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NNLO corrections to $\bar{B} \to X_u \ell \bar{\nu}$ in the shape-function region

H. M. Asatrian[(a)], C. Greub[(b)], and B. D. Pecjak[(c)]

[(a)] *Yerevan Physics Institute, 375036 Yerevan, Armenia*

[(b)] *Center for Research and Education in Fundamental Physics, Institute for Theoretical Physics, Univ. Bern, CH-Bern, Switzerland*

[(c)] *Theory Group, Deutsches Elektronen-Synchrotron DESY, D-22603 Hamburg, Germany*

Abstract

The inclusive decay $\bar{B} \to X_u \ell \bar{\nu}$ is of much interest because of its potential to constrain the CKM element $|V_{ub}|$. Experimental cuts required to suppress charm background restrict measurements of this decay to the shape-function region, where the hadronic final state carries a large energy but only a moderate invariant mass. In this kinematic region, the differential decay distributions satisfy a factorization formula of the form $H \cdot J \otimes S$, where S is the non-perturbative shape function, and the object $H \cdot J$ is a perturbatively calculable hard-scattering kernel. In this paper we present the calculation of the hard function H at next-to-next-to-leading order (NNLO) in perturbation theory. Combined with the known NNLO result for the jet function J, this completes the perturbative part of the NNLO calculation for this process.

1 Introduction

The inclusive decay $\bar{B} \to X_u \ell \bar{\nu}$ is of much interest because of its potential to constrain the CKM element $|V_{ub}|$. Due to experimental cuts required to suppress charm background, measurements of this decay are available only in the shape-function region, where the hadronic final state is collimated into a single jet carrying a large energy on the order of m_b, and a moderate invariant mass squared on the order of $m_b \Lambda_{\rm QCD}$. Much theoretical effort has been put into establishing a factorization formalism which enables the calculation of differential decay rates in this kinematic region. Early work in QCD was based on diagrammatic approaches [1, 2], whereas more recent papers [3–5] are based on soft-collinear effective theory (SCET) [6–8]. The main result of these works can be summarized in the following factorization formula for an arbitrary differential decay rate:

$$d\Gamma \sim H \cdot J \otimes S\,, \tag{1}$$

where the symbol $\otimes$ denotes a convolution. The perturbative information is contained in the hard function H, which is related to physics at the hard scale m_b, and the jet function J, which is related to physics at the intermediate scale $m_b \Lambda_{\rm QCD}$. The object S is a non-perturbative shape function describing the internal soft dynamics of the B meson [9, 10]. The factorization formula is valid up to corrections in $\Lambda_{\rm QCD}/m_b$, which have been studied in detail in [11–13]. The hard and jet functions to next-to-leading order (NLO) in perturbation theory have been known for some time [3, 4], and the jet function at next-to-next-to-leading order (NNLO) was obtained in [14].

The main purpose of this paper is to complete the perturbative part of the NNLO corrections to the factorization formula (1) by obtaining the hard function to this order. The organization is as follows. In Section 2, we briefly outline how to obtain the hard function through a matching calculation in SCET. The task is to extract three Wilson coefficients C_i, which arise from integrating out the hard scale m_b by matching the semi-leptonic $b \to u$ transition current from QCD onto SCET. The discussion there makes clear that the principle technical challenge is to calculate the two-loop QCD corrections to the $b \to u$ current. This loop calculation is the subject of Section 3, where we explain our calculational procedure and give explicit results in terms of a set of harmonic polylogarithms. The method relies on a reduction to master integrals through integration-by-parts relations, which are then solved using differential equations. In Section 4, we use our results to obtain the Wilson coefficients C_i at NNLO; a phenomenological analysis of partial decay rates and the impact on the determination of $|V_{ub}|$ is in progress and will be presented in future work. We conclude in Section 5.

2 The hard function in SCET

The QCD effects in inclusive semi-leptonic B decays are contained in the hadronic tensor $W^{\mu\nu}$, from which any differential decay distribution can be derived. It is defined as the discontinuity of the forward matrix element of the current correlator $T^{\mu\nu}$, which is the time-ordered product of two semi-leptonic $b \to u$ currents, $J^\mu = \bar{u}\gamma^\mu(1-\gamma_5)b$:

$$W^{\mu\nu} = \frac{1}{\pi}\,\mathrm{Im}\,\frac{\langle \bar{B}(v)|T^{\mu\nu}|\bar{B}(v)\rangle}{2M_B}\,, \qquad T^{\mu\nu} = i\int d^4x\, e^{iq\cdot x}\,\mathrm{T}\big\{J^{\dagger\mu}(0)J^\nu(x)\big\}\,. \tag{2}$$

Here q is the momentum carried by the lepton pair and v is the velocity of the B meson. Using the SCET formalism it is possible to show that the hadronic tensor obeys the factorization formula

$$W^{\mu\nu} = \sum_{i,j=1}^{3} H_{ij}(\bar{n}\cdot p)\text{tr}\left(\bar{\Gamma}_j \frac{\not{p}_-}{2}\Gamma_i^\nu \frac{1+\not{v}}{2}\right) J\otimes S\,. \tag{3}$$

We have introduced the vector $p \equiv m_b v - q$, which in the parton model is the momentum of the final-state jet into which the b quark decays, as well as its light-cone decomposition,

$$p^\mu = (n\cdot p)\frac{\bar{n}^\mu}{2} + p_\perp^\mu + (\bar{n}\cdot p)\frac{n^\mu}{2} \equiv p_+^\mu + p_-^\mu + p_\perp^\mu\,, \tag{4}$$

where n and $\bar{n}$ are two light-like vectors satisfying $\bar{n}\cdot n = 2$. The object H_{ij} is defined as

$$H_{ij}(\bar{n}\cdot p) = C_i(\bar{n}\cdot p)C_j(\bar{n}\cdot p)\,, \tag{5}$$

where the Wilson coefficients C_i arise from matching the semi-leptonic $b\to u$ current from QCD onto SCET. In position space and to leading order in the heavy-quark limit, this matching is of the form

$$e^{-im_b v\cdot x}\bar{u}(x)\gamma^\mu(1-\gamma_5)b(x) = \sum_{i=1}^{3}\int ds\,\tilde{C}_i(s)\bar{\chi}(x+s\bar{n})\Gamma_i^\mu \mathcal{H}(x_-), \tag{6}$$

where we have followed the SCET conventions of [4]. The Γ_i^μ are a set of three Dirac structures, which we shall choose as

$$\Gamma_1^\mu = \gamma^\mu(1-\gamma_5), \qquad \Gamma_2^\mu = v^\mu(1+\gamma_5), \qquad \Gamma_3^\mu = \frac{n^\mu}{n\cdot v}(1+\gamma_5)\,. \tag{7}$$

In practice, the matching calculation is carried out in momentum space and yields results for the Fourier-transformed coefficients, which read

$$C_i(\bar{n}\cdot p) = \int ds\, e^{is\bar{n}\cdot p}\,\tilde{C}_i(s)\,. \tag{8}$$

The matching coefficients are obtained by evaluating UV-renormalized matrix elements of both sides of (6), corresponding to calculations in full QCD and SCET. The calculation is simplest when the external states are chosen as on-shell quarks and both UV and IR divergences are regulated in dimensional regularization in $d=4-2\epsilon$ dimensions. In that case the loop corrections to the SCET matrix elements are given by scaleless integrals and vanish, so that the result is just its tree-level value multiplied by renormalization factors from operator and wave-function renormalization. The QCD result is written in terms of three Dirac structures multiplied by scalar form factors, which we shall define according to

$$\begin{aligned}\langle u(p)|J^\mu|b(p_b)\rangle &= D_1\bar{u}(p)\gamma^\mu(1-\gamma_5)u(p_b) + D_2\bar{u}(p)\frac{p_b^\mu}{m_b}(1+\gamma_5)u(p_b) \\ &+ D_3\bar{u}(p)\frac{p^\mu}{m_b}(1+\gamma_5)u(p_b)\,,\end{aligned} \tag{9}$$

where $u(p)$ and $u(p_b)$ are on-shell spinor wave functions, p_b and p are the momenta of the b and u quarks respectively, and $p^2 = 0$, $p_b^2 = m_b^2$. We shall always work in the reference frame where the perpendicular components of the external momenta vanish, and where $p_b^\mu = m_b v^\mu$ and $p^\mu = (\bar{n} \cdot p) n^\mu / 2$. Then the three Dirac structures multiplying the D_i correspond to those in (7) in an obvious way.

