Fermionic Corrections to the Three-Loop Matching Coefficient of the Vector Current

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Abstract

In this paper we consider the matching coefficient of the vector current between Quantum Chromodynamics (QCD) and Non-Relativistic QCD (NRQCD) to three-loop order in perturbation theory. We evaluate the fermionic corrections containing a closed massless fermion loop. The results are building blocks both for the bottom and top quark system at threshold. We explain in detail the methods used for the evaluation of the Feynman diagrams, classify the occurring master integrals and provide results for the latter. The numerical effects are significant. They have the tendency to improve the behaviour of the perturbative series — both for the bottom and top quark system.

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1 Introduction

One of the main goals of a future international linear collider (ILC) is the precise measurement of the top quark threshold. Next to a precise extraction of the strong coupling an unrivaled determination of the top quark mass and its width is possible. This would open up a new chapter in the electroweak precision physics which leads to very strong checks of the Standard Model or possible extensions.

The theoretical calculations are based on an effective theory [1,2] (for a review see [3]) which enables the simultaneous expansion in the two small parameters present in threshold phenomena, the strong coupling $\alpha_s$ and the velocity of the heavy quarks, $v$. Furthermore, a resummation of correction terms like $(\alpha_s/v)^n$ to all orders is possible in perturbation theory. In a first step the effective theory is constructed in a matching procedure where it is required that the Green functions agree with the corresponding ones in full QCD in the limit of infinitely heavy top quark mass. In a second step the Green function in the effective theory has to be evaluated leading to the desired cross section.

Experimental studies [4] have shown that an uncertainty of less than 3% is necessary for the theoretical predictions for the cross section of the reaction $e^+e^-\rightarrow t\bar{t}$ in the threshold region, i.e. for $\sqrt{s} \approx 350$ GeV. This has not yet been achieved.

As far as the strong coupling is concerned currently the analysis is complete to next-to-next-to-leading order (NNLO) [5] demonstrating the urgent need for the third-order corrections. This huge enterprise has been started already some years ago and many building blocks have been evaluated starting from the determination of the third-order Hamiltonian [6], third-order corrections to the energy levels and wave functions [7–9] up to the evaluation of the contributions from the Coulomb potential to the non-relativistic Green function [9]. Next to fixed-order corrections also the resummation of next-to-next-to leading logarithmic terms has been considered and quite some progress has been achieved [10–13].

In order to reach a theory-uncertainty below 3% it is also necessary to worry about electroweak effects which can be parametrically as big as the third-order QCD terms. First results in this context are available [14,15] which show that indeed numerical effects in the region of a few percent are possible.

In this paper a further building block needed for the N$^3$LO analysis is provided: the fermionic corrections to the matching coefficient of the vector current. More precisely we compute the three-loop contributions to the matching coefficient containing at least one closed loop of massless fermions which we enumerate by $n_l$.

The paper is organized as follows: in the next section we describe in detail the theoretical framework and the methods used for the calculation. In particular, we classify the occurring integrals and discuss their evaluation. Sections 3 and 4 contain a detailed discussion about the wave function and matching coefficient up to order $\alpha_s^n n_l$, respectively. In Section 5 we briefly discuss the phenomenological impact of our result and Section 6 contains our conclusions and outlook. In the Appendix a complete list of master integrals is provided — both for the "natural" and the $\epsilon$-finite basis.
2 Method

The matching coefficient establishing the relation between the quark current in the full and effective theory constitutes a building block for all threshold phenomena involving the coupling of a photon or $Z$ boson to heavy quarks. We define the currents through

$$
\begin{align*}
    j^\mu_v &= \bar{Q} \gamma^\mu Q, \\
    j^i &= \phi^\dagger \sigma^i \chi,
\end{align*}
$$

and generically denote the heavy quark by $Q$. $\phi$ and $\chi$ are two-component Pauli spinors for quark and anti-quark, respectively. The definition of the matching coefficient is established through

$$
\begin{align*}
    j^k_v &= c_v(\mu) \tilde{j}^k + \frac{d_v(\mu)}{6m_Q^2} \phi^\dagger \sigma^k \bar{D}^2 \chi + \ldots,
\end{align*}
$$

where $k = 1, 2, 3$ denotes the spacial components. $\bar{D}$ contains the space-like components of the gauge-covariant derivative involving the gluon fields and the ellipsis stand for operators of higher mass dimension. The second term on the r.h.s. of Eq. (2) is already of NNLO with $d_v = 1 + \mathcal{O}(\alpha_s)$. The Wilson coefficients $c_v$ and $d_v$ may be expressed as series in $\alpha_s$ and represent the contributions from the hard modes which have been integrated out in order to arrive at the effective theory. Note that both the higher order terms in the inverse heavy quark mass and the time-like component is not of interest for the aim of this paper. The purpose of this paper is the evaluation of the fermionic correction to the non-singlet contribution of $c_v$ containing at least one closed massless quark loop. The one-loop corrections to $d_v$ contain no contribution proportional to $n_l$.

In order to compute $c_v$ it is obvious to consider the $Q\bar{Q}\gamma$ vertex which in the following is denoted by $\Gamma_v$. This effectively transforms Eq. (2) into

$$
Z_2 \Gamma_v = c_v \tilde{Z}_2 \tilde{Z}_v^{-1} \tilde{\Gamma}_v + \ldots,
$$

where we have on the left- and right-hand side quantities of the full and effective theory, respectively, and the ellipses denote terms suppressed by inverse powers of the heavy quark mass. In Eq. (3) it is understood that the couplings and masses in $\Gamma_v$ are renormalized.

Since $c_v$ takes into account the degrees of freedom which have been integrated out from the full theory it depends in our case only on $\alpha_s$ and — for dimensional reasons — on $\ln(\mu^2/m_Q^2)$. In particular, $c_v$ does not explicitly depend on the momenta of the external particles. Thus, it is useful to apply the so-called threshold expansion [16, 17] to Eq. (3) which has the consequence that $\Gamma_v$ has to be evaluated for $s = 4m_Q^2$ since all except the hard region cancel in Eq. (3). Furthermore, on the right-hand side only tree contributions have to be considered. In particular we have $\tilde{Z}_2 = 1$.

Starting from two-loop order the matching procedure exhibits infra-red divergences which are compensated by ultra-violet divergences of the effective theory rendering physical quantities finite. In Eq. (3) the renormalization constant $\tilde{Z}_v$ which generates the
anomalous dimension of $\tilde{j}_v$ takes over this part. Note that the vector current in the full theory does not get renormalized.

