig}\beta_0\right) + f_1^{[i]} + \epsilon \widetilde{G_1^{[i]}}, \qquad (4.26)$$

$$G_2^{[i]} = 2\left(B_2^{[i]} - 2\delta_{ig}\beta_1\right) + f_2^{[i]} + \beta_0 \widetilde{G_1^{[i]}}(\epsilon = 0) + \widetilde{\epsilon G_2^{[i]}}, \qquad (4.27)$$

$$G_{3}^{[i]} = 2\left(B_{3}^{[i]} - 3\delta_{ig}\beta_{2}\right) + f_{3}^{[i]} + \beta_{1}\widetilde{G_{1}^{[i]}}(\epsilon=0) + \beta_{0}\left(\widetilde{G_{2}^{[i]}}(\epsilon=0) - \beta_{0}\widetilde{G_{1}^{[i]}}(\epsilon=0)\right) + \epsilon\widetilde{G}_{3}^{[i]},$$
(4.28)

where i = q, g and

$$\widetilde{F} = \epsilon^{-1} \left[F - F(\epsilon = 0) \right].$$
(4.29)

Here (and only here), the functions $B_n^{[i]}$ (not to be confused with the ones given in eqs. (4.34)–(4.36)) denote the coefficients of term with $\delta(1-x)$ in the *n*-loop diago-

nal $\overline{\text{MS}}$ splitting functions $P_{ii}^{(n-1)}$ [44, 45], while the universal functions $f_n^{[i]}$ exhibit the same maximally non-Abelian color structure as the $A_n^{[i]}$ [43] up to the factor C_A/C_F , i.e., $f_i^{[g]} = C_A/C_F f_i^{[q]}$, see ref. [28] for details. With the help of eqs. (4.26)–(4.28) one could translate the exponentiated form factor in eq. (3.11) for heavy quarks immediately e.g. to the case of gluinos \tilde{g} with mass $m_{\tilde{g}}$, all resummation coefficients up to three loops being known.

For completeness, let us finally mention also the functions H and S of eq. (3.21) as well as B and h from eq. (3.24). The function H is already known through two loops from refs. [56, 59], while the function S was evaluated in refs. [54, 55] to one loop. Using eq. (3.22) and matching it to the fixed-order calculation for \mathcal{F}_2 we can extract in particular the two-loop coefficient S_2 from the term $\alpha_s^2/\epsilon L^0$. The explicit results for $H(a_s)$ of the massive form factor in eq. (3.22) read,

$$H_1 = -4C_F \,, \tag{4.30}$$

$$H_2 = C_F C_A \left(\frac{220}{27} + 8\zeta_2 - 36\zeta_3\right) + n_f C_F \frac{8}{27}, \qquad (4.31)$$

and for $S(a_s)$

$$S_1 = -4C_F, (4.32)$$

$$S_2 = C_F C_A \left(-\frac{1396}{27} + 8\zeta_2 + 20\zeta_3 \right) + n_f C_F \frac{232}{27}.$$
(4.33)

In order to have a self-contained presentation, we also give the perturbative expansions of the coefficients $B(a_s)$,

$$B_{1} = -3C_{F}, \qquad (4.34)$$

$$B_{2} = C_{F}^{2} \left(-\frac{3}{2} + 12\zeta_{2} - 24\zeta_{3} \right) + C_{F}C_{A} \left(-\frac{3155}{54} + \frac{44}{3}\zeta_{2} + 40\zeta_{3} \right) + C_{F}n_{f} \left(\frac{247}{27} - \frac{8}{3}\zeta_{2} \right), \qquad (4.35)$$

$$B_{3} = C_{F}^{3} \left(-\frac{29}{2} - 18\zeta_{2} - 68\zeta_{3} - \frac{288}{5}\zeta_{2}^{2} + 32\zeta_{2}\zeta_{3} + 240\zeta_{5} \right) + C_{A}C_{F}^{2} \left(-46 + 287\zeta_{2} - \frac{712}{3}\zeta_{3} - \frac{272}{5}\zeta_{2}^{2} - 16\zeta_{2}\zeta_{3} - 120\zeta_{5} \right) + C_{A}^{2}C_{F} \left(-\frac{599375}{729} + \frac{32126}{81}\zeta_{2} + \frac{21032}{27}\zeta_{3} - \frac{652}{15}\zeta_{2}^{2} - \frac{176}{3}\zeta_{2}\zeta_{3} - 232\zeta_{5} \right) + C_{F}^{2}n_{f} \left(\frac{5501}{54} - 50\zeta_{2} + \frac{32}{9}\zeta_{3} \right) + C_{F}n_{f}^{2} \left(-\frac{8714}{729} + \frac{232}{27}\zeta_{2} - \frac{32}{27}\zeta_{3} \right) + C_{A}C_{F}n_{f} \left(\frac{160906}{729} - \frac{9920}{81}\zeta_{2} - \frac{776}{9}\zeta_{3} + \frac{208}{15}\zeta_{2}^{2} \right),$$