To determine the Wilson coefficients C_i we also need the SCET matrix element, for which we can make an important simplification. In general, the result involves a renormalization matrix Z_{ij} applied to the bare SCET current operators. However, we can use that the partonic expression for the quantity $J \otimes S$ in the factorization formula (3) for the hadronic tensor is independent of the coefficients H_{ij} that multiply it. This implies that the operator renormalization matrix is just the unit matrix multiplied by a single scalar factor Z_J. Moreover, for on-shell matching the wave function renormalization factors in SCET are unity, and the SCET spinor wave functions correspond to those in QCD. Therefore, the coefficients C_i can be obtained through the relations

$$\begin{aligned} C_i(\bar{n} \cdot p) &= \lim_{\epsilon \to 0} Z_J^{-1}(\epsilon, m_b, \bar{n} \cdot p, \mu) D_i(\epsilon, m_b, \bar{n} \cdot p, \mu) \qquad (i = 1, 2)\,, \\ C_3(\bar{n} \cdot p) &= \lim_{\epsilon \to 0} Z_J^{-1}(\epsilon, m_b, \bar{n} \cdot p, \mu) \frac{p_b \cdot p}{m_b^2} D_3(\epsilon, m_b, \bar{n} \cdot p, \mu)\,. \end{aligned} \tag{10}$$

The renormalization factor Z_J can be determined in two different ways. The first is to require that the matching relation (10) is free of IR poles in dimensional regularization, which allows one to deduce the UV structure of the SCET currents from the IR structure of the D_i. A second method is to determine the UV poles of the object $J \otimes S$ in the parton model, using the two-loop anomalous dimensions for the jet and soft functions, calculated in [14] and [15,16]. Agreement between the two methods is an important check on the factorization formalism, and also on the two-loop calculation of each function. The agreement will be verified in Section 4 below.

We end this section by pointing out a subtlety in the matching calculation related to heavy-quark loops, which first becomes relevant at NNLO. Whereas the partonic matrix elements in QCD are calculated as an expansion in α_s in the $\overline{\text{MS}}$ renormalization scheme in a five-flavor theory, where $n_f = n_l + n_h$ with $n_h = 1$ for the b quark, in SCET b-quark loops are absent and the matrix elements are calculated as an expansion in a four-flavor theory. To match results in the two theories as in (10), it is necessary to express the UV renormalized results in five-flavor QCD in terms of the four-flavor parameters of SCET. To achieve this, one renormalizes the coupling constant in the $n_f = n_h + n_l$ flavor theory according to $\alpha_s^{\text{bare}} = Z_\alpha^{n_h + n_l} \alpha_s$, with (see e.g. [17])

$$Z_\alpha^{n_h + n_l} = 1 - \frac{\alpha_s}{4\pi\epsilon} \left[\frac{11}{3} C_A - \frac{4}{3} T_R n_f + \frac{4}{3} T_R n_h (1 - N_\epsilon) \right]. \tag{11}$$

The function N_ϵ is fixed such that α_s is the $\overline{\text{MS}}$-renormalized coupling in the *four* flavor theory. Its value is

$$N(\epsilon) = e^{\gamma \epsilon} \left(\frac{\mu^2}{m_b^2} \right)^\epsilon \Gamma(1 + \epsilon)\,. \tag{12}$$

Results for the scalar amplitudes D_i in this renormalization scheme can be obtained from those in the $\overline{\text{MS}}$ scheme in five-flavor QCD by making the replacement

$$\alpha_s \to \alpha_s \left(1 + \frac{\alpha_s}{4\pi} \frac{8}{3} T_R n_h \left[L + \epsilon \left(L^2 + \frac{\pi^2}{24} \right) + \epsilon^2 \left(\frac{2L^3}{3} + \frac{\pi^2}{12} L - \frac{\zeta_3}{6} \right) \right] \right) + \dots\,, \tag{13}$$

where $L = \ln \mu/m_b$. After applying this decoupling to the D_i, dependence on n_h in the pole terms, and thus Z_J, drops out. This must be the case, since heavy quark loops do not exist in SCET, where the b quark field is treated as in HQET. This same procedure was used in the completely analogous case of matching the $b \to s$ current at $q^2 = 0$ in [18].

From the above discussion, it is obvious that the main technical obstacle to obtaining the Wilson coefficients C_i is the calculation of the QCD form factors D_i. This will be the subject of the next section.

3 Two-loop QCD corrections to the $b \to u$ current

In this section we perform the calculation of the renormalized scalar form factors D_i at two-loop order. We begin by outlining the calculational procedure in Section 3.1, and then give the final results in Section 3.2.

3.1 Calculational procedure

In this section we describe some technical details involved in obtaining the two-loop QCD corrections to the $b \to u$ current. The main task is to evaluate the bare two-loop amplitude by calculating the Feynman diagrams in Figure 1. This bare amplitude contains both UV and IR divergences. The UV divergences are removed by counterterms related to b and u-quark wave-function renormalization (on-shell scheme), coupling constant renormalization ($\overline{\rm MS}$ scheme), and mass renormalization (on-shell scheme).

The calculation of the individual two-loop Feynman diagrams proceeds as follows. First, by doing tensor decomposition, we extract the contributions of each diagram to the form factors D_i in (9). At this level, these contributions are written as linear combinations of certain scalar integrals. Second, this rather large set of scalar integrals is reduced to a much smaller set of master integrals using the Laporta algorithm [19], which is based on the integration-by-parts identities introduced in [20,21]. A very useful tool for performing this reduction is the integral reduction program AIR [22], written in `Maple`, and we have used this program in our calculation.

A typical master integral depends on m_b, the dimensionless variable $\hat{s} = (p_b - p)^2/m_b^2$, and the parameter $\epsilon = (4-d)/2$ of dimensional regularization. Some of the simpler master integrals (those with three or less propagators), are easily solved using the standard technique of Feynman parameterization. In most cases, it is straightforward to obtain exact results in ϵ, which involve hypergeometric functions or their generalizations. These can be expanded around $\epsilon \to 0$ using the `Mathematica` program `HypExp` [23,24]. For the more difficult master integrals, we have used the differential equation technique [25] (for a recent review, see [26]). This involves solving a set of differential equations obtained by differentiating the master integrals with respect to the variable $\hat{s}$. The solutions to the differential equations determine the master integrals as a Laurent series in ϵ, up to their values at the boundary point $\hat{s} = 0$. In some cases, these constants can be determined by requiring that the coefficients in the Laurent expansion are finite in the limit $\hat{s} \to 0$. In other cases, there is no choice but to calculate the ϵ-expansion of the two-loop master integral at the point $\hat{s} = 0$. The solutions to the differential equations involve the harmonic polylogarithms (HPLs) introduced in [27]. For their numerical implementation and also some symbolic manipulations, we used the `Mathematica` package `HPL` [28].

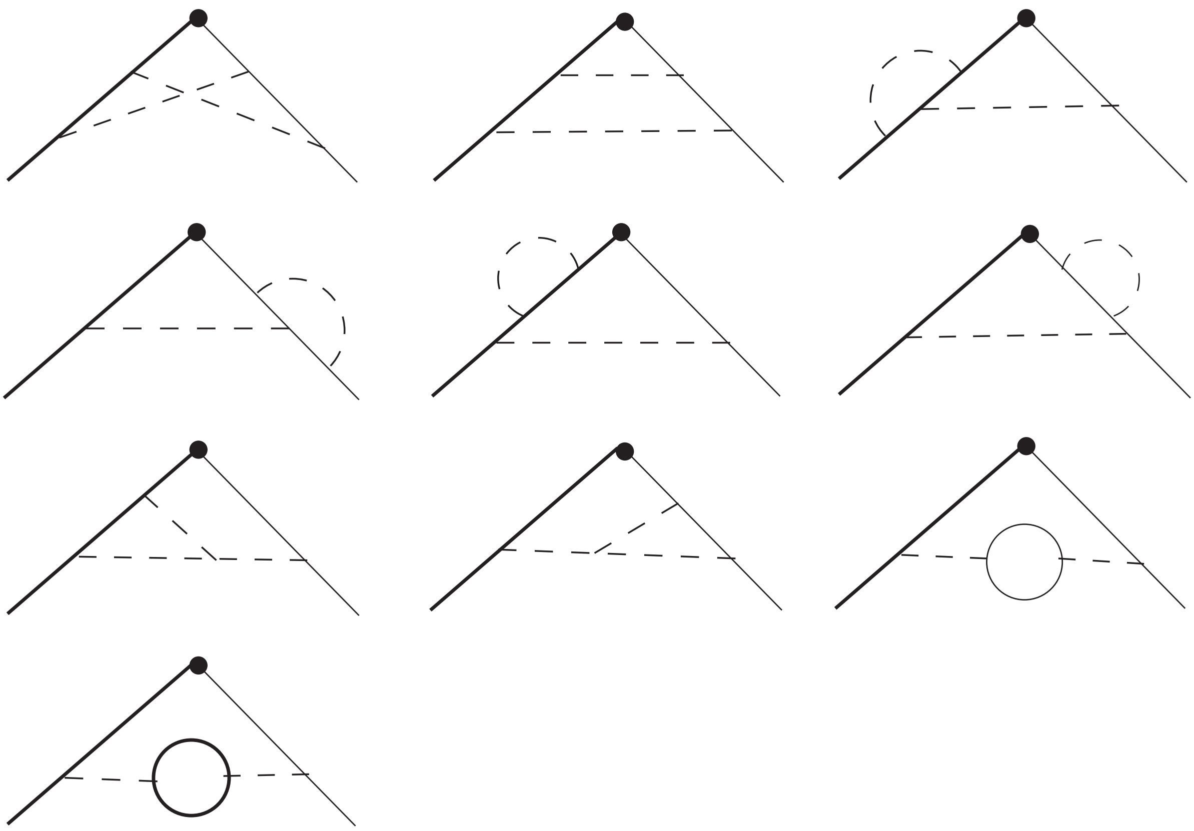

Figure 1: Two-loop corrections to the $b \to u$ left-handed current. The incoming b-quark and the outgoing u-quark are represented by thick and thin solid lines, respectively, while dashed lines represent gluons. Fermionic bubbles with b-quarks and lighter quarks (the latter being treated as massless) are shown by thick and thin circles. Diagrams where the light fermionic bubbles are replaced by gluons and ghost-particles are not shown explicitly, but they are taken into account.