Sample Feynman diagrams contributing to the one-, two- and three-loop fermionic part of $c_v$ are shown in Fig. 1. Due to the special kinematic situation with $s = q^2 = 4m_Q^2$ and on-shell heavy quark lines it is possible to perform a partial fractioning in the integrands corresponding to the various types of diagrams and map all occurring integrals to one of the following functions:

\[
J^{(2)}_{\pm}(n_1, \ldots, n_5) = \left( \frac{\mu^{2\epsilon}}{i\pi^{d/2}} \right)^2 \int \frac{d^dk \, d^dl}{(k^2)^{n_1}(l^2)^{n_2}((k-l)^2)^{n_3}(k^2 + q \cdot k)^{n_4}(l^2 \pm q \cdot l)^{n_5}},
\]

\[
L^{(2)}_{\pm}(n_1, \ldots, n_5) = \left( \frac{\mu^{2\epsilon}}{i\pi^{d/2}} \right)^2 \int \frac{d^dk \, d^dl}{(k^2)^{n_1}(l^2)^{n_2}(k^2 + q \cdot (k+l))^2(k^2 + q \cdot k)^{n_4}(l^2 \pm q \cdot l)^{n_5}},
\]

\[
J^{(3)}_{\pm}(n_1, \ldots, n_9) = \left( \frac{\mu^{2\epsilon}}{i\pi^{d/2}} \right)^3 \int \frac{d^dk \, d^dl \, dp}{(p^2 + q \cdot l)^{-n_8}} \times \frac{(k^2 + q \cdot k)^{n_7}(p^2 \pm q \cdot p)^{n_9}}{(k^2)^{n_1}(l^2)^{n_2}((k-l)^2)^{n_3}(k^2 + q \cdot k)^{n_4}(l^2 \pm q \cdot l)^{n_5}(p^2 + q \cdot p)^{n_6}((p-k)^2)^{n_7}((p-l)^2)^{n_8}},
\]

\[
L^{(3, n_1)}_{\pm}(n_1, \ldots, n_9) = \left( \frac{\mu^{2\epsilon}}{i\pi^{d/2}} \right)^3 \int \frac{d^dk \, d^dl \, dp}{(p^2 + q \cdot l)^{-n_8}} \times \frac{(k^2 + q \cdot k)^{n_7}(p^2 \pm q \cdot p)^{n_9}}{(k^2)^{n_1}(l^2)^{n_2}((k-l)^2)^{n_3}(k^2 + q \cdot k)^{n_4}(l^2 \pm q \cdot l)^{n_5}(p^2 + q \cdot p)^{n_6}((p-k)^2)^{n_7}((p-l)^2)^{n_8}}.
\]

For convenience we have also listed the two-loop functions $J^{(2)}_{\pm}$ and $L^{(2)}_{\pm}$ originally defined in Ref. [16]. The three-loop functions $J^{(3)}_{\pm}$ and $L^{(3, n_1)}_{\pm}$ contain irreducible scalar products...
which are shown as numerators in the three-loop integrals in Eq. (4). The corresponding indices can only adopt values less or equal to zero. Furthermore, only two out of the three indices $n_6$, $n_7$ and $n_8$ in $L^{(3,n_l)}_{\pm}$ can have positive values. Note that the integrals $J^{(2)}_\pm$, $L^{(2)}_\pm$ and $J^{(3)}_\pm$ are actually two-point functions whereas the integrals $J^{(2)}_\mp$, $L^{(2)}_\mp$, $J^{(3)}_\mp$ and $L^{(3,n_l)}_{\pm}$ correspond to vertices.

All Feynman diagrams are generated with QGRAF [18]. The various topologies are identified with the help of Q2e and exp [19,20] which also adapts the notation in order to match the one of Eq. (4).

In a next step the reduction of the various functions to so-called master integrals has to be achieved. For this step we have chosen two approaches: the Laporta method [21,22] and Baikov’s method [23,24] in the formulation of [25]. The application of these methods reduces the three-loop integrals to twelve master integrals. Since some of the master integrals are only known numerically it is very useful to construct a so-called $\epsilon$-finite basis [26]. Details of this procedure and the results for the master integrals are given in Appendix A. Let us in the following provide more details on our implementation of each of the two reduction methods.

### 2.1 Implementation of the Laporta algorithm

The Laporta algorithm is based on the integration-by-parts (IBP) relations [27] where in a first step a huge system of equations is created by inserting numerical integer values into the relations. After assigning a weight specifying the complexity to each occurring integral the system of equations is solved step-by-step. In this way an arbitrary integral is expressed in terms of master integrals which cannot be further reduced.

To date there is only one publicly available computer code, AIR [28], where the Laporta algorithm is implemented. We have successfully applied AIR to the two-loop diagrams. However, the three-loop integrals of Eq. (4) cannot be treated with the help of AIR.

For this reason we have chosen to write a new implementation of Laporta’s algorithm, Crusher [29]. It is written in C++ and uses GiNaC [30] for simple manipulations like taking derivatives of polynomial quantities. In the practical implementation of the Laporta algorithm one of the most time-consuming operations is the simplification of the coefficients appearing in front of the individual integrals. This task is performed with the help of Fermat [31] where a special interface has been used (see Ref. [32]). The main features of the implementation are the automated generation of the IBP identities and a complete symmetrization of the diagrams. Using Crusher we solved approximately forty million equations to reduce all integrals to master integrals.

### 2.2 Baikov’s method

Baikov’s method is also based on the IBP relations. Here, however, one explicitly constructs the coefficient functions of the master integrals as parametric integrals over some polynomial, which encodes the topology of the initial integral. The integrations can then
be performed as Cauchy integrations around the origin or as contour integrations
between the roots of the polynomial. The results are rational functions depending on
the dimension and the kinematical invariants.

In some cases, however, it is not possible to perform the integrations in this way. In
these cases one has to solve the integration-by-parts relations for the parametric
integrals. They are similar to the relations for the initial integral, however, they depend
on less indices and are thus in general significantly simpler. Since the relations can still be quite
complicated, it is convenient to again use Laporta’s algorithm. In the current calculation
the program AIR was used for this task.

In order to perform the calculations, the algorithms for each integral were
implemented in FORM [33]. In a first step, however, everything was implemented in
Mathematica. This is very convenient since it is possible to produce almost all needed
Mathematica code automatically. Once the program is finished, it can be easily translated
to FORM and the Mathematica version can be used for debugging.

The two-loop calculation was done entirely with this method. In the three-loop case,
however, it turned out that a complete solution of the recurrence relations for the coef-
ficient functions is not possible with AIR. The calculation was therefore done with the
Laporta method described above. We used Baikov’s method only for the
part and to
cross-check some of the coefficient functions.