$$(4.36)$$

and for $h(a_s)$

$$h_1 = -3C_F + \epsilon C_F (-16 + 2\zeta_2) + \epsilon^2 C_F \left(-32 + 3\zeta_2 + \frac{28}{3}\zeta_3 \right) + \epsilon^3 C_F \left(-64 + 8\zeta_2 \right)$$
(4.37)

$$\begin{split} &+14\zeta_{3}+\frac{47}{10}\zeta_{2}^{2}\right)+\epsilon^{4}C_{F}\left(-128+16\zeta_{2}+\frac{112}{3}\zeta_{3}+\frac{141}{20}\zeta_{2}^{2}-\frac{14}{3}\zeta_{2}\zeta_{3}+\frac{124}{5}\zeta_{5}\right)\\ &+\epsilon^{5}C_{F}\left(-256+32\zeta_{2}+\frac{224}{3}\zeta_{3}+\frac{94}{5}\zeta_{2}^{2}-7\zeta_{2}\zeta_{3}+\frac{186}{5}\zeta_{5}+\frac{949}{140}\zeta_{2}^{3}-\frac{98}{9}\zeta_{3}^{2}\right),\\ h_{2}&=C_{F}^{2}\left(-\frac{3}{2}+12\zeta_{2}-24\zeta_{3}\right)+C_{F}C_{A}\left(-\frac{215}{6}-\frac{88}{3}\zeta_{2}+12\zeta_{3}\right)+n_{f}C_{F}\left(\frac{19}{3}+\frac{16}{3}\zeta_{2}\right) \quad (4.38)\\ &+\epsilon C_{F}^{2}\left(-\frac{1}{2}+116\zeta_{2}-120\zeta_{3}-\frac{176}{5}\zeta_{2}^{2}\right)+\epsilon C_{F}C_{A}\left(-\frac{70165}{162}-\frac{575}{9}\zeta_{2}+\frac{520}{3}\zeta_{3}\right)\\ &+\frac{176}{5}\zeta_{2}^{2}\right)+\epsilon n_{f}C_{F}\left(\frac{5813}{81}+\frac{74}{9}\zeta_{2}-\frac{16}{3}\zeta_{3}\right)+\epsilon^{2}C_{F}^{2}\left(\frac{109}{4}+437\zeta_{2}-736\zeta_{3}-\frac{432}{5}\zeta_{2}^{2}\right)\\ &+112\zeta_{2}\zeta_{3}-48\zeta_{5}\right)+\epsilon^{2}C_{F}C_{A}\left(-\frac{1547797}{972}-\frac{7297}{27}\zeta_{2}+\frac{24958}{27}\zeta_{3}+\frac{653}{6}\zeta_{2}^{2}-\frac{356}{3}\zeta_{2}\zeta_{3}\\ &+204\zeta_{5}\right)+\epsilon^{2}n_{f}C_{F}\left(\frac{129389}{486}+\frac{850}{27}\zeta_{2}-\frac{1204}{27}\zeta_{3}-\frac{7}{3}\zeta_{2}^{2}\right)+\epsilon^{3}C_{F}^{2}\left(\frac{1287}{8}+\frac{2991}{2}\zeta_{2}\right)\\ &-3614\zeta_{3}-508\zeta_{2}^{2}+104\zeta_{2}\zeta_{3}-72\zeta_{5}+\frac{6864}{35}\zeta_{2}^{3}+1072\zeta_{3}^{2}\right)+\epsilon^{3}C_{F}C_{A}\left(\frac{31174909}{5832}\right)\\ &-\frac{155701}{162}\zeta_{2}+\frac{308810}{81}\zeta_{3}+\frac{100907}{180}\zeta_{2}^{2}-\frac{478}{3}\zeta_{2}\zeta_{3}+840\zeta_{5}-\frac{1618}{35}\zeta_{2}^{3}-\frac{2276}{3}\zeta_{3}^{2}\right)\\ &+\epsilon^{3}n_{f}C_{F}\left(\frac{2628821}{2916}+\frac{8405}{81}\zeta_{2}-\frac{16340}{81}\zeta_{3}-\frac{1873}{90}\zeta_{2}^{2}-\frac{44}{3}\zeta_{2}\zeta_{3}-48\zeta_{5}\right),\\ h_{3}=C_{F}^{3}\left(-\frac{29}{2}-18\zeta_{2}-68\zeta_{3}-\frac{288}{5}\zeta_{2}^{2}+32\zeta_{2}\zeta_{3}+240\zeta_{5}\right)+C_{F}^{2}C_{A}\left(-\frac{94}{3}\right) \\ &+\frac{1235}{3}\zeta_{2}-\frac{2296}{3}\zeta_{3}+\frac{856}{15}\zeta_{2}^{2}-16\zeta_{2}\zeta_{3}-120\zeta_{5}\right)+C_{F}C_{A}^{2}\left(-\frac{16540}{27}-\frac{22286}{27}\zeta_{2}\\ &+\frac{1544}{3}\zeta_{3}+\frac{1592}{15}\zeta_{2}^{2}-40\zeta_{5}\right)+n_{f}C_{F}^{2}\left(\frac{239}{6}-\frac{146}{3}\zeta_{2}+\frac{400}{3}\zeta_{3}-\frac{208}{15}\zeta_{2}^{2}\right)\\ &+n_{f}C_{F}C_{A}\left(\frac{5516}{27}+\frac{7216}{27}\zeta_{2}-\frac{224}{3}\zeta_{3}-\frac{296}{15}\zeta_{2}^{2}\right)+n_{f}^{2}C_{F}\left(-\frac{406}{27}-\frac{536}{27}\zeta_{2}\right), \end{split}$$