We have checked our results in several ways. First, we have used the numerical method of sector decomposition [29] to evaluate the master integrals for various values of $\hat{s}$, and checked that they agree with the analytic results. For this we have used self-written code, and also the publicly available C++ program described in [30]. Second, we have obtained results as a double series in $\epsilon \to 0$, $\hat{s} \to 0$ using two different techniques. One is to expand each master integral as a series in $\hat{s} \to 0$ before doing the loop integrals using sector decomposition, the other is to obtain results for each diagram at $\hat{s} = 0$ and then recover the $\hat{s}$-dependence using differential equations. We then checked that these agree numerically with the expansion of the analytic results in the same limit, up to the first five or six terms around $\hat{s} \to 0$. Finally, we were able to transform our basis of master integrals into that used for the two-loop calculation of the vertex corrections in $B \to \pi\pi$, presented in [31, 32]. For some of the master integrals, we used these results to help convert numerical results for the boundary conditions into analytic results in terms of constants like π.

To illustrate the method of differential equations in our application, we take as an example the first diagram in the second row in Figure 1. In this case we have four master integrals h_1, h_2 , h_3 and h_4, reading

$$\begin{aligned} h_1(\hat{s}) &= \int \frac{d^d\ell}{(2\pi)^d} \frac{d^d r}{(2\pi)^d} \frac{1}{[(\ell+p_b)^2-m_b^2]\,[(l+r+p)^2]\,[(r+p)^2]}\,, \\ h_2(\hat{s}) &= \int \frac{d^d\ell}{(2\pi)^d} \frac{d^d r}{(2\pi)^d} \frac{1}{[(\ell+p_b)^2-m_b^2]\,[(\ell+p)^2]\,[(l+r+p)^2]\,[(r+p)^2]}\,, \\ h_3(\hat{s}) &= \int \frac{d^d\ell}{(2\pi)^d} \frac{d^d r}{(2\pi)^d} \frac{1}{[(\ell+p_b)^2-m_b^2]\,[r^2]\,[(l+r+p)^2]}\,, \\ h_4(\hat{s}) &= \int \frac{d^d\ell}{(2\pi)^d} \frac{d^d r}{(2\pi)^d} \frac{1}{[(\ell+p_b)^2-m_b^2]\,[r^2]\,[(\ell+p)^2]\,[(l+r+p)^2]}\,. \end{aligned} \quad (14)$$

They satisfy the differential equations

$$\begin{aligned} \frac{dh_1(\hat{s})}{d\hat{s}} &= 0\,, \\ \frac{dh_2(\hat{s})}{d\hat{s}} &= -\frac{1}{4}\frac{(4d+4d\hat{s}-16\hat{s}-12)}{\hat{s}(1-\hat{s})}\,h_2(\hat{s}) - \frac{1}{4}\frac{(-3d+8)}{m_b^2\,\hat{s}(1-\hat{s})}\,h_1(\hat{s})\,, \\ \frac{dh_3(\hat{s})}{d\hat{s}} &= \frac{1}{4}\frac{(d-4)}{\hat{s}}\,h_3(\hat{s}) - \frac{1}{4}\frac{m_b^2\,(1-\hat{s})(d-4)}{\hat{s}}\,h_4(\hat{s})\,, \\ \frac{dh_4(\hat{s})}{d\hat{s}} &= -\frac{1}{4}\frac{(3d+5d\hat{s}-8-20\hat{s})}{\hat{s}(1-\hat{s})}\,h_4(\hat{s}) - \frac{1}{4}\frac{(-3d+8)}{m_b^2\,\hat{s}(1-\hat{s})}\,h_3(\hat{s})\,. \end{aligned} \quad (15)$$

Obviously, h_1 has to be calculated using the standard technique of Feynman parameterization. The dependence of h_2 on $\hat{s}$ can then be determined by solving the second differential equation, in which h_1 plays the role of a given inhomogeneity. The requirement that h_2 is non-singular for $\hat{s} \to 0$ uniquely determines the function $h_2(\hat{s})$. The $\hat{s}$ dependence of the functions h_3 and h_4 can be obtained by solving the corresponding two differential equations simultaneously (as an expansion in ϵ). Specifying $h_3(\hat{s}=0)$ by means of standard Feynman parameterization and imposing the additional requirement that $h_4(\hat{s})$ is non-singular for $\hat{s} \to 0$, uniquely determines $h_3(\hat{s})$ and $h_4(\hat{s})$.

3.2 Renormalized scalar form factors

We now give results for the UV-renormalized form factors in (9), which we expand in α_s according to

$$D_i = \delta_{i1} + \frac{\alpha_s}{4\pi}\,D_i^{(1)} + \left(\frac{\alpha_s}{4\pi}\right)^2 D_i^{(2)} + \ldots\,.$$

We start by listing the results of the one-loop contributions. To this end we further decompose the quantities $D_i^{(1)}$ as

$$D_i^{(1)} = C_F\left[\frac{R^{(1)}_{(-2),i}}{\epsilon^2} + \frac{R^{(1)}_{(-1),i}}{\epsilon} + R^{(1)}_{(0),i} + R^{(1)}_{(1),i}\epsilon + R^{(1)}_{(2),i}\epsilon^2\right]\,. \quad (16)$$

The Laurent expansion coefficients of the poles and constant term have been known for some time [7], whereas the terms proportional to ϵ and ϵ^2 are new. Note that terms up to ϵ^2 are needed to correctly extract the Wilson coefficients C_i through (10). The explicit results for the $R^{(i)}$ in (16) read (recall $\hat{s} = (p_b - p)^2/m_b^2$)

$$
\begin{aligned}
R^{(1)}_{(-2),1} &= -1 \\
R^{(1)}_{(-1),1} &= -\frac{5}{2} - 2L - 2F_4 \\
R^{(1)}_{(0),1} &= -6 - 5L - 2L^2 - \frac{\pi^2}{12} - 3F_4 - 4LF_4 + \frac{F_4}{\hat{s}} - 2F_5 - 4F_{10} \\
R^{(1)}_{(1),1} &= -12 - 12L - 5L^2 - \frac{4L^3}{3} - \frac{5\pi^2}{24} - \frac{L\pi^2}{6} - 8F_4 - 6LF_4 - 4L^2F_4 - \frac{\pi^2 F_4}{6} + \\
&\quad \frac{4F_4}{\hat{s}} + \frac{2LF_4}{\hat{s}} - 3F_5 - 4LF_5 + \frac{F_5}{\hat{s}} - 2F_6 - 6F_{10} - 8LF_{10} + \frac{2F_{10}}{\hat{s}} - 4F_{11} - \\
&\quad 4F_{13} - 8F_{17} + \frac{\zeta(3)}{3} \\
R^{(1)}_{(2),1} &= -24 - 24L - 12L^2 - \frac{10L^3}{3} - \frac{2L^4}{3} - \frac{\pi^2}{2} - \frac{5L\pi^2}{12} - \frac{L^2\pi^2}{6} - \frac{\pi^4}{160} - 16F_4 - \\
&\quad 16LF_4 - 6L^2F_4 - \frac{8L^3F_4}{3} - \frac{\pi^2 F_4}{4} - \frac{1}{3}L\pi^2F_4 + \frac{8F_4}{\hat{s}} + \frac{8LF_4}{\hat{s}} + \frac{2L^2F_4}{\hat{s}} + \\
&\quad \frac{\pi^2 F_4}{12\hat{s}} - 8F_5 - 6LF_5 - 4L^2F_5 - \frac{\pi^2 F_5}{6} + \frac{4F_5}{\hat{s}} + \frac{2LF_5}{\hat{s}} - 3F_6 - 4LF_6 + \\
&\quad \frac{F_6}{\hat{s}} - 2F_7 - 16F_{10} - 12LF_{10} - 8L^2F_{10} - \frac{\pi^2 F_{10}}{3} + \frac{8F_{10}}{\hat{s}} + \frac{4LF_{10}}{\hat{s}} - 6F_{11} - \\
&\quad 8LF_{11} + \frac{2F_{11}}{\hat{s}} - 4F_{12} - 6F_{13} - 8LF_{13} + \frac{2F_{13}}{\hat{s}} - 4F_{14} - 4F_{15} - 12F_{17} - \\
&\quad 16LF_{17} + \frac{4F_{17}}{\hat{s}} - 8F_{18} - 8F_{19} - 8F_{20} - 16F_{21} + \frac{5\zeta(3)}{6} + \frac{2}{3}L\zeta(3) + \frac{2}{3}F_4\zeta(3)
\end{aligned}
$$