3 Wave function renormalization constant

According to Eq. (3) the wave function renormalization constant in the on-shell scheme
$Z_2$ constitutes a crucial input for the computation of $c_v$. It has been computed to two-
and three-loop approximation in Refs. [34] and [35], respectively. We have repeated the
calculation of the two-loop and fermionic three-loop contributions which are needed for
the present calculation and find complete agreement with the literature. For completeness
we repeat the result for $Z_2$ which can be cast into the form

$$Z_2 = 1 + \frac{\alpha_s(\mu)}{\pi} \left( \frac{e^\gamma E}{4\pi} \right)^{-\epsilon} \delta Z_2^{(1)} + \left( \frac{\alpha_s(\mu)}{\pi} \right)^2 \left( \frac{e^\gamma E}{4\pi} \right)^{-2\epsilon} \delta Z_2^{(2)}$$

$$+ \left( \frac{\alpha_s(\mu)}{\pi} \right)^3 \left( \frac{e^\gamma E}{4\pi} \right)^{-3\epsilon} \left( \delta Z_2^{(3,nl)} + \text{non-$n_l$ terms} \right) + \mathcal{O}(\alpha_s^4) ,$$

with

$$\delta Z_2^{(1)} = -C_F \left[ \frac{3}{4\epsilon} + 1 + \frac{3}{4} L_\mu + \left( 2 + \frac{1}{16} \pi^2 + L_\mu + \frac{3}{8} L_\mu^2 \right) \epsilon \right.$$

$$\left. + \left( 4 + \frac{1}{12} \pi^2 - \frac{1}{4} \zeta(3) + \left( 2 + \frac{1}{16} \pi^2 \right) L_\mu + \frac{1}{2} L_\mu^2 + \frac{1}{8} L_\mu^3 \right) \epsilon^2 \right] ,$$

(5)
\[ \delta Z_2^{(2)} = \left[ \frac{11}{32\epsilon^2} - \frac{127}{192\epsilon} - \frac{1705}{384} + \frac{5}{16} \pi^2 - \frac{1}{2} \pi^2 \ln 2 + \frac{3}{4} \zeta(3) - \frac{215}{96} L_\mu - \frac{11}{32} L_\mu^2 \right. \\
+ \left( -\frac{9907}{768} + \frac{769}{1152} \pi^2 - \frac{23}{8} \pi^2 \ln 2 + \pi^2 \ln^2 2 + \frac{129}{16} \zeta(3) - \frac{7}{40} \pi^4 + \frac{1}{2} \ln^4 2 + 12a_4 \right. \\
+ \left( -\frac{2057}{192} + \frac{109}{192} \pi^2 - \pi^2 \ln 2 + \frac{3}{2} \zeta(3) \right) L_\mu - \frac{259}{96} L_\mu^2 - \frac{11}{32} L_\mu^3 \right] C_A C_F \\
+ \left[ \frac{9}{32\epsilon^2} + \left( \frac{51}{16} + \frac{9}{16} L_\mu \right) \frac{1}{\epsilon} + \frac{433}{128} - \frac{49}{64} \pi^2 + \pi^2 \ln 2 - \frac{3}{2} \zeta(3) + \frac{51}{32} L_\mu + \frac{9}{16} L_\mu^2 \right. \\
+ \left( \frac{211}{256} - \frac{339}{128} \pi^2 + \frac{23}{4} \pi^2 \ln 2 - 2 \pi^2 \ln^2 2 - \frac{297}{16} \zeta(3) + \frac{7}{20} \pi^4 - \ln^4 2 - 24a_4 \right. \\
+ \left( \frac{433}{64} - \frac{49}{32} \pi^2 + 2 \pi^2 \ln 2 - 3 \zeta(3) \right) L_\mu + \frac{51}{32} L_\mu^2 + \frac{3}{8} L_\mu^3 \right] C_F^2 \\
+ \left[ \left( \frac{1}{16} + \frac{1}{4} L_\mu \right) \frac{1}{\epsilon} + \frac{947}{288} - \frac{5}{16} \pi^2 + \frac{11}{24} L_\mu + \frac{3}{8} L_\mu^2 + \left( \frac{17971}{1728} \frac{445}{288} \pi^2 \right. \\
+ 2 \pi^2 \ln 2 - \frac{85}{12} \zeta(3) + \left( \frac{1043}{144} - \frac{29}{48} \pi^2 \right) L_\mu + \frac{5}{8} L_\mu^2 + \frac{7}{24} L_\mu^3 \right] C_F T \\
+ \left[ \frac{1}{8\epsilon^2} + \frac{11}{48\epsilon} + \frac{113}{96} + \frac{1}{12} \pi^2 + \frac{19}{24} L_\mu + \frac{1}{8} L_\mu^2 \right. \\
+ \left( \frac{851}{192} + \frac{127}{288} \pi^2 + \zeta(3) + \left( \frac{145}{48} + \frac{3}{16} \pi^2 \right) L_\mu + \frac{23}{24} L_\mu^2 + \frac{1}{8} L_\mu^3 \right] C_F T_{n_l} \right] (7)
\[ \delta Z^{[3,nl]}_2 = C_F T n_l \left\{ \left[ \frac{11}{72\epsilon^3} - \frac{169}{432\epsilon^2} + \left( \frac{313}{1296} + \frac{1}{4}\zeta(3) \right) \frac{1}{\epsilon} ight] + \frac{111791}{15552} + \frac{13}{48} \pi^2 + \frac{47}{36} \pi^2 \text{ln}^2 2 - \frac{2}{9} \pi^2 \text{ln}^2 2 - \frac{35}{72} \zeta(3) + \frac{19}{1080} \pi^4 - \frac{1}{9} \text{ln}^4 2 - \frac{8}{3} a_4 \ight. \\
+ \left( \frac{169}{27} - \frac{1}{3} \pi^2 \text{ln}^2 2 + \frac{1}{4}\zeta(3) \right) L_{\mu} + \frac{469}{288} L_{\mu}^2 + \frac{11}{72} L_{\mu}^3 \right\} C_A \\
+ \left[ \frac{3}{32\epsilon^3} + \left( -\frac{19}{192} + \frac{3}{32} L_{\mu} \right) \frac{1}{\epsilon^2} + \left( -\frac{235}{384} - \frac{7}{128} \pi^2 - \frac{1}{4}\zeta(3) - \frac{41}{64} L_{\mu} - \frac{3}{64} L_{\mu}^2 \right) \frac{1}{\epsilon} ight] \\
- \frac{3083}{2304} + \frac{2845}{2304} \pi^2 - \frac{47}{18} \pi^2 \text{ln}^2 2 + \frac{4}{9} \pi^2 \text{ln}^2 2 + \frac{473}{96} \zeta(3) + \frac{229}{2160} \pi^4 + \frac{2}{9} \text{ln}^4 2 - \frac{16}{3} a_4 \\
+ \left( -\frac{1475}{384} + \frac{133}{384} \pi^2 - \frac{2}{3} \pi^2 \text{ln}^2 2 + \frac{1}{4}\zeta(3) \right) L_{\mu} - \frac{179}{128} L_{\mu}^2 - \frac{11}{64} L_{\mu}^3 \right\} C_F \\
+ \left[ \left( \frac{1}{36} + \frac{1}{12} L_{\mu} \right) \frac{1}{\epsilon^2} + \left( -\frac{5}{216} + \frac{1}{144} \pi^2 - \frac{1}{9} L_{\mu} + \frac{1}{24} L_{\mu}^2 \right) \frac{1}{\epsilon} ight] \\
- \frac{4721}{1296} + \frac{19}{54} \pi^2 - \frac{1}{36}\zeta(3) + \left( -\frac{329}{108} + \frac{25}{144} \pi^2 \right) L_{\mu} - \frac{7}{12} L_{\mu}^2 - \frac{5}{72} L_{\mu}^3 \right] T \\
+ \left[ \left( \frac{1}{36\epsilon^3} + \frac{11}{216\epsilon^2} + \frac{5}{1296\epsilon} - \frac{5767}{7776} - \frac{19}{108} \pi^2 - \frac{7}{18}\zeta(3) \right) \ight. \\
- \frac{167}{216} + \frac{1}{36}\pi^2 \right] L_{\mu} - \frac{19}{72} L_{\mu}^2 - \frac{1}{18} L_{\mu}^3 \right\} T n_l \right\} . \tag{8} \]