where the function B is known to three loops from refs. [37, 39, 53, 62], while the function h has been derived by matching eq. (3.24) to the respective fixed-order calculation starting from the single pole terms α_s^n/ϵ .

5. Applications

Here we want to demonstrate how the previous considerations can be applied to derive the structure of the singularities and all large Sudakov logarithms in higher order QCD corrections to partonic scattering processes. Let us start with the general $2 \rightarrow n$ scattering processes of partons p_i in eq. (2.1) and consider eq. (2.7) in a perturbative expansion in α_s . We want to present the explicit relations between corresponding amplitudes with and without parton masses $\{m_i\}$, in our notation $|\mathcal{M}_{p,\{m_i\}}\rangle$ and $|\mathcal{M}_{p,\{m_i=0\}}\rangle$. Throughout this section, we consider (ultraviolet) renormalized quantities and we define

$$|\mathcal{M}_{\mathrm{p}}\rangle = \sum_{i=0}^{\infty} \left(a_{\mathrm{s}}\right)^{i} |\mathcal{M}_{\mathrm{p}}^{(i)}\rangle, \qquad (5.1)$$

and any overall powers of a_s typical say, for jet cross-sections at hadron colliders, have been absorbed in the notation. We can then express eq. (2.7) for a general process (2.1) in an expansion to second order in α_s as,

$$|\mathcal{M}_{\mathbf{p},\{m_i\}}^{(0)}\rangle = |\mathcal{M}_{\mathbf{p},\{m_i=0\}}^{(0)}\rangle,$$
(5.2)

$$|\mathcal{M}_{\mathbf{p},\{m_i\}}^{(1)}\rangle = \frac{1}{2} \sum_{i \in \{\text{all legs}\}} Z_{[i]}^{(1)} |\mathcal{M}_{\mathbf{p},\{m_i=0\}}^{(0)}\rangle + |\mathcal{M}_{\mathbf{p},\{m_i=0\}}^{(1)}\rangle, \qquad (5.3)$$