$$
\begin{aligned}
R^{(1)}_{(-2),2} &= R^{(1)}_{(-1),2} = 0 \\
R^{(1)}_{(0),2} &= \frac{2}{\hat{s}} - \frac{2F_4}{\hat{s}^2} + \frac{2F_4}{\hat{s}} \\
R^{(1)}_{(1),2} &= \frac{4}{\hat{s}} + \frac{4L}{\hat{s}} - \frac{2F_4}{\hat{s}^2} - \frac{4LF_4}{\hat{s}^2} + \frac{2F_4}{\hat{s}} + \frac{4LF_4}{\hat{s}} - \frac{2F_5}{\hat{s}^2} + \frac{2F_5}{\hat{s}} - \frac{4F_{10}}{\hat{s}^2} + \frac{4F_{10}}{\hat{s}} \\
R^{(1)}_{(2),2} &= \frac{8}{\hat{s}} + \frac{8L}{\hat{s}} + \frac{4L^2}{\hat{s}} + \frac{\pi^2}{6\hat{s}} - \frac{4F_4}{\hat{s}^2} - \frac{4LF_4}{\hat{s}^2} - \frac{4L^2F_4}{\hat{s}^2} - \frac{\pi^2F_4}{6\hat{s}^2} + \frac{4F_4}{\hat{s}} + \frac{4LF_4}{\hat{s}} + \\
&\quad \frac{4L^2F_4}{\hat{s}} + \frac{\pi^2F_4}{6\hat{s}} - \frac{2F_5}{\hat{s}^2} - \frac{4LF_5}{\hat{s}^2} + \frac{2F_5}{\hat{s}} + \frac{4LF_5}{\hat{s}} - \frac{2F_6}{\hat{s}^2} + \frac{2F_6}{\hat{s}} - \frac{4F_{10}}{\hat{s}^2} - \\
&\quad \frac{8LF_{10}}{\hat{s}^2} + \frac{4F_{10}}{\hat{s}} + \frac{8LF_{10}}{\hat{s}} - \frac{4F_{11}}{\hat{s}^2} + \frac{4F_{11}}{\hat{s}} - \frac{4F_{13}}{\hat{s}^2} + \frac{4F_{13}}{\hat{s}} - \frac{8F_{17}}{\hat{s}^2} + \frac{8F_{17}}{\hat{s}}
\end{aligned}
$$

$$
\begin{aligned}
R^{(1)}_{(-2),3} &= R^{(1)}_{(-1),3} = 0 \\
R^{(1)}_{(0),3} &= -\frac{2}{\hat{s}} + \frac{2F_4}{\hat{s}^2} - \frac{4F_4}{\hat{s}} \\
R^{(1)}_{(1),3} &= -\frac{4}{\hat{s}} - \frac{4L}{\hat{s}} + \frac{2F_4}{\hat{s}^2} + \frac{4LF_4}{\hat{s}^2} - \frac{10F_4}{\hat{s}} - \frac{8LF_4}{\hat{s}} + \frac{2F_5}{\hat{s}^2} - \frac{4F_5}{\hat{s}} + \frac{4F_{10}}{\hat{s}^2} - \frac{8F_{10}}{\hat{s}} \\
R^{(1)}_{(2),3} &= -\frac{8}{\hat{s}} - \frac{8L}{\hat{s}} - \frac{4L^2}{\hat{s}} - \frac{\pi^2}{6\hat{s}} + \frac{4F_4}{\hat{s}^2} + \frac{4LF_4}{\hat{s}^2} + \frac{4L^2F_4}{\hat{s}^2} + \frac{\pi^2F_4}{6\hat{s}^2} - \frac{20F_4}{\hat{s}} - \frac{20LF_4}{\hat{s}} - \\
&\quad \frac{8L^2F_4}{\hat{s}} - \frac{\pi^2F_4}{3\hat{s}} + \frac{2F_5}{\hat{s}^2} + \frac{4LF_5}{\hat{s}^2} - \frac{10F_5}{\hat{s}} - \frac{8LF_5}{\hat{s}} + \frac{2F_6}{\hat{s}^2} - \frac{4F_6}{\hat{s}} + \frac{4F_{10}}{\hat{s}^2} + \\
&\quad \frac{8LF_{10}}{\hat{s}^2} - \frac{20F_{10}}{\hat{s}} - \frac{16LF_{10}}{\hat{s}} + \frac{4F_{11}}{\hat{s}^2} - \frac{8F_{11}}{\hat{s}} + \frac{4F_{13}}{\hat{s}^2} - \frac{8F_{13}}{\hat{s}} + \frac{8F_{17}}{\hat{s}^2} - \frac{16F_{17}}{\hat{s}}
\end{aligned}
$$

In these equations $L = \ln \mu/m_b$, while the quantities $F_1, \ldots, F_{21}$ denote the following harmonic polylogarithms:

$$
\begin{aligned}
F = \quad & [\mathrm{HPL}(\{-2\},\hat{s}), \mathrm{HPL}(\{-1\},1-\hat{s}), \mathrm{HPL}(\{-1\},\hat{s}), \mathrm{HPL}(\{1\},\hat{s}), \mathrm{HPL}(\{2\},\hat{s}), \\
& \mathrm{HPL}(\{3\},\hat{s}), \mathrm{HPL}(\{4\},\hat{s}), \mathrm{HPL}(\{-2,2\},\hat{s}), \mathrm{HPL}(\{-1,2\},\hat{s}), \mathrm{HPL}(\{1,1\},\hat{s}), \\
& \mathrm{HPL}(\{1,2\},\hat{s}), \mathrm{HPL}(\{1,3\},\hat{s}), \mathrm{HPL}(\{2,1\},\hat{s}), \mathrm{HPL}(\{2,2\},\hat{s}), \mathrm{HPL}(\{3,1\},\hat{s}), \\
& \mathrm{HPL}(\{-1,0,0\},1-\hat{s}), \mathrm{HPL}(\{1,1,1\},\hat{s}), \mathrm{HPL}(\{1,1,2\},\hat{s}), \mathrm{HPL}(\{1,2,1\},\hat{s}), \\
& \mathrm{HPL}(\{2,1,1\},\hat{s}), \mathrm{HPL}(\{1,1,1,1\},\hat{s})] \; . \qquad (17)
\end{aligned}
$$

We now turn to the order α_s^2 contributions $D_i^{(2)}$, which we decompose according to

$$
D_i^{(2)} = C_F \left[\frac{R^{(2)}_{(-4),i}}{\epsilon^4} + \frac{R^{(2)}_{(-3),i}}{\epsilon^3} + \frac{R^{(2)}_{(-2),i}}{\epsilon^2} + \frac{R^{(2)}_{(-1),i}}{\epsilon} + R^{(2)}_{(0),i} \right] . \qquad (18)
$$

The (infrared) singular pieces yield relatively compact expressions. We find

$$
\begin{aligned}
R^{(2)}_{(-4),1} &= \frac{C_F}{2} \\
R^{(2)}_{(-3),1} &= C_F \left(\frac{5}{2} + 2L + 2F_4 \right) + \frac{11C_A}{4} - n_l T_R \\
R^{(2)}_{(-2),1} &= C_F \left(\frac{73}{8} + 10L + 4L^2 + \frac{\pi^2}{12} + 8F_4 + 8LF_4 - \frac{F_4}{\hat{s}} + 2F_5 + 8F_{10} \right) + \\
&\quad C_A \left(\frac{49}{18} + \frac{11L}{3} + \frac{\pi^2}{12} + \frac{11F_4}{3} \right) + \frac{8}{3} L n_h T_R + \left(-\frac{10}{9} - \frac{4L}{3} - \frac{4F_4}{3} \right) n_l T_R \\
R^{(2)}_{(-1),1} &= C_F \left(\frac{213}{8} - \frac{19\zeta(3)}{3} + \frac{73L}{2} + 20L^2 + \frac{16L^3}{3} + \frac{11\pi^2}{12} + \frac{L\pi^2}{3} + \frac{55F_4}{2} + 32LF_4 + \right. \\
&\quad 16L^2F_4 + \frac{\pi^2F_4}{3} - \frac{13F_4}{2\hat{s}} - \frac{4LF_4}{\hat{s}} + 8F_5 + 8LF_5 - \frac{F_5}{\hat{s}} + 2F_6 + 28F_{10} + \\
&\quad \left. 32LF_{10} - \frac{6F_{10}}{\hat{s}} + 8F_{11} + 12F_{13} + 32F_{17} \right) + C_A \left(-\frac{1549}{216} + \frac{11\zeta(3)}{2} - \frac{67L}{9} - \right. \\
&\quad \left. \frac{7\pi^2}{24} + \frac{L\pi^2}{3} - \frac{67F_4}{9} + \frac{\pi^2F_4}{3} \right) + \left(\frac{20L}{3} + 8L^2 + \frac{\pi^2}{9} + \frac{16LF_4}{3} \right) n_h T_R + \\
&\quad \left(\frac{125}{54} + \frac{20L}{9} + \frac{\pi^2}{6} + \frac{20F_4}{9} \right) n_l T_R
\end{aligned}
$$