where \( L_{\mu} = \text{ln}(\mu^2/m^2) \), \( C_F = (N_c^2 - 1)/(2N_c) \), \( C_A = N_c \), \( T = 1/2 \) and \( n_l = n_f - 1 \) is the number of light-quark flavours. \( N_c = 3 \) and \( \alpha_s \) is the strong coupling renormalized in the \( \overline{\text{MS}} \) scheme with \( n_f \) active flavours. \( \zeta(3) \) is Riemann’s \( \zeta \) function with the value \( \zeta(3) = 1.202057 \ldots \) \( \gamma_E \) is Euler’s constant with the value \( \gamma_E = 0.577216 \ldots \) and \( a_4 = \text{Li}_4(1/2) = 0.517479 \ldots \) Note that \( \delta Z_2^{(1)} \) and \( \delta Z_2^{(2)} \) are given to order \( \epsilon^2 \) and \( \epsilon \), respectively, which is needed for the three-loop calculation of \( c_v \).

The integrals needed for \( Z_2 \) constitute a subset of the ones needed for \( c_v \). In fact, from Eq. (11) only the integral types with a “+” sign contribute. We also want to mention that our calculation poses the first independent check of the \( n_l \) part of Ref. [35].

### 4 Matching coefficient

It is convenient to cast the perturbative expansion of the matching coefficient in the form

\[ c_v = 1 + \frac{\alpha_s(\mu)}{\pi} c_v^{(1)} + \left( \frac{\alpha_s(\mu)}{\pi} \right)^2 c_v^{(2)} + \left( \frac{\alpha_s(\mu)}{\pi} \right)^3 c_v^{(3)} + \mathcal{O}(\alpha_s^4), \tag{9} \]
where the one- [36] and two-loop [37, 38] (see also Ref. [39]) terms are given by

\[
c_v^{(1)} = -2C_F
\]

\[
c_v^{(2)} = \left( -\frac{151}{72} + \frac{89}{144}\pi^2 - \frac{5}{6}\pi^2\ln 2 - \frac{13}{4}\zeta(3) \right) C_A C_F
\]

\[
+ \left( \frac{23}{8} - \frac{79}{36}\pi^2 + \pi^2\ln 2 - \frac{1}{2}\zeta(3) \right) C_F^2 + \left( \frac{22}{9} - \frac{2}{9}\pi^2 \right) C_F T
\]

\[
+ \frac{11}{18} C_F T n_t - \frac{1}{2} \left[ 4\beta_0 + \pi^2 \left( \frac{1}{2} C_A + \frac{1}{3} C_F \right) \right] C_F \ln \frac{\mu^2}{m_Q^2}, \tag{10}
\]

with \( \beta_0 = (11 C_A/3 - 4 T n_f/3)/4 \). Note that the terms proportional to \( \beta_0 \ln \frac{\mu^2}{m_Q^2} \) are connected to the choice \( \alpha_s(\mu) \) in Eq. (9) whereas the ones proportional to \( \pi^2 \ln \frac{\mu^2}{m_Q^2} \) originate from the separation of hard and soft scales in the construction of NRQCD.

The decomposition of \( c_v^{(3)} \) according to the colour structures is given by

\[
c_v^{(3)} = C_F T n_t \left( C_F c_{FFL} + C_A c_{FAL} + T c_{FHL} + T n_t c_{FLL} \right) + \text{non-}\ n_t \ \text{terms}. \tag{11}
\]

In the notation of Eq. (8) it is understood that in \( \Gamma_v \) the renormalization of the coupling constant and heavy quark mass is already performed. The renormalization of the coupling constant can be done straightforwardly by replacing the bare coupling with the renormalization constant times the renormalized coupling. The mass renormalization, however, is more intricate since we are dealing with on-shell integrals. It is therefore convenient to calculate the counterterms directly by considering one- and two-loop diagrams with zero-momentum insertions in the massive fermion lines. Sample diagrams are shown in Fig. 1(d) and (h). The vertex denoted by a cross is replaced by the mass renormalization constant in the on-shell scheme. One-loop diagrams with two insertions are not needed at the order considered in this paper.

Starting from three-loop level the wave function renormalization constant begins to depend on the QCD gauge parameter, \( \xi \) [35]. However, it is interesting to note that the colour structures entering our result (cf. Eq. (3)) are independent of \( \xi \). As a consequence the quantity \( \Gamma_v \) also has to be independent of \( \xi \) which is indeed the case in our calculation. Actually, the \( \xi \) dependence remaining in the sum of all genuine three-loop diagrams contributing to \( \Gamma_v \) is canceled by the contribution where a two-loop mass counterterm is inserted in the one-loop vertex diagram (cf. Fig. 1(d)). Note that the mass counterterm contribution from the two-loop fermionic diagram (cf. Fig. 1(h)) is \( \xi \) independent. The cancellation of the gauge parameter serves as a welcome check for the correctness of our result.

As already mentioned above, after taking into account all counterterm contributions there are still infra-red divergences left in the quantity \( Z_2 \Gamma_v \) and thus in \( c_v Z_v^{-1} \). This is a consequence of the threshold expansion accompanied by dimensional regularization which is used to extract the matching coefficient. Alternatively it would have been possible to choose a cut-off for the momentum integrations which finally results in a factorization scale.
separating the hard and soft momenta. In our approach the infra-red poles are absorbed into \( \tilde{Z}_v \) which we define in the \( \overline{\text{MS}} \) scheme. As a consequence the matching coefficient itself is finite but scale dependent. In the physical quantities this scale dependence gets canceled against the corresponding contributions from the effective theory. Of course, one has to make sure that for the subtraction of the poles in the effective theory the same scheme is used as in the full theory.

For the renormalization constant \( \tilde{Z}_v \) we obtain

\[
\tilde{Z}_v = 1 + \left( \frac{\alpha_s(\mu)}{\pi} \right)^2 \left( \frac{1}{12} C_F^2 + \frac{1}{8} C_F C_A \right) \frac{\pi^2}{\epsilon} + \left( \frac{\alpha_s(\mu)}{\pi} \right)^3 C_F T n_l \left[ \left( \frac{1}{54} C_F + \frac{1}{36} C_A \right) \frac{\pi^2}{\epsilon^2} - \left( \frac{25}{324} C_F + \frac{37}{432} C_A \right) \frac{\pi^2}{\epsilon} \right] + \ldots ,
\]

(12)

where the ellipses stand for non-\( n_l \) and \( O(\alpha_s^4) \) terms.