$$|\mathcal{M}_{\mathbf{p},\{m_i\}}^{(2)}\rangle = \frac{1}{2} \sum_{i \in \{\text{all legs}\}} \left(Z_{[i]}^{(2)} - \frac{1}{4} \left(Z_{[i]}^{(1)} \right)^2 \right) |\mathcal{M}_{\mathbf{p},\{m_i=0\}}^{(0)}\rangle + \frac{1}{2} \sum_{i \in \{\text{all legs}\}} Z_{[i]}^{(1)} |\mathcal{M}_{\mathbf{p},\{m_i=0\}}^{(1)}\rangle + |\mathcal{M}_{\mathbf{p},\{m_i=0\}}^{(2)}\rangle,$$
(5.4)

which holds in the small mass limit up to terms suppressed with the parton masses m_i^2 . Of course, in the case of massless external lines the respective higher order corrections to the Z-factors in eqs. (5.3), (5.4) mostly vanish. Also recall that the amplitude $|\mathcal{M}_{\rm p}\rangle$ is a vector in color space whereas the Z-factors from eq. (2.8) are in this respect simply functions. Non-trivial color dependence of singularities on the other hand typically arises from soft gluon exchange and therefore carries over directly from underlying massless hard scattering amplitude $|\mathcal{M}_{\rm p,\{m_i=0\}}\rangle$. Finally, it has been emphasized already in the previous discussions, that eqs. (5.2)–(5.4) require to organize the contributions to the massive amplitude $|\mathcal{M}_{\rm p,\{m_i\}}\rangle$ in terms of flavor classes, i.e. whether or not the heavy parton lines are external. An analogous distinction holds for the gluon factor $Z_{[g]}^{(m|0)}$ when heavy quarks are included for instance as self-energy corrections to the external gluons, see eqs. (5.15), (5.16) below. The explicit results for $Z_{[q]}^{(1)}$ and $Z_{[q]}^{(2)}$ in eqs. (4.2), (4.3) hold for the cases ll, hl.

In the light of eqs. (5.2)-(5.4) let us briefly come back to the relation between the factor $Z^{(m|0)}$ and the perturbative fragmentation functions [19]. Although this connection may come at first as a surprise, the two functions are actually intimately related in the context of QCD amplitudes. First of all, both are process-independent. Secondly, one may compare both approaches in a computation of a one-particle inclusive cross-section of a massive parton based on an amplitude such as eq. (2.2). The result takes the form of a convolution of massless cross-section times the perturbative fragmentation function. (We refer the reader to the discussion in refs. [57, 68] for complete details on this point). Alternatively, we can use eq. (2.7) to relate the massive amplitude to the massive one. As is clear e.g. from the perturbative expansion in eqs. (5.2)–(5.4) the proportionality factor between $|\mathcal{M}_{\mathrm{p},\{m_i\}}\rangle$ and $|\mathcal{M}_{\mathrm{p},\{m_i=0\}}\rangle$ is independent of the kinematics and is also not affected by the subsequent phase-space integration. Furthermore, this holds separately for virtual and the corresponding real radiation contributions.

relation between massive amplitudes and their massless counterpart in eq. (2.7) represents the appropriate generalization of the formalism of Mele and Nason [19] at the amplitude level.

In an equivalent formulation, we can also consider the perturbative expansion of eq. (2.4). To that end, we repeat the decomposition of the amplitude $|\mathcal{M}_{\mathbf{p},\{m_i\}}\rangle$ from eqs. (5.2)–(5.4) up to two loops in terms of products of the functions $\mathcal{J}^{[\mathbf{p}]}$, $\mathcal{S}^{[\mathbf{p}]}$ and $\mathcal{H}^{[\mathbf{p}]}$.

$$\left|\mathcal{M}_{\mathbf{p},\{m_i\}}^{(0)}\right\rangle = \left|\mathcal{H}_{\mathbf{p}}^{(0)}\right\rangle,\tag{5.5}$$

$$|\mathcal{M}_{\mathbf{p},\{m_i\}}^{(1)}\rangle = \frac{1}{2} \sum_{i \in \{\text{all legs}\}} \mathcal{F}_1^{[i]} |\mathcal{H}_{\mathbf{p}}^{(0)}\rangle + \mathcal{S}_1^{[\mathbf{p}]} |\mathcal{H}_{\mathbf{p}}^{(0)}\rangle + |\mathcal{H}_{\mathbf{p}}^{(1)}\rangle,$$
(5.6)