$$
\begin{aligned}
R^{(2)}_{(-4),2} &= R^{(2)}_{(-3),2} = 0 \\
R^{(2)}_{(-2),2} &= C_F\left(-\frac{2}{\hat{s}} + \frac{2F_4}{\hat{s}^2} - \frac{2F_4}{\hat{s}}\right) \\
R^{(2)}_{(-1),2} &= C_F\left(-\frac{9}{\hat{s}} - \frac{8L}{\hat{s}} + \frac{7F_4}{\hat{s}^2} + \frac{8LF_4}{\hat{s}^2} - \frac{11F_4}{\hat{s}} - \frac{8LF_4}{\hat{s}} + \frac{2F_5}{\hat{s}^2} - \frac{2F_5}{\hat{s}} + \frac{12F_{10}}{\hat{s}^2} - \frac{12F_{10}}{\hat{s}}\right)
\end{aligned}
$$

$$
\begin{aligned}
R^{(2)}_{(-4),3} &= R^{(2)}_{(-3),3} = 0 \\
R^{(2)}_{(-2),3} &= C_F\left(\frac{2}{\hat{s}} - \frac{2F_4}{\hat{s}^2} + \frac{4F_4}{\hat{s}}\right) \\
R^{(2)}_{(-1),3} &= C_F\left(\frac{9}{\hat{s}} + \frac{8L}{\hat{s}} - \frac{7F_4}{\hat{s}^2} - \frac{8LF_4}{\hat{s}^2} + \frac{24F_4}{\hat{s}} + \frac{16LF_4}{\hat{s}} - \frac{2F_5}{\hat{s}^2} + \frac{4F_5}{\hat{s}} - \frac{12F_{10}}{\hat{s}^2} + \frac{24F_{10}}{\hat{s}}\right) .
\end{aligned}
$$

On the other hand, the expressions for the infrared finite parts $R^{(2)}_{(0),i}$ are rather lengthy. It is convenient to further decompose them according to

$$
R^{(2)}_{(0),i} = \sum_{j,k} \frac{C_F f^{\mathrm{a}}_{i,j,k} + C_A f^{\mathrm{na}}_{i,j,k} + n_l T_R f^{\mathrm{nl}}_{i,j,k} + n_h T_R f^{\mathrm{nh}}_{i,j,k}}{\hat{s}^j (1-\hat{s})^k} .
$$

In the following we list the functions $f^{\mathrm{a}}_{i,j,k}$, $f^{\mathrm{na}}_{i,j,k}$, $f^{\mathrm{nl}}_{i,j,k}$ and $f^{\mathrm{nh}}_{i,j,k}$, $(i = 1,2,3)$ for all values j,k for which they are nonzero. We find

$$
\begin{aligned}
f^a_{1,0,0} &= \frac{1327}{16} + \frac{16\zeta(3)}{3} + \frac{213L}{2} - \frac{76\zeta(3)L}{3} + 73L^2 + \frac{80L^3}{3} + \frac{16L^4}{3} + \frac{97\pi^2}{48} - 4\ln(2)\pi^2 + \\
&\quad \frac{11L\pi^2}{3} + \frac{2L^2\pi^2}{3} - \frac{449\pi^4}{720} - \frac{4\pi^2 F_1}{3} + \frac{10\pi^2 F_3}{3} + \frac{153F_4}{2} - \frac{28\zeta(3)F_4}{3} + 110LF_4 + \\
&\quad 64L^2F_4 + \frac{64L^3F_4}{3} + \frac{10\pi^2F_4}{3} + \frac{4}{3}L\pi^2F_4 - \frac{19F_5}{2} + 32LF_5 + 16L^2F_5 + \frac{\pi^2F_5}{3} - \\
&\quad 12F_6 + 8LF_6 - 6F_7 - 16F_8 + 40F_9 + 59F_{10} + 112LF_{10} + 64L^2F_{10} + \frac{4\pi^2F_{10}}{3} + \\
&\quad 28F_{11} + 32LF_{11} - 8F_{12} + 60F_{13} + 48LF_{13} + 12F_{14} + 12F_{15} + 104F_{17} + 128LF_{17} + \\
&\quad 32F_{18} + 48F_{19} + 56F_{20} + 128F_{21} \\
f^a_{1,1,0} &= \frac{2\pi^2F_3}{3} - \frac{49F_4}{2} - 26LF_4 - 8L^2F_4 + \frac{5\pi^2F_4}{6} - \frac{15F_5}{2} - 4LF_5 + F_6 + 8F_9 - \\
&\quad 25F_{10} - 24LF_{10} - 4F_{11} - 10F_{13} - 28F_{17} \\
f^a_{1,0,1} &= -30\zeta(3) + \frac{28\pi^2}{3} + 16\ln(2)\pi^2 + \frac{3\pi^4}{5} + \pi^2F_2 - \frac{20\pi^2F_3}{3} + \frac{28\pi^2F_4}{3} + 90F_5 - \\
&\quad 4\pi^2F_5 + 12F_6 + 8F_7 - 80F_9 + 50F_{10} + 24F_{11} - 78F_{13} - 8F_{14} + 16F_{15} + 2F_{16} \\
f^a_{1,0,2} &= -\frac{59\pi^2}{3} - \frac{277\pi^4}{90} - \frac{8\pi^2F_1}{3} + \frac{8\pi^2F_3}{3} - \frac{68\pi^2F_4}{3} - 50F_5 + \frac{62\pi^2F_5}{3} + 24F_6 - \\
&\quad 20F_7 - 32F_8 + 32F_9 - 56F_{11} + 112F_{13} + 52F_{14} - 104F_{15} \\
f^a_{1,0,3} &= \frac{152\pi^4}{45} + \frac{8\pi^2F_1}{3} - 3\pi^2F_2 - \frac{68\pi^2F_5}{3} + 6F_6 + 24F_7 + 32F_8 - 6F_{13} - 56F_{14} + \\
&\quad 112F_{15} - 6F_{16}
\end{aligned}
$$

$$
\begin{aligned}
f^{na}_{1,0,0} &= -\frac{89437}{1296}+\frac{19\zeta(3)}{18}-\frac{3925L}{54}+22\zeta(3)L-\frac{299L^2}{9}-\frac{44L^3}{9}-\frac{815\pi^2}{216}+2\ln(2)\pi^2- \\
&\quad \frac{16L\pi^2}{9}+\frac{2L^2\pi^2}{3}+\frac{31\pi^4}{120}+\frac{2\pi^2F_1}{3}-\frac{5\pi^2F_3}{3}-\frac{2545F_4}{54}+14\zeta(3)F_4-\frac{466LF_4}{9}- \\
&\quad \frac{44L^2F_4}{3}-\frac{28\pi^2F_4}{9}+\frac{4}{3}L\pi^2F_4-\frac{116F_5}{9}-\frac{44LF_5}{3}+\frac{4\pi^2F_5}{3}+\frac{20F_6}{3}+8F_8- \\
&\quad 20F_9-\frac{349F_{10}}{9}-\frac{88LF_{10}}{3}+\frac{4\pi^2F_{10}}{3}-\frac{44F_{11}}{3}+8F_{12}-\frac{62F_{13}}{3}-\frac{88F_{17}}{3} \\
f^{na}_{1,1,0} &= -\frac{1}{3}\pi^2F_3+\frac{269F_4}{18}+\frac{22LF_4}{3}-\frac{2\pi^2F_4}{3}+\frac{11F_5}{3}-4F_9+\frac{13F_{10}}{3} \\
f^{na}_{1,0,1} &= 15\zeta(3)+13\pi^2-8\ln(2)\pi^2+\frac{3\pi^4}{5}-\frac{\pi^2F_2}{2}+\frac{10\pi^2F_3}{3}+\frac{47\pi^2F_4}{6}+12F_5- \\
&\quad 4\pi^2F_5-31F_6+8F_7+40F_9+17F_{10}+13F_{11}-11F_{13}-8F_{14}+16F_{15}-F_{16} \\
f^{na}_{1,0,2} &= -\frac{67\pi^2}{6}-\frac{86\pi^4}{45}+\frac{4\pi^2F_1}{3}-\frac{4\pi^2F_3}{3}-\frac{29\pi^2F_4}{3}-17F_5+\frac{38\pi^2F_5}{3}+30F_6- \\
&\quad 36F_7+16F_8-16F_9-14F_{11}+28F_{13}+20F_{14}-40F_{15} \\
f^{na}_{1,0,3} &= \frac{263\pi^4}{180}-\frac{4\pi^2F_1}{3}+\frac{3\pi^2F_2}{2}-\frac{29\pi^2F_5}{3}-3F_6+30F_7-16F_8+3F_{13}-14F_{14}+ \\
&\quad 28F_{15}+3F_{16}
\end{aligned}
$$