Our final result for \( c_v^{(3)} \) reads

\[
c_{FFL} = 46.7(1) + \left( -\frac{17}{12} + \frac{61}{36} \pi^2 - \frac{2}{3} \pi^2 \ln 2 + \frac{1}{3} \zeta(3) \right) L_\mu + \frac{1}{18} \pi^2 L_\mu^2 ,
\]

\[
c_{FAL} = 39.6(1) + \left( \frac{181}{54} - \frac{67}{432} \pi^2 + \frac{5}{9} \pi^2 \ln 2 + \frac{13}{6} \zeta(3) \right) L_\mu + \left( \frac{11}{9} + \frac{1}{12} \pi^2 \right) L_\mu^2 ,
\]

\[
c_{FHL} = -\frac{557}{162} + \frac{26}{81} \pi^2 + \left( -\frac{55}{27} + \frac{4}{27} \pi^2 \right) L_\mu - \frac{4}{9} L_\mu^2 ,
\]

\[
c_{FLL} = -\frac{163}{162} - \frac{4}{27} \pi^2 - \frac{11}{27} L_\mu - \frac{2}{9} L_\mu^2 .
\]

(13)

The uncertainties assigned to the numerical constants in \( c_{FFL} \) and \( c_{FAL} \) are based on a conservative estimate. Note that the precision of these quantities is more than enough for all phenomenological applications. Inserting the numerical values for the colour factors we obtain for \( \mu = m_Q \)

\[
c_v^{(3)} \approx -0.823 n_l^2 + 121. n_l + \text{non-} n_l \text{ terms} .
\]

(14)

The coefficients in Eq. (13) correspond to an expansion parameter \( \alpha_s(\mu) \), as given in Eq. (9). Choosing instead \( \alpha_s(m_Q) \) leads to

\[
\bar{c}_{FFL} = 46.7(1) + \frac{25}{108} \pi^2 L_\mu - \frac{1}{18} \pi^2 L_\mu^2 ,
\]

\[
\bar{c}_{FAL} = 39.6(1) + \frac{37}{144} \pi^2 L_\mu - \frac{1}{12} \pi^2 L_\mu^2 ,
\]

\[
\bar{c}_{FHL} = -\frac{557}{162} + \frac{26}{81} \pi^2 ,
\]

\[
\bar{c}_{FLL} = -\frac{163}{162} - \frac{4}{27} \pi^2 .
\]

(15)
The dependence on $L_{\mu}$ in Eq. (15) is canceled against contributions from the effective theory. They agree with the ones of Ref. [40].

5 Phenomenological applications

Let us in this section estimate the numerical effect of our new terms on the bottom and top system. In particular we consider the decay of the $\Upsilon(1S)$ bound state to leptons and the production of top quark pairs close to threshold.

Next to the matching coefficient considered in the previous Sections a crucial ingredient for these quantities is the wave function at the origin. Currently the second order is known completely [41–45] and at order $\alpha_s^3$ the quadratically [46,47] and linearly [12,40] enhanced logarithms and the corrections proportional to $\beta_0^3$ [8,9] are available. It is convenient to introduce the quantity

$$\rho_1 = \frac{|\psi_1(0)|^2}{|\psi_C(0)|^2} = C_F^2 \alpha_s^3 m_q^2/(8\pi n^3).$$

Let us for completeness list the results for principle quantum number $n = 1$

$$\rho_1 = 1 + \frac{\alpha_s(\mu_s)}{\pi} \left[ \left( 4 - \frac{2}{3} \pi^2 \right) \beta_0 + \frac{3}{4} a_1 \right] + \left( \frac{\alpha_s(\mu_s)}{\pi} \right)^2 \left\{ \frac{-C_A C_F}{2} + \left( -2 + \frac{2}{3} S(S+1) \right) C_F^2 \right\} \left( \frac{\pi^2}{2} \right)^2 \ln(C_F \alpha_s(\mu_s))$$

$$+ \left( -\frac{5}{3} \pi^2 + 20 \zeta(3) + \frac{1}{9} \right) \beta_0^2 + \left( 4 - \frac{2}{3} \pi^2 \right) \beta_1 + \left( \frac{5}{2} - \frac{2}{3} \pi^2 \right) \beta_0 a_1$$

$$+ \frac{3}{16} a_1^2 + \frac{3}{16} a_2 + \frac{9}{4} \pi^2 C_A C_F + \left( \frac{33}{8} - \frac{13}{9} S(S+1) \right) \pi^2 C_F^2 \right\}$$

$$+ \left( \frac{\alpha_s(\mu_s)}{\pi} \right)^3 \left\{ \pi^2 C_2 \ln^2 (C_F \alpha_s(\mu_s)) + \pi^2 C_1 \ln(C_F \alpha_s(\mu_s)) + C_0^3 \ln \right\},$$ (16)

with

$$C_2 = \left( -2 C_A C_F + \left( -4 + \frac{4}{3} S(S+1) \right) C_F^2 \right) \beta_0 - \frac{2}{3} C_A^2 C_F$$

$$+ \left( \frac{41}{12} + \frac{7}{12} S(S+1) \right) C_A C_F^2 - \frac{3}{2} C_F^3,$$ (17)

Note that in Ref. [40] there is a typo in the coefficient of the $L_{\mu}^2$ term. The “$-3/2$” should read “$+1$.”
\[ C_1 = \left[ \left( -3 + \frac{2}{3} \pi^2 \right) C_A C_F + \left( \frac{4}{3} \pi^2 - \left( \frac{10}{9} + \frac{4}{9} \pi^2 \right) S(S+1) \right) C_F^2 \right] \beta_0 \\
+ \left[ -\frac{3}{4} C_A C_F + \left( -\frac{9}{4} + \frac{2}{3} S(S+1) \right) C_F^2 \right] a_1 + \frac{1}{4} C_A^3 + \left( \frac{59}{36} - 4 \ln 2 \right) C_A^2 C_F \\
+ \left( \frac{143}{36} - 4 \ln 2 - \frac{19}{108} S(S+1) \right) C_A C_F^2 + \left( -\frac{35}{18} + 8 \ln 2 - \frac{1}{3} S(S+1) \right) C_F^3 \\
+ \left( -\frac{32}{15} + 2 \ln 2 + (1 - \ln 2) S(S+1) \right) C_F^2 T + \frac{49}{36} C_A C_F T n_l \\
+ \left( \frac{8}{9} - \frac{10}{27} S(S+1) \right) C_F^2 T n_l \\ (18) \]

and

\[ C_{\beta_0}^3 = \beta_0^3 \left[ -20 + \frac{22}{3} \pi^2 + 112 \zeta(3) - \frac{7}{5} \pi^4 - 12 \pi^2 \zeta(3) - 40 \zeta(5) - 16 \zeta(3)^2 \\
+ \frac{4}{105} \pi^6 \right], \quad (19) \]

where \( \mu_s = C_F m_q \alpha_s(\mu_s) \) is the soft scale. It is straightforward to obtain the result for general \( \alpha_s(\mu) \) using standard renormalization group analyses. In Eqs. (16)–(18) \( S \) is the spin quantum number which is equal to one in our applications. The ellipses in Eq. (16) represent yet unknown corrections like, e.g., the pure ultrasoft contributions.