$$|\mathcal{M}_{\mathbf{p},\{m_i\}}^{(2)}\rangle = \frac{1}{2} \sum_{i \in \{\text{all legs}\}} \left(\mathcal{F}_2^{[i]} - \frac{1}{4} \left(\mathcal{F}_1^{[i]} \right)^2 + \frac{1}{2} \mathcal{F}_1^{[i]} \mathcal{S}_1^{[\mathbf{p}]} \right) |\mathcal{H}_{\mathbf{p}}^{(0)}\rangle$$
(5.7)

$$+\frac{1}{2}\sum_{i\in \{\text{all legs}\}} \mathcal{F}_1^{[i]}|\mathcal{H}_p^{(1)}\rangle + \mathcal{S}_2^{[p]}|\mathcal{H}_p^{(0)}\rangle + \mathcal{S}_1^{[p]}|\mathcal{H}_p^{(1)}\rangle + |\mathcal{H}_p^{(2)}\rangle,$$

where the perturbative expansions of $S^{[p]}$ and $|\mathcal{H}_p\rangle$ are defined analogous to eq. (5.1). Of course, the same qualifications from section 3 about the distinct flavor classes contributing to the massive form factor \mathcal{F} also apply here. Now, in the factorization ansatz of eq. (2.4) the function $|\mathcal{H}_p\rangle$ is a vector and $S^{[p]}$ is a matrix in color space. Thus, their products in eqs. (5.6), (5.7) are in the sense of matrix multiplication and all dependence on singular color correlations rests entirely in the function $S^{[p]}$.

As we remarked above (and as is well known in the literature [11, 24, 46]) the matrix $\mathcal{S}^{[p]}$ is subject of a renormalization group equation which allows for an all-order exponentiation of the soft contributions. The solution for $\mathcal{S}^{[p]}$ results in a path-ordered exponential due to mixing of the color structures under soft gluon exchange,

$$\mathcal{S}^{[p]}\left(\{k_i\}, \frac{Q^2}{\mu^2}, \alpha_{\rm s}(\mu^2), \epsilon\right) = \Pr \exp \left[-\frac{1}{2} \int_{0}^{Q^2} \frac{dk^2}{k^2} \Gamma^{[p]}\left(\bar{a}(k^2, \epsilon)\right)\right],$$
(5.8)

where P denotes the path ordering. Here, $\Gamma^{[p]}$ is the so-called soft anomalous dimension, which is a matrix in the space of color tensors (see eqs. (2.2), (2.4)). Of course, the running coupling $\bar{\alpha}_s$ in the argument of $\Gamma^{[p]}$ is to be taken in *d* dimensions. For $2 \to n$ hard scattering processes with massless partons $\Gamma^{[p]}$ is currently known up to two loops [24, 66, 69, 70] and to one loop results for reactions with massive partons [71, 72]. In the latter case, one can show in particular, that the soft anomalous dimension $\Gamma^{[p]}$ has a smooth limit for $m \to 0$.

To summarize, we have given in eqs. (5.2)-(5.4) and (5.5)-(5.7) two equivalent formulations. Both allow to obtain all large logarithms of Sudakov type together with the dimensionally regulated soft poles in ϵ and any given QCD amplitude for $2 \rightarrow n$ scattering with parton masses $\{m_i\}$ can be constructed by either method. In particular eq. (5.8) can be used to derive explicit expressions for $S_1^{[p]}$ and $S_2^{[p]}$ in eqs. (5.5)–(5.7) in terms of the perturbative expansion for the soft anomalous dimension $\Gamma^{[p]}$. Most of the other ingredients are explicitly presented in this paper. Next, let us discuss the consistency of eq. (2.7) with the results of ref. [2]. In that reference the structure of both soft and collinear singularities for any one-loop amplitude was presented for arbitrary values of parton masses. In the approach of ref. [2] any one-loop n-parton amplitude can be written as:

$$|\mathcal{M}_{\rm p}^{(1)}\rangle = I_n^{(m)}(\epsilon, \mu^2, \{m_i^2\}) |\mathcal{M}_{\rm p}^{(0)}\rangle + |\mathcal{M}_{\rm p}^{(1), \rm fin}\rangle, \qquad (5.9)$$