$$
\begin{aligned}
f^{nl}_{1,0,0} &= \frac{6629}{324}+\frac{26\zeta(3)}{9}+\frac{682L}{27}+\frac{100L^2}{9}+\frac{16L^3}{9}+\frac{85\pi^2}{54}+\frac{8L\pi^2}{9}+\frac{418F_4}{27}+ \\
&\quad \frac{152LF_4}{9}+\frac{16L^2F_4}{3}+\frac{8\pi^2F_4}{9}+\frac{76F_5}{9}+\frac{16LF_5}{3}+\frac{8F_6}{3}+\frac{152F_{10}}{9}+\frac{32LF_{10}}{3}+ \\
&\quad \frac{16F_{11}}{3}+\frac{16F_{13}}{3}+\frac{32F_{17}}{3} \\
f^{nl}_{1,1,0} &= -\frac{38F_4}{9}-\frac{8LF_4}{3}-\frac{4F_5}{3}-\frac{8F_{10}}{3}
\end{aligned}
$$

$$
\begin{aligned}
f^{nh}_{1,0,0} &= \frac{7951}{162}-\frac{28\zeta(3)}{9}+16L+20L^2+\frac{112L^3}{9}-\frac{41\pi^2}{54}+\frac{2L\pi^2}{3}+\frac{530F_4}{27}+8LF_4+ \\
&\quad 16L^2F_4+\frac{2\pi^2F_4}{9}-\frac{76F_5}{9}+\frac{16LF_5}{3}+\frac{8F_6}{3}+\frac{32LF_{10}}{3} \\
f^{nh}_{1,1,0} &= -\frac{38F_4}{9}-\frac{8LF_4}{3}-\frac{4F_5}{3} \\
f^{nh}_{1,0,1} &= -\frac{508}{9}-\frac{64\pi^2}{9}-\frac{440F_4}{9}+\frac{104F_5}{3} \\
f^{nh}_{1,0,2} &= \frac{128}{9}+16\zeta(3)+\frac{32\pi^2}{3}+\frac{128F_4}{9}-48F_5-16F_6 \\
f^{nh}_{1,0,3} &= -16\zeta(3)-\frac{64\pi^2}{27}+\frac{128F_5}{9}+16F_6
\end{aligned}
$$

$$
\begin{aligned}
f^{a}_{2,1,0} &= -31 - 36L - 16L^2 + 3\pi^2 + \frac{4\pi^2 F_3}{3} - 24F_4 - 44LF_4 - 16L^2F_4 - \frac{19\pi^2 F_4}{3} + \\
&\quad 23F_5 - 8LF_5 + 18F_6 + 16F_9 + 50F_{10} - 48LF_{10} - 24F_{11} + 12F_{13} - 56F_{17} \\
f^{a}_{2,2,0} &= -\frac{4}{3}\pi^2 F_3 + 16F_4 + 28LF_4 + 16L^2F_4 - \frac{5\pi^2 F_4}{3} + 13F_5 + 8LF_5 - 2F_6 - 16F_9 - \\
&\quad 2F_{10} + 48LF_{10} + 8F_{11} + 20F_{13} + 56F_{17} \\
f^{a}_{2,3,0} &= 8F_{10} \\
f^{a}_{2,0,1} &= -4\zeta(3) + \frac{28\pi^2}{3} - 2\pi^2 F_2 + \frac{8\pi^2 F_3}{3} - \frac{20\pi^2 F_4}{3} + 44F_5 + 32F_9 + 100F_{10} - \\
&\quad 24F_{11} + 44F_{13} - 4F_{16} \\
f^{a}_{2,0,2} &= 32\zeta(3) - \frac{118\pi^2}{3} - \frac{12\pi^4}{5} - 8\pi^2 F_2 + \frac{16\pi^2 F_3}{3} - \frac{136\pi^2 F_4}{3} - 100F_5 + 16\pi^2 F_5 + \\
&\quad 32F_6 - 32F_7 + 64F_9 - 112F_{11} + 208F_{13} + 32F_{14} - 64F_{15} - 16F_{16} \\
f^{a}_{2,0,3} &= \frac{304\pi^4}{45} + \frac{16\pi^2 F_1}{3} - 6\pi^2 F_2 - \frac{136\pi^2 F_5}{3} + 12F_6 + 48F_7 + 64F_8 - 12F_{13} - \\
&\quad 112F_{14} + 224F_{15} - 12F_{16}
\end{aligned}
$$

$$
\begin{aligned}
f^{na}_{2,1,0} &= \frac{269}{9} + \frac{44L}{3} - 2\pi^2 - \frac{2\pi^2 F_3}{3} + \frac{257F_4}{9} + \frac{44LF_4}{3} - \frac{10\pi^2 F_4}{3} + \frac{46F_5}{3} + 4F_6 - 8F_9 + \\
&\quad \frac{86F_{10}}{3} - 4F_{11} + 8F_{13} \\
f^{na}_{2,2,0} &= \frac{2\pi^2 F_3}{3} - \frac{203F_4}{9} - \frac{44LF_4}{3} + \frac{4\pi^2 F_4}{3} - \frac{22F_5}{3} + 8F_9 - \frac{26F_{10}}{3} \\
f^{na}_{2,0,1} &= 2\zeta(3) + \frac{2\pi^2}{3} + \pi^2 F_2 - \frac{4\pi^2 F_3}{3} - \frac{5\pi^2 F_4}{3} + 32F_5 + 10F_6 - 16F_9 + 34F_{10} + \\
&\quad 2F_{11} - 2F_{13} + 2F_{16} \\
f^{na}_{2,0,2} &= -16\zeta(3) - \frac{67\pi^2}{3} - \frac{6\pi^4}{5} + 4\pi^2 F_2 - \frac{8\pi^2 F_3}{3} - \frac{58\pi^2 F_4}{3} - 34F_5 + 8\pi^2 F_5 + \\
&\quad 68F_6 - 16F_7 - 32F_9 - 28F_{11} + 64F_{13} + 16F_{14} - 32F_{15} + 8F_{16} \\
f^{na}_{2,0,3} &= \frac{263\pi^4}{90} - \frac{8\pi^2 F_1}{3} + 3\pi^2 F_2 - \frac{58\pi^2 F_5}{3} - 6F_6 + 60F_7 - 32F_8 + 6F_{13} - 28F_{14} + \\
&\quad 56F_{15} + 6F_{16}
\end{aligned}
$$

$$
\begin{aligned}
f^{nl}_{2,1,0} &= -\frac{76}{9} - \frac{16L}{3} - \frac{52F_4}{9} - \frac{16LF_4}{3} - \frac{8F_5}{3} - \frac{16F_{10}}{3} \\
f^{nl}_{2,2,0} &= \frac{52F_4}{9} + \frac{16LF_4}{3} + \frac{8F_5}{3} + \frac{16F_{10}}{3}
\end{aligned}
$$

$$
\begin{aligned}
f^{nh}_{2,1,0} &= -\frac{76}{9} - \frac{16L}{3} - \frac{292F_4}{9} - \frac{16LF_4}{3} - \frac{8F_5}{3} \\
f^{nh}_{2,2,0} &= \frac{52F_4}{9} + \frac{16LF_4}{3} + \frac{8F_5}{3} \\
f^{nh}_{2,0,1} &= -\frac{104}{3} + \frac{32\pi^2}{9} - \frac{80F_4}{3} - \frac{16F_5}{3} \\
f^{nh}_{2,0,2} &= \frac{64\pi^2}{9} - \frac{32F_5}{3} \\
f^{nh}_{2,0,3} &= -32\zeta(3) + 32F_6
\end{aligned}
$$