For completeness we provide the one- and two-loop coefficients of the \( \beta \) function and the static potential which are given by

\[ \beta_0 = \frac{1}{4} \left( \frac{11}{3} C_A - \frac{4}{3} T n_l \right), \]
\[ \beta_1 = \frac{1}{16} \left( \frac{34}{3} C_A^2 - \frac{20}{3} C_A T n_l - 4 C_F T n_l \right), \]
\[ a_1 = \frac{31}{9} C_A - \frac{20}{9} T n_l, \]
\[ a_2 = \left( \frac{4343}{162} + 4 \pi^2 + \frac{22}{3} \zeta(3) - \frac{1}{4} \pi^4 \right) C_A^2 - \left( \frac{1798}{81} + \frac{56}{3} \zeta(3) \right) C_A T n_l \\
- \left( \frac{55}{3} - 16 \zeta(3) \right) C_F T n_l + \left( \frac{20}{9} T n_l \right)^2. \quad (20) \]

\section*{5.1 Bottom system}

The leptonic decay of the \( \Upsilon(1S) \) state can be cast in the form [41–45]

\[ \Gamma(\Upsilon(1S) \to l^+ l^-) = \Gamma^{LO} \rho_1 \left[ C_v^2(m_b) + \frac{C_F^2 \alpha_s^2(\mu_s)}{12} c_v(m_b) (d_v(m_b) + 3) \right] + \ldots, \quad (21) \]
with $\Gamma^{\text{LO}} = 4\pi N_c Q_b^2 \alpha^2 |\psi_1^C(0)|^2 / (3m_b^2)$, $Q_b = -1/3$, $N_c = 3$, $\alpha$ is Sommerfeld’s fine-structure constant and nonperturbative contributions to Eq. (21) are ignored.

Inserting the perturbative expansion for $\rho_1$ and $c_v$ we obtain

$$\Gamma_1 \approx \Gamma^{\text{LO}}_1 (1 - 1.70 \alpha_s(m_b) - 7.98 \alpha_s^2(m_b) + 30.0 \alpha_s^3(m_b)|_{m_l} + \ldots)$$

$$\times \left[1 - 0.30 \alpha_s(\mu_s) + \alpha_s^2(\mu_s) (17.2 - 5.19 \ln \alpha_s(\mu_s))\right.$$ 

$$+ \alpha_s^3(\mu_s) \left(-14.4 \ln^2 \alpha_s(\mu_s) + 0.17 \ln \alpha_s(\mu_s) - 34.9 |_{\beta_0^3}\right) + \ldots], \quad (22)$$

where in the matching coefficient $\mu = m_b$ has been chosen and the corresponding strong coupling is defined with five and $\alpha_s(\mu_s)$ with four active flavours.

Starting from $\alpha_s(M_Z) = 0.118$ we have used the program RunDec [48] to obtain $\alpha_s(m_b) = 0.2096$ and $\alpha_s(\mu_s) = 0.2967$ with $m_b = 5.3$ GeV and $\mu_s = 2.0967$ GeV which leads to

$$\Gamma_1 \approx \Gamma^{\text{LO}}_1 (1 - 0.446\text{NLO} + 1.75\text{NNLO} - 1.20\text{NNLO}^\prime + \ldots), \quad (23)$$

where Eq. (22) is expanded and terms of order $\alpha_s^4$ are dropped consistently. The prime reminds that the third-order corrections are not complete. Apart from the new contribution to $c_v$ and the known third-order corrections to $\rho_1$ we have also included all interference terms which are proportional to powers of $n_l$. Note that the new corrections are responsible for the reduction of $N^3\text{LO}^\prime$ terms from $-1.67$ to $-1.20$ which amounts to about 47% of the Born cross section. However, in total the fermionic corrections tend to further reduce the strong increase of the perturbative coefficients leading to an overall correction factor of approximately 10%.

We have performed the numerical analysis also for $m_b = 4.8$ GeV. There are changes in the individual contributions to $\Gamma_1$ (c.f. Eq. (23)) of the order of a few per cent, however, the final correction factor remains the same.

### 5.2 Top system

In the top-quark case, the nonperturbative effects are negligible. However, the effect of the top-quark total decay width $\Gamma_1$ has to be properly taken into account [49], as it is relatively large and smears out the Coulomb-like resonances below threshold. The NNLO analysis of the cross section [5] shows that only the ground-state pole gives rise to a prominent resonance.

A crucial quantity in connection to the threshold production of top quark pairs is the peak of the normalized cross section $R = \sigma(e^+e^- \rightarrow t\bar{t})/\sigma(e^+e^- \rightarrow \mu^+\mu^-)$. It is dominated by the contribution from the would-be toponium ground-state, which can be cast in the from

$$R_1(e^+e^- \rightarrow t\bar{t}) = R_1^{\text{LO}} \rho_1 \left[c_v^2(m_t) + \frac{C_F^2 \alpha_s^2(\mu_s)}{12} c_v(m_t) (d_v(m_t) + 3)\right] + \ldots, \quad (24)$$
with the leading order term $R_{1}^{\text{LO}} = 6\pi N_c Q_t^2 |\psi_C^t(0)|^2 / (m_t^2 \Gamma_t)$. The contributions from the higher Coulomb-like poles and the continuum are not included in Eq. (24).

The analog equations to Eqs. (22) and (23) read

$$R_1 \approx R_{1}^{\text{LO}} (1 - 1.70 \alpha_s(m_t) - 7.89 \alpha_s^2(m_t) + 37.2 \alpha_s^3(m_t)|_n + \ldots) \times \left[ 1 - 0.43 \alpha_s(\mu_s) + \alpha_s^2(\mu_s) (16.1 - 5.19 \ln \alpha_s(\mu_s)) + \alpha_s^3(\mu_s) \left( -13.8 \ln^2 \alpha_s(\mu_s) + 2.06 \ln \alpha_s(\mu_s) - 27.2 |\beta_3^0| + \ldots \right) \right],$$

(25)

where $\alpha_s(m_t)$ and $\alpha_s(\mu_s)$ are defined with six and five active flavours, respectively. Using again $\alpha_s(M_Z) = 0.118$ one gets $\alpha_s(m_t) = 0.1075$ and $\alpha_s(\mu_s) = 0.1398$ with $m_t = 175$ GeV and $\mu_s = 32.625$ GeV and finally

$$R_1 \approx R_{1}^{\text{LO}} (1 - 0.243_{\text{NLO}} + 0.435_{\text{NNLO}} - 0.195_{\text{N^3LO'}} + \ldots).$$

(26)

The fermionic corrections to $c_v$ are responsible for a reduction of the third-order coefficient from $-0.268$ to $-0.195$ and thus amount to moderate 7% of the leading order term. Similarly as for the bottom quark case also for the top quark the perturbative series is alternating and the third-order coefficient tends to stabilize the expansion. It is interesting to note that after the inclusion of our new terms the total corrections amount to less than 1%.

6 Conclusions and outlook

This paper deals with the question of establishing a relation for the vector current between full QCD and NRQCD. The corresponding matching coefficient, $c_v$, constitutes a building block in all threshold phenomena involving a vector coupling. The main result of this paper is the fermionic three-loop contribution to $c_v$ which contains a closed light fermion loop. The numerical effect of the new terms is relatively big and amounts to about 47% for the bottom and to about 7% for the top quark system. However, their inclusion leads to a reduction of the overall corrections. E.g., in the case of the top quark the corrections to the normalization at the peak of the production cross section amount to less than 1% after including all currently known perturbative terms.