where $|\mathcal{M}_{\mathbf{p}}^{(0)}\rangle$ is the Born amplitude for the process under consideration. The amplitude $|\mathcal{M}_{\mathbf{p}}^{(1),\mathrm{fin}}\rangle$ contains only one-loop corrections which are finite in the limits $m_i \to 0$ and $\epsilon \to 0$. In the following we will adapt the results of ref. [2] to the $\overline{\mathrm{MS}}$ coupling evaluated at a renormalization scale μ . We will also assume conventional dimensional regularization for simplicity. In the small mass limit the operator $I_n^{(m)}$ then takes the form (recall that all non-vanishing masses m_i are assumed to have a common value m):

$$I_n^{(m)}(\epsilon,\mu^2,\{m_i^2\}) = \frac{\exp(\epsilon\gamma_{\rm E})}{\Gamma(1-\epsilon)} \left\{ \sum_{j\neq k=1}^n T_j \cdot T_k \ \mathcal{V}_{jk}(s_{jk};m_j,m_k;\epsilon) - \sum_{j=1}^n \Gamma_j(\mu,m_j;\epsilon) + \dots \right\},\tag{5.10}$$

where T_k are the generators of the gauge group and s_{jk} the kinematical invariants. The dots denote mass-independent terms and the functions \mathcal{V}_{jk} are associated to pairs of external partons. One has three possible combinations in each pair of partons with two, one or none of them being massive. Thus, three separate functions \mathcal{V}_{jk} are needed for these three cases. Similarly, the functions Γ_j are different, depending on whether the parton j is massive or massless, i.e. quark, gluon, gluino and so on.

For the sake of comparison with the Z-factor in eq. (2.8) we write \mathcal{V}_{jk} and Γ_j as

$$\mathcal{V}_{jk}^{(2 \text{ massive partons})} = 2\,\Delta_V + \mathcal{V}_{jk}^{(0)} \tag{5.11}$$

$$\mathcal{V}_{jk}^{(1 \text{ massive parton})} = \Delta_V + \mathcal{V}_{jk}^{(0)} \tag{5.12}$$

$$\Gamma_q^{(m)} = \Delta_q + \Gamma_q^{(0)} \tag{5.13}$$

$$\Gamma_g^{(m)} = \eta_h \,\Delta_g + \Gamma_g^{(0)} \,, \tag{5.14}$$

where the functions Δ_V , Δ_q and Δ_g are independent of the invariants s_{jk} , i.e. they are the same for each external parton (or pair of external partons).³ Therefore one can apply the color algebra to express the sum over the products of color generators multiplying these functions directly in terms of the corresponding Casimir operators (see ref. [2]). In this way, all process dependent factors are separated into functions that are independent of the mass. All mass dependence on the other hand enters only in a process-independent way. Combining the above results one gets

$$I_n^{(m)}(\epsilon,\mu^2,m^2) = I_n^{(0)}(\epsilon,\mu^2) + \sum_{j=1}^{n_h} f_q(\epsilon,\mu^2,m^2) + \sum_{j=1}^{n_g} n_h f_g(\epsilon,\mu^2,m^2), \qquad (5.15)$$

where $I_n^{(0)}$ is the appropriate operator for purely massless amplitudes [10] evaluated for $n_f = n_l + n_h$ light flavors. The function f_q is given by one half of the function $Z_{[q]}^{(1)}$ (and of

³The superscripts (m) and (0) refer to quantities evaluated in the massive, respectively massless case.

course restricted to constant terms at order ϵ^0) presented in eq. (4.2). For the function f_g we find

$$f_g(\epsilon, \mu^2, m^2) = -\frac{1}{3} \left(\frac{1}{\epsilon} + \ln\left(\frac{\mu^2}{m^2}\right) \right), \qquad (5.16)$$

which, when restricted to constant terms at order ϵ^0 , is related to the function $Z_{[g]}^{(1)}$ in eq. (4.5) through $n_h f_g(\epsilon, \mu^2, m^2) = Z_{[g]}^{(1)}/2$.

Finally, we briefly comment on Abelian gauge theories with fermion masses like Quantum Electrodynamics (QED). These provide other prominent examples for the considerations of the present article. For instance one arrives at QED (with massive electrons) after the usual identification of the color factors, $C_F = 1$, $C_A = 0$ and $T_f = 1$ instead of our QCD convention $T_f n_f = n_f/2$ There, the complete calculation of the two-loop radiative photonic corrections in QED to Bhabha scattering in the small mass limit have already been performed [20-22]. This included also a complete matching at two loops, i.e. the computation of the constant terms which are not logarithmically enhanced. The latter also required the constant terms from the massless, dimensionally regularized amplitudes of ref. [73]. An extension of the results of the present article (and the exponentiation in particular) in this direction is a possibility which we leave for a future publication.