$$
\begin{aligned}
f^{a}_{3,1,0} &= 31+36L+16L^2-3\pi^2-\frac{8\pi^2F_3}{3}+75F_4+96LF_4+32L^2F_4+\frac{14\pi^2F_4}{3}- \\
&\quad 12F_5+16LF_5-20F_6-32F_9+96LF_{10}+32F_{11}+8F_{13}+112F_{17} \\
f^{a}_{3,2,0} &= \frac{4\pi^2F_3}{3}-16F_4-28LF_4-16L^2F_4+\frac{5\pi^2F_4}{3}-13F_5-8LF_5+2F_6+16F_9+ \\
&\quad 2F_{10}-48LF_{10}-8F_{11}-20F_{13}-56F_{17} \\
f^{a}_{3,3,0} &= -8F_{10} \\
f^{a}_{3,0,1} &= -40\zeta(3)-\frac{16\pi^2}{3}+16\ln(2)\pi^2+4\pi^2F_2-\frac{16\pi^2F_3}{3}-4F_4+\frac{28\pi^2F_4}{3}+12F_5- \\
&\quad 8F_6-64F_9-48F_{10}+8F_{11}-56F_{13}+8F_{16} \\
f^{a}_{3,0,2} &= 12\zeta(3)-\frac{248\pi^2}{3}-\frac{12\pi^4}{5}+6\pi^2F_2+\frac{8\pi^2F_3}{3}-\frac{116\pi^2F_4}{3}-284F_5+16\pi^2F_5+ \\
&\quad 32F_6-32F_7+32F_9-300F_{10}-88F_{11}+188F_{13}+32F_{14}-64F_{15}+12F_{16} \\
f^{a}_{3,0,3} &= -64\zeta(3)+118\pi^2+\frac{716\pi^4}{45}+\frac{32\pi^2F_1}{3}+16\pi^2F_2-16\pi^2F_3+136\pi^2F_4+ \\
&\quad 300F_5-\frac{320\pi^2F_5}{3}-112F_6+128F_7+128F_8-192F_9+336F_{11}- \\
&\quad 640F_{13}-256F_{14}+512F_{15}+32F_{16} \\
f^{a}_{3,0,4} &= -\frac{304\pi^4}{15}-16\pi^2F_1+18\pi^2F_2+136\pi^2F_5-36F_6-144F_7-192F_8+36F_{13}+ \\
&\quad 336F_{14}-672F_{15}+36F_{16}
\end{aligned}
$$

$$
\begin{aligned}
f^{na}_{3,1,0} &= -\frac{269}{9}-\frac{44L}{3}+2\pi^2+\frac{4\pi^2F_3}{3}-\frac{592F_4}{9}-\frac{88LF_4}{3}+\frac{14\pi^2F_4}{3}-\frac{68F_5}{3}-4F_6+ \\
&\quad 16F_9-\frac{112F_{10}}{3}+4F_{11}-8F_{13} \\
f^{na}_{3,2,0} &= -\frac{2}{3}\pi^2F_3+\frac{203F_4}{9}+\frac{44LF_4}{3}-\frac{4\pi^2F_4}{3}+\frac{22F_5}{3}-8F_9+\frac{26F_{10}}{3} \\
f^{na}_{3,0,1} &= -6+20\zeta(3)+\frac{38\pi^2}{3}-8\ln(2)\pi^2-2\pi^2F_2+\frac{8\pi^2F_3}{3}-18F_4+\frac{16\pi^2F_4}{3}-16F_6+ \\
&\quad 32F_9-4F_{10}+16F_{11}-12F_{13}-4F_{16} \\
f^{na}_{3,0,2} &= -6\zeta(3)-\frac{118\pi^2}{3}-\frac{12\pi^4}{5}-3\pi^2F_2-\frac{4\pi^2F_3}{3}-\frac{89\pi^2F_4}{3}-144F_5+16\pi^2F_5+ \\
&\quad 82F_6-32F_7-16F_9-102F_{10}-54F_{11}+102F_{13}+32F_{14}-64F_{15}-6F_{16} \\
f^{na}_{3,0,3} &= 32\zeta(3)+67\pi^2+\frac{398\pi^4}{45}-\frac{16\pi^2F_1}{3}-8\pi^2F_2+8\pi^2F_3+58\pi^2F_4+102F_5-\frac{176\pi^2F_5}{3}- \\
&\quad 196F_6+160F_7-64F_8+96F_9+84F_{11}-184F_{13}-96F_{14}+192F_{15}-16F_{16} \\
f^{na}_{3,0,4} &= -\frac{263\pi^4}{30}+8\pi^2F_1-9\pi^2F_2+58\pi^2F_5+18F_6-180F_7+96F_8-18F_{13}+84F_{14}- \\
&\quad 168F_{15}-18F_{16}
\end{aligned}
$$

$$
\begin{aligned}
f^{nl}_{3,1,0} &= \frac{76}{9}+\frac{16L}{3}+\frac{152F_4}{9}+\frac{32LF_4}{3}+\frac{16F_5}{3}+\frac{32F_{10}}{3} \\
f^{nl}_{3,2,0} &= -\frac{52F_4}{9}-\frac{16LF_4}{3}-\frac{8F_5}{3}-\frac{16F_{10}}{3}
\end{aligned}
$$

$$
\begin{aligned}
f^{nh}_{3,1,0} &= \frac{76}{9}+\frac{16L}{3}+\frac{392F_4}{9}+\frac{32LF_4}{3}+\frac{16F_5}{3}\\
f^{nh}_{3,2,0} &= -\frac{52F_4}{9}-\frac{16LF_4}{3}-\frac{8F_5}{3}\\
f^{nh}_{3,0,1} &= -\frac{32}{3}-\frac{16\pi^2}{9}+\frac{80F_4}{3}+\frac{32F_5}{3}\\
f^{nh}_{3,0,2} &= \frac{568}{3}+\frac{32\pi^2}{3}+\frac{496F_4}{3}-48F_5\\
f^{nh}_{3,0,3} &= -64\zeta(3)-\frac{320\pi^2}{9}+\frac{352F_5}{3}+64F_6\\
f^{nh}_{3,0,4} &= 96\zeta(3)-96F_6\,.
\end{aligned}
$$

4 Two-loop results for the Wilson coefficients C_i

In this section we give results for the Wilson coefficients C_i, valid to NNLO in α_s. To calculate them, we take the UV-renormalized form factors D_i obtained in the previous section, translate them to four-flavor QCD using (13), and evaluate the matching condition (10). This procedure allows us to determine both the Wilson coefficients C_i and the renormalization factor Z_J. The form of the renormalization factor is completely determined by the renormalization-group equations for heavy-to-light currents in SCET, and thus provides important checks on our result. We shall first say a few words about these, and then list results for the Wilson coefficients C_i.

The renormalization factor Z_J is determined from our calculation by requiring that the matching relation (10) is finite in the limit $\epsilon \to 0$. However, as explained in Section 2, it can also be determined by the UV poles of the object $J \otimes S$ in the parton model. Expressions at two loops can be derived from the renormalization factors for the jet and soft functions calculated in [14, 16]. Either way, the result depends only on logs of the form $L_p \equiv \ln \mu/\bar{n}\cdot p$ and reads

$$
Z_J = 1+\frac{C_F\alpha_s}{4\pi}\left[-\frac{1}{\epsilon^2}+\frac{1}{\epsilon}\left(-\frac{5}{2}-2L_p\right)\right]+\left(\frac{\alpha_s}{4\pi}\right)^2 C_F\sum_{i=1}^{4}\frac{Z^{(2)}_{(-i)}}{\epsilon^i} \tag{19}
$$

where the two-loop coefficients are

$$
\begin{aligned}
Z^{(2)}_{(-4)} &= \frac{C_F}{2}\\
Z^{(2)}_{(-3)} &= C_F\left(\frac{5}{2}+2L_p\right)+\frac{11C_A}{4}-n_lT_R\\
Z^{(2)}_{(-2)} &= C_F\left(\frac{25}{8}+5L_p+2L_p^2\right)+C_A\left(\frac{49}{18}+\frac{\pi^2}{12}+\frac{11L_p}{3}\right)+n_lT_R\left(-\frac{10}{9}-\frac{4L_p}{3}\right)\\
Z^{(2)}_{(-1)} &= C_F\left(\frac{-3}{8}+\frac{\pi^2}{2}-6\zeta_3\right)+C_A\left(-\frac{1549}{216}-\frac{7\pi^2}{24}+\frac{11}{2}\zeta_3+L_p\left[-\frac{67}{9}+\frac{\pi^2}{3}\right]\right)\\
&\quad +n_lT_R\left(\frac{125}{54}+\frac{\pi^2}{6}+\frac{20L_p}{9}\right).
\end{aligned} \tag{20}
$$

In SCET, the hard function is derived from the matrix of Wilson coefficients $H_{ij} = C_iC_j$

and satisfies the renormalization-group equation [4]

$$\frac{d}{d\ln\mu}H_{ij}(\bar{n}\cdot p,\mu) = 2\left[\gamma'(\alpha_s) + \Gamma_{\rm cusp}(\alpha_s)\ln\frac{\bar{n}\cdot p}{\mu}\right] H_{ij}(\bar{n}\cdot p,\mu)\,. \qquad (21)$$

It is easy to show that the anomalous dimension derived from the explicit expressions in (20) are consistent with (21), with

$$\begin{aligned}\gamma' &= -5\frac{C_F\alpha_s}{4\pi} - 8C_F\left(\frac{\alpha_s}{4\pi}\right)^2\left[C_F\left(\frac{3}{16}-\frac{\pi^2}{4}+3\zeta_3\right)+C_A\left(\frac{1549}{432}+\frac{7\pi^2}{48}-\frac{11}{4}\zeta_3\right)\right.\\ &\quad \left. -n_l T_R\left(\frac{125}{108}+\frac{\pi^2}{12}\right)\right]. \qquad (22)\end{aligned}$$

This result is consistent with that given in [33], and the piece of the anomalous dimension proportional to the logarithmic term is consistent with the two-loop cusp anomalous dimension from [34].