Several steps still have to be taken in order to arrive at the complete analysis of the top-anti-top quark system at threshold. Next to the non-fermionic pieces to $c_v$ the major building blocks which are still missing are the ultra-soft corrections and the three-loop static potential.

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Figure 2: Three-loop master integrals. Bold lines denote massive lines with mass $2m_Q$, thin lines denote massive lines with mass $m_Q$ and dashed lines denote massless lines. All external lines are on-shell. A dot on a line denotes a squared propagator.

A Results for the master integrals

The master integrals for the three-loop functions of Eq. (4) are shown in Fig. 2. For the self-energy integrals $I_1 - I_6$ the external momentum squared equals the square of the heavy quark mass, $q^2 = m_Q^2$. For the integrals $I_7$ and $I_8$ we have $q^2 = 4m_Q^2$. The momenta $q_1$ and $q_2$ flowing out of the vertex diagrams on the right fulfill $q_1^2 = q_2^2 = m_Q^2$ with $(q_1 + q_2)^2 = 4m_Q^2$. In Minkowski space the results for the master integrals read

$$I_1 = J^{(3)}_+ (0, 1, 0, 1, 1, 0, 1, 0, 1)$$

$$= m_Q^2 \left( \frac{\mu^2}{m_Q^2} e^{-\gamma_E} \right)^{3\varepsilon} \left\{ \frac{1}{3\varepsilon^3} + \frac{5}{3\varepsilon^2} + \left( 4 + \frac{3}{4} \pi^2 \right) \frac{1}{\varepsilon} - \frac{10}{3} + \frac{11}{4} \pi^2 + \frac{25}{3} \zeta(3) + \left( -\frac{302}{3} + 2\pi^2 + \frac{89}{3} \zeta(3) + \frac{3059}{1440} \pi^4 \right) \varepsilon + \left( -734 - \frac{69}{2} \pi^2 + 16 \zeta(3) + \frac{9751}{1440} \pi^4 \right) \varepsilon + \frac{107}{4} \pi^2 \zeta(3) + \frac{2309}{5} \zeta(5) \right\} \varepsilon^2 + \mathcal{O}(\varepsilon^3),$$

(27)

$$I_2 = J^{(3)}_+ (0, 1, 1, 1, 0, 1, 1, 0, 0)$$

$$= -m_Q^2 \left( \frac{\mu^2}{m_Q^2} \right)^{3\varepsilon} \frac{\Gamma^4(1-\varepsilon) \Gamma^2(\varepsilon) \Gamma(3\varepsilon - 1) \Gamma(3 - 6\varepsilon)}{\Gamma^2(2 - 2\varepsilon) \Gamma(3 - 4\varepsilon)},$$

(28)
\[ I_3 = L_{+}^{(3,n_1)}(0, 0, 1, 1, 1, 1, 0, 1, 0) \]
\[ = m_Q^2 \left( \frac{\mu^2}{m_Q^2} e^{-\gamma_E} \right)^{3\epsilon} \left\{ \frac{2}{3\epsilon^3} + \frac{10}{3\epsilon^2} + \left( \frac{26}{3} + \frac{1}{2\pi^2} \right) \frac{1}{\epsilon} + 2 + \frac{9}{2}\pi^2 + \frac{14}{3}\zeta(3) \right. \]
\[ + \left( -\frac{398}{3} + \frac{53}{2}\pi^2 - 16\pi^2 \ln 2 + \frac{238}{3}\zeta(3) + \frac{287}{720}\pi^4 \right) \epsilon + \left( -1038 + \frac{259}{2}\pi^2 \right) \]
\[ -160\pi^2 \ln 2 + \frac{128}{3}\pi^2 \ln 2 + \frac{1862}{3}\zeta(3) + \frac{323}{720}\pi^4 + \frac{7}{2}\pi^2 \zeta(3) + \frac{478}{5}\zeta(5) \]
\[ + \frac{64}{3} \ln^4 2 + 512a_4 \right\} \epsilon^2 + \mathcal{O}(\epsilon^3) \}, \tag{29} \]

\[ I_4 = J_{+}^{(3)}(0, 0, 0, 1, 1, 0, 1, 0, 1) \]
\[ = m_Q^4 \left( \frac{\mu^2}{m_Q^2} \right)^{3\epsilon} \frac{\Gamma^2(1 - \epsilon)\Gamma(\epsilon)\Gamma^2(2\epsilon - 1)\Gamma(3\epsilon - 2)}{\Gamma(4\epsilon - 2)\Gamma(2 - \epsilon)}, \tag{30} \]

\[ I_5 = J_{+}^{(3)}(0, 1, 0, 1, 0, 0, 1, 0, 1) \]
\[ = m_Q^4 \left( \frac{\mu^2}{m_Q^2} \right)^{3\epsilon} \frac{\Gamma(1 - \epsilon)\Gamma(\epsilon)\Gamma(2\epsilon - 1)\Gamma(3\epsilon - 2)}{\Gamma(2 - \epsilon)\Gamma(3 - 3\epsilon)}, \tag{31} \]

\[ I_6 = J_{+}^{(3)}(0, 0, 1, 1, 1, 0, 1, 0, 0) \]
\[ = m_Q^4 \left( \frac{\mu^2}{m_Q^2} \right)^{3\epsilon} \frac{\Gamma^3(1 - \epsilon)\Gamma(2\epsilon - 1)\Gamma(3\epsilon - 2)\Gamma(5 - 6\epsilon)}{\Gamma(3 - 3\epsilon)\Gamma(4 - 4\epsilon)}, \tag{32} \]

\[ I_7 = J_{+}^{(3)}(0, 0, 0, 1, 1, 0, 1, 0, 1) \]
\[ = m_Q^4 \left( \frac{\mu^2}{m_Q^2} e^{-\gamma_E} \right)^{3\epsilon} \left\{ \frac{1}{3\epsilon^3} + \frac{1}{2\epsilon^2} + \left( -\frac{17}{36} + \frac{1}{12}\pi^2 \right) \frac{1}{\epsilon} - 6.6827387(1) \]
\[ - 56.300353(1)\epsilon - 209.48231(1)\epsilon^2 + \mathcal{O}(\epsilon^3) \right\}, \tag{33} \]

\[ I_8 = J_{+}^{(3)}(0, 0, 0, 2, 1, 0, 1, 0, 1) \]
\[ = -m_Q^2 \left( \frac{\mu^2}{m_Q^2} e^{-\gamma_E} \right)^{3\epsilon} \left\{ \frac{1}{3\epsilon^3} + \frac{2}{3\epsilon^2} + \left( -\frac{8}{3} + \frac{5}{6}\pi^2 \right) \frac{1}{\epsilon} + 10.797602(1) \]
\[ + 62.250613(1)\epsilon + \mathcal{O}(\epsilon^2) \right\}, \tag{34} \]