6. Summary

In this article we have presented a first discussion of the singular behavior of on-shell QCD amplitudes with massive particles beyond one loop. We have performed a systematic study of both, the soft singularities typically showing up as poles in ϵ in dimensional regularization and the structure of the large Sudakov (or quasi-collinear) type logarithms of the parton masses, which become dominant in the high energy limit. Working in the small mass limit, we have consistently omitted power corrections in the parton masses.

We have presented in eqs. (2.4) and (2.7) a general framework for the factorization of *n*-parton amplitudes in QCD which incorporates massive partons. The factorization formula, which we have organized in terms of flavor classes, is universal and is valid for any amplitude. We have emphasized the strong similarities between scattering amplitudes with massless and massive partons in the limit where all parton masses are much smaller than the relevant kinematic invariants of the scattering process. In this regime, the factorization formula can be used to directly obtain (apart from vanishing corrections when the masses tend to zero) the massive amplitude from the corresponding massless amplitude, without explicitly computing the former. To that end we have introduced the factor $Z^{(m|0)}$ as the building block of the proportionality. In the case of heavy quarks we have linked $Z_{[q]}^{(m|0)}$ to the virtual corrections in the formalism of perturbative fragmentation function thus generalizing the approach of ref. [19] to the level of amplitudes. Finally, we have explicitly illustrated the predictive power of the factorization ansatz for examples from $2 \to n$ scattering processes in QCD.

Improved insight into the structure underlying the factorization of amplitudes in the soft and (quasi)-collinear momentum regions have enabled us to derive an exponential (3.12)

for the form factor of heavy quarks. We have used this new result to predict the fixedorder expansion of the massive form factor to up three loops and, in comparing massless and massive amplitudes, we have observed an apparent universality of the respective resummation coefficients G which we find worth mentioning. Furthermore, on the basis of eq. (2.4) and the exponentiations for the functions $\mathcal{J}^{[p]}$ and $\mathcal{S}^{[p]}$ we have shown how to extend our predictions to the perturbative expansion of general *n*-parton amplitudes in QCD with massive partons.

Thus, the results of the present paper such as eq. (2.8) can be useful to either check explicit evaluations of amplitudes at higher loops or make predictions to higher orders in perturbation theory. The material presented can also help to organize calculations, say at NNLO, in terms of divergent, but analytically computable, parts and finite remainders that can be integrated numerically. In the context of general calculations for differential observables with massive partons at NNLO our factorization formula may also facilitate the combination of the respective tree-level and one-loop real emission amplitudes with the virtual contributions in a process independent manner.

We will return to these issues as well as potential connections to threshold resummation for processes with massive partons in future work.

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A. The complete form factor \mathcal{F} at one loop

Here, we give the complete result for one-loop QCD corrections to order ϵ^2 to the form factor of a heavy quark at the scale $\mu^2 = m^2$ in terms of harmonic polylogarithms $H_{m_1,...,m_w}(x)$, see also section 3 and eq. (4.8) for definitions. The variable x with $0 \le x \le 1$ for space-like $q^2 = -Q^2 < 0$ is given by

$$x = \frac{\sqrt{Q^2 + 4m^2} - \sqrt{Q^2}}{\sqrt{Q^2 + 4m^2} + \sqrt{Q^2}}.$$
 (A.1)

For \mathcal{F}_1 we find⁴

$$\mathcal{F}_{1} = \frac{1}{\epsilon} C_{F} \left\{ -2 + 2 \left(1 - \frac{1}{1-x} - \frac{1}{1+x} \right) H_{0} \right\} + C_{F} \left\{ -4 + \left(3 - \frac{4}{1-x} - \frac{2}{1+x} \right) H_{0} \right\}$$
(A.2)

⁴We thank J. Gluza for providing us with the integral SE212m of refs. [12, 13] to order ϵ^3 , see also http://www-zeuthen.desy.de/theory/research/bhabha/.