We now give final results for the Wilson coefficients C_i, which we decompose according to

$$C_i = C_i^{(0)} + \frac{\alpha_s}{4\pi}C_i^{(1)} + \left(\frac{\alpha_s}{4\pi}\right)^2 C_i^{(2)}\,. \qquad (23)$$

We find

$$\begin{aligned}C_1^{(0)} &= 1,\; C_2^{(0)} = C_3^{(0)} = 0\,, \qquad (24)\\ C_i^{(1)} &= R^{(1)}_{(0),i}\,,\; C_i^{(2)} = R^{(2)}_{(0),i} + C_F^2 K_{i,1} + C_F n_h T_R K_{i,2}\;(i=1,2)\,,\\ C_3^{(1)} &= \frac{1-\hat{s}}{2}R^{(1)}_{(0),3},\; C_3^{(2)} = \frac{1-\hat{s}}{2}\left(R^{(2)}_{(0),3} + C_F^2 K_{3,1} + C_F n_h T_R K_{3,2}\right)\,,\end{aligned}$$

where the $R^{(k)}_{(0),j}$ were given in Section 3, and functions $K_{i,1}$ and $K_{i,2}$ read

$$\begin{aligned}K_{1,1} &= -54 - \frac{49\pi^2}{48} - \frac{\pi^4}{160} - 60F_4 - \frac{13\pi^2F_4}{12} + \frac{18F_4}{\hat{s}} + \frac{\pi^2F_4}{12\hat{s}} - \frac{31F_5}{2} - \frac{\pi^2F_5}{6} + \\ &\quad \frac{13F_5}{2\hat{s}} - 8F_6 + \frac{F_6}{\hat{s}} - 2F_7 - 63F_{10} - \pi^2F_{10} + \frac{29F_{10}}{\hat{s}} - 22F_{11} + \frac{4F_{11}}{\hat{s}} - \\ &\quad 8F_{12} - 28F_{13} + \frac{6F_{13}}{\hat{s}} - 8F_{14} - 12F_{15} - 68F_{17} + \frac{16F_{17}}{\hat{s}} - 24F_{18} - 32F_{19} - \\ &\quad 32F_{20} - 80F_{21} + \frac{5\zeta(3)}{3} + \frac{4}{3}F_4\zeta(3) + \\ &\quad L\left(-78 - \frac{5\pi^2}{4} - 71F_4 - \pi^2F_4 + \frac{21F_4}{\hat{s}} - 22F_5 + \frac{4F_5}{\hat{s}} - 8F_6 - 68F_{10} + \frac{16F_{10}}{\hat{s}} - \right.\\ &\quad \left. 24F_{11} - 32F_{13} - 80F_{17} + \frac{4\zeta(3)}{3}\right) + \\ &\quad L^2\left(-\frac{97}{2} - \frac{\pi^2}{2} - 38F_4 + \frac{6F_4}{\hat{s}} - 12F_5 - 40F_{10}\right) + L^3\left(-\frac{50}{3} - \frac{40F_4}{3}\right) - \frac{10L^4}{3}\,,\end{aligned}$$

$$\begin{aligned}K_{1,2} &= -\frac{5\pi^2}{18} - \frac{2\pi^2F_4}{9} + \frac{4\zeta(3)}{9} + L\left(-16 - \frac{2\pi^2}{3} - 8F_4 + \frac{8F_4}{3\hat{s}} - \frac{16F_5}{3} - \frac{32F_{10}}{3}\right) - \\ &\quad L^2\left(20 + 16F_4\right) - \frac{112L^3}{9}\,,\end{aligned}$$

$$
\begin{aligned}
K_{2,1} &= \frac{18}{\hat{s}}+\frac{\pi^2}{6\hat{s}}-\frac{9F_4}{\hat{s}^2}-\frac{\pi^2F_4}{6\hat{s}^2}+\frac{17F_4}{\hat{s}}+\frac{\pi^2F_4}{6\hat{s}}-\frac{7F_5}{\hat{s}^2}+\frac{7F_5}{\hat{s}}-\frac{2F_6}{\hat{s}^2}+\frac{2F_6}{\hat{s}}-\frac{22F_{10}}{\hat{s}^2}+ \\
&\quad \frac{22F_{10}}{\hat{s}}-\frac{8F_{11}}{\hat{s}^2}+\frac{8F_{11}}{\hat{s}}-\frac{12F_{13}}{\hat{s}^2}+\frac{12F_{13}}{\hat{s}}-\frac{32F_{17}}{\hat{s}^2}+\frac{32F_{17}}{\hat{s}}+ \\
&\quad L\left(\frac{26}{\hat{s}}-\frac{18F_4}{\hat{s}^2}+\frac{26F_4}{\hat{s}}-\frac{8F_5}{\hat{s}^2}+\frac{8F_5}{\hat{s}}-\frac{32F_{10}}{\hat{s}^2}+\frac{32F_{10}}{\hat{s}}\right)+L^2\left(\frac{12}{\hat{s}}-\frac{12F_4}{\hat{s}^2}+\frac{12F_4}{\hat{s}}\right),
\end{aligned}
$$

$$
K_{2,2} = L\left(\frac{16}{3\hat{s}}-\frac{16F_4}{3\hat{s}^2}+\frac{16F_4}{3\hat{s}}\right),
$$

$$
\begin{aligned}
K_{3,1} &= -\frac{18}{\hat{s}}-\frac{\pi^2}{6\hat{s}}+\frac{9F_4}{\hat{s}^2}+\frac{\pi^2F_4}{6\hat{s}^2}-\frac{53F_4}{\hat{s}}-\frac{\pi^2F_4}{3\hat{s}}+\frac{7F_5}{\hat{s}^2}-\frac{20F_5}{\hat{s}}+\frac{2F_6}{\hat{s}^2}-\frac{4F_6}{\hat{s}}+\frac{22F_{10}}{\hat{s}^2}- \\
&\quad \frac{80F_{10}}{\hat{s}}+\frac{8F_{11}}{\hat{s}^2}-\frac{16F_{11}}{\hat{s}}+\frac{12F_{13}}{\hat{s}^2}-\frac{24F_{13}}{\hat{s}}+\frac{32F_{17}}{\hat{s}^2}-\frac{64F_{17}}{\hat{s}}+ \\
&\quad L\left(-\frac{26}{\hat{s}}+\frac{18F_4}{\hat{s}^2}-\frac{68F_4}{\hat{s}}+\frac{8F_5}{\hat{s}^2}-\frac{16F_5}{\hat{s}}+\frac{32F_{10}}{\hat{s}^2}-\frac{64F_{10}}{\hat{s}}\right)+ \\
&\quad L^2\left(-\frac{12}{\hat{s}}+\frac{12F_4}{\hat{s}^2}-\frac{24F_4}{\hat{s}}\right),
\end{aligned}
$$

$$
K_{3,2} = L\left(-\frac{16}{3\hat{s}}+\frac{16F_4}{3\hat{s}^2}-\frac{32F_4}{3\hat{s}}\right).
$$

The terms proportional to the explicit factors of n_h in (24) stem from converting the results of the renormalized form factors D_i from the five-flavor to the four-flavor theory. As a final check, we have confirmed that the μ-dependence in the C_i is such that the renormalization-group equation (21) is satisfied.

5 Conclusions

We have presented results for the short-distance Wilson coefficients needed to complete the calculation of partial decay rates in $\bar{B} \to X_u \ell \bar{\nu}$ at NNLO in α_s and to leading order in $1/m_b$, for decay kinematics limited to the shape-function region. The technical challenge was to compute the two-loop QCD corrections to the semi-leptonic $b \to u$ transition current. To do this, we used the Laporta algorithm to perform a reduction to master integrals, which were solved using the method of differential equations. We then performed a matching calculation from QCD onto SCET to translate these results into the Wilson coefficients needed to compute the hard function in the factorization formula (1) at NNLO. In a companion paper, we shall perform an analysis of partial decay rates with arbitrary kinematic cuts at NNLO, and study the implications on the determination of $|V_{ub}|$ from inclusive decays.

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Note Added: After our calculation was completed, the paper [35] appeared, where the UV-renormalized two-loop corrections to the $b \to u$ current were presented. We have compared with their results and found agreement with those given in Section 3.

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