$$\begin{split} +& 2 \left(1 - \frac{1}{1 - x} - \frac{1}{1 + x}\right) (\mathcal{H}_{0,0} - 2\mathcal{H}_{-1,0} - \zeta_2) \right\} + \epsilon C_F \left\{-8 + \left(1 - \frac{1}{1 - x} - \frac{1}{1 + x}\right) (8\mathcal{H}_0 \\ +& 8\mathcal{H}_{-1,-1,0} - 4\zeta_3 + 4\mathcal{H}_{-1}\zeta_2 - 4\mathcal{H}_{-1,0,0} - \mathcal{H}_0\zeta_2 - 4\mathcal{H}_{0,-1,0} + 2\mathcal{H}_{0,0,0}) \\ +& \left(3 - \frac{4}{1 - x} - \frac{2}{1 + x}\right) (\mathcal{H}_{0,0} - 2\mathcal{H}_{-1,0}) - 2 \left(2 - \frac{2}{1 - x} - \frac{1}{1 + x}\right) \zeta_2 \right\} + \epsilon^2 C_F \left\{-16 \\ -& \frac{4}{3} \left(4 - \frac{6}{1 - x} - \frac{3}{1 + x}\right) \zeta_3 + \left(3 - \frac{4}{1 - x} - \frac{2}{1 + x}\right) \left(2\mathcal{H}_{-1}\zeta_2 + 4\mathcal{H}_{-1,-1,0} - 2\mathcal{H}_{-1,0,0}\right) \\ -& \frac{1}{2}\mathcal{H}_0\zeta_2 - 2\mathcal{H}_{0,-1,0} + \mathcal{H}_{0,0,0}\right) + \left(1 - \frac{1}{1 - x} - \frac{1}{1 + x}\right) \left(-\frac{14}{5}\zeta_2^2 + 8\mathcal{H}_{-1}\zeta_3 - 8\mathcal{H}_{-1,-1}\zeta_2 \\ -& 16\mathcal{H}_{-1,-1,-1,0} + 8\mathcal{H}_{-1,-1,0,0} - 16\mathcal{H}_{-1,0} + 2\mathcal{H}_{-1,0}\zeta_2 + 8\mathcal{H}_{-1,0,-1,0} - 4\mathcal{H}_{-1,0,0,0} + 16\mathcal{H}_0 \\ -& \frac{14}{3}\mathcal{H}_0\zeta_3 + 4\mathcal{H}_{0,-1}\zeta_2 + 8\mathcal{H}_{0,-1,-1,0} - 4\mathcal{H}_{0,-1,0,0} + 8\mathcal{H}_{0,0} - \mathcal{H}_{0,0}\zeta_2 - 4\mathcal{H}_{0,0,-1,0} \\ +& 2\mathcal{H}_{0,0,0,0}\right) - 2\left(5 - \frac{4}{1 - x} - \frac{4}{1 + x}\right)\zeta_2\right\}.$$

In eq. (A.2) all harmonic polylogarithms $H_{m_1,...,m_w}(x)$, $m_j = 0, \pm 1$ are understood to be of argument x. For the rest, our notation follows ref. [76] to which the reader is referred for a detailed discussion.

Next we present the one-loop result for the virtual contribution to the perturbative fragmentation function to all orders in ϵ [57]:

$$D_1^{\text{virt}}(z) = a_{\text{s}} C_F \frac{2\epsilon^2 - 3\epsilon + 2}{(1 - 2\epsilon)\epsilon} \exp(\epsilon\gamma_{\text{E}}) \Gamma(\epsilon) \left(\frac{\mu^2}{m^2}\right)^{\epsilon} \delta(1 - z).$$
(A.3)

As one can easily verify, the expansion of the coefficient of the delta-function in ϵ coincides to all known powers with the factor $Z_{[q]}^{(1)}$ in eq. (4.2), which suggests that eq. (A.3) is indeed the proper generalization to all orders in ϵ .

Finally, we discuss the derivation of the one-loop heavy quark insertion in the tree-level gluon form factor. It is clear that this diagram coincides with the one loop contribution to $Z_{[g]}^{(1)}$. We find it particularly convenient to evaluate this diagram in a physical light-cone gauge. Following the procedure outlined in refs. [57, 58] we obtain to all orders in ϵ :

$$Z_{[g]}^{(1)} = a_{\rm s} n_h \left(-\frac{2}{3}\right) \exp(\epsilon \gamma_{\rm E}) \Gamma(\epsilon) \left(\frac{\mu^2}{m^2}\right)^{\epsilon}.$$
 (A.4)

Upon expansion in ϵ eq. (4.5) is derived.

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