\[ I_9 = J_{+}^{(3)}(0, 1, 0, 1, 1, 0, 1, 0, 1) \]
\[ = m_Q^2 \left( \frac{\mu^2}{m_Q^2} e^{-\gamma_E} \right)^{3\epsilon} \left\{ \frac{1}{3\epsilon^3} + \frac{5}{3\epsilon^2} + \left( \frac{10}{3} + \frac{3}{4}\pi^2 \right) \frac{1}{\epsilon} + 33.8328(4) + 152.870(4)\epsilon \]
\[ + \mathcal{O}(\epsilon^2) \right\}, \tag{35} \]
\[ I_{10} = J_{+}^{(3, n)}(0, 0, 1, 1, 0, 1, 1, 0) \]
\[ = m_{Q}^{2} \left( \frac{\mu^{2}}{m_{Q}^{2}} e^{-\gamma E} \right)^{3\epsilon} \left\{ \frac{2}{3\epsilon^{3}} + \frac{10}{3\epsilon^{2}} + \left( 8 + \frac{1}{2} \pi^{2} \right) \frac{1}{\epsilon} + 52.5698(4) + 145.087(4) \epsilon \right. \]
\[ + 562.250(14) \epsilon^{2} + O(\epsilon^{3}) \right\}, \tag{36} \]
\[ I_{11} = J_{-}^{(3)}(0, 1, 0, 1, 0, 1, 0, 1) \]
\[ = m_{Q}^{2} \left( \frac{\mu^{2}}{m_{Q}^{2}} e^{-\gamma E} \right)^{3\epsilon} \left\{ \frac{1}{2\epsilon^{3}} + \frac{11}{6\epsilon^{2}} + \left( -\frac{1}{6} + \frac{29}{24} \pi^{2} \right) \frac{1}{\epsilon} + 34.791(4) + 154.08(2) \epsilon \right. \]
\[ + O(\epsilon^{2}) \right\}, \tag{37} \]
\[ I_{12} = J_{-}^{(3)}(0, 1, 0, 1, 0, 1, 0, 2) \]
\[ = \left( \frac{\mu^{2}}{m_{Q}^{2}} e^{-\gamma E} \right)^{3\epsilon} \left\{ \frac{1}{6\epsilon^{3}} + \frac{1}{2\epsilon^{2}} + \left( \frac{1}{6} + \frac{7}{24} \pi^{2} \right) \frac{1}{\epsilon} + 7.024(4) + 32.04(2) \epsilon \right. \]
\[ + O(\epsilon^{2}) \right\}, \tag{38} \]

where \( \zeta(5) = 1.036927 \ldots \) and \( a_{4} = \text{Li}_{4}(1/2) = 0.517479 \ldots \)

\( I_{1} \) was calculated in Ref. [35]. We have repeated the calculation described in the reference with the program \textsc{XSummer} [51] and find complete agreement. The results for \( I_{3} - I_{6} \) can be found in Ref. [21]. We have checked the result for \( I_{3} \) numerically with the help of a one-fold Mellin-Barnes [52, 53] representation and find complete agreement. Note, that \( I_{2}, I_{4}, I_{5} \) and \( I_{6} \) are quite simple to evaluate and are available for general \( \epsilon \). Nevertheless the result for \( I_{6} \) as given in Ref. [35] is not correct whereas the correct result can be found in Ref. [21]. The pole part of \( I_{7} \) agrees with the result of Ref. [54].

The remaining master integrals, \( I_{7} - I_{12} \), have been evaluated with the help of the Mellin-Barnes method where the evaluation of the integrals has been performed with the program \textsc{MB} [55]. \( I_{7} \) and \( I_{8} \) can be expressed in terms of a one-fold Mellin-Barnes representation and are thus known with a quite high precision. On the other hand, \( I_{10} \) is represented by a two-fold and \( I_{9}, I_{11} \) and \( I_{12} \) even by a three-fold integration which results in less accurate results. The quoted uncertainties in the above equations correspond to twice the Vegas error given by \textsc{MB} for the multi-dimensional integrals and to a conservative estimate in case of the one-dimensional integrals \( I_{7} \) and \( I_{8} \). Note that the latter errors are negligible.

As can be seen in the above results some of the master integrals are needed to higher order in \( \epsilon \) which on one hand makes the calculation very tedious and on the other hand leads to less accurate results. For this reason we decided to change basis and switch — at least for some of the integrals — to the so-called \( \epsilon \)-finite master integrals [26] which have the advantage that the coefficient function is finite and thus the integral itself is only needed to order \( \epsilon^{0} \).
Figure 3: $\epsilon$-finite master integrals. The same coding as in Fig. 2 is adopted.

Since $I_1$—$I_6$ are known analytically, a replacement is, of course, not necessary. Furthermore, for $I_7$ and $I_8$ the numerical precision is sufficient for our calculation. As far as the remaining four integrals are concerned, we found it convenient to replace $I_9$ and $I_{12}$ by the integrals shown in Fig. 3. Their numerical evaluation with the help of MB is straightforward leading to the results

$$I_f^9 = J_1^{(3)}(0, 1, 1, 1, 1, 0, 1, 0, 1, 1) = \left(\frac{\mu^2}{m_Q^2} e^{-\gamma_E}\right)^{3\epsilon} \left\{ \frac{1}{6\epsilon^3} + \frac{3}{2\epsilon^2} + \left(\frac{55}{6} + \frac{3}{8}\pi^2\right) \frac{1}{\epsilon} + 64.678(8) + O(\epsilon) \right\},$$

$$I_f^{12} = J_1^{(3)}(0, 1, 0, 1, 1, 1, 1, 0, 1, 1) = \left(\frac{\mu^2}{m_Q^2} e^{-\gamma_E}\right)^{3\epsilon} \left\{ \frac{2.4041(4)}{\epsilon} + 8.1(2) + O(\epsilon) \right\}.$$

Switching from $I_9$ and $I_{12}$ to $I_f^9$ and $I_f^{12}$ reduces the number of coefficients which are only known numerically from 17 to 14. In particular the $1/\epsilon$-poles of $I_9$ and $I_{12}$ have been determined in analytical form from the $\epsilon$-finite integrals via the corresponding IBP relations.

A further reduction is achieved after exploiting the locality and incorporating the knowledge of the linear $\ln(\mu^2/m_Q^2)$ term in $c_v$ [40] which we have checked numerically in a first step. In this way the analytical result for the $1/\epsilon$-pole of $I_{11}$ has been determined.

In total ten (eleven) numerical coefficients contribute to our final result given in Eqs. (13) and (14) using the $\epsilon$-finite (“normal”) basis.

In the end it turned out, that the numerical precision is better using the “normal” basis. The reason is, that the uncertainty of the $\epsilon^0$-coefficient of $I_f^{12}$ is by far the largest. Still, it was useful to consider the $\epsilon$-finite basis since it enabled us to determine analytical results for two integral coefficients of the “normal” basis.

References

[1] W. E. Caswell and G. P. Lepage, Phys. Lett. B 167 (1986) 437.
[2] G. T. Bodwin, E. Braaten and G. P. Lepage, Phys. Rev. D 51 (1995) 1125 [Erratum-ibid. D 55 (1997) 5853] arXiv:hep-ph/9407339.

[3] N. Brambilla et al., arXiv:hep-ph/0412158.

[4] M. Martinez and R. Miquel, Eur. Phys. J. C 27 (2003) 49 arXiv:hep-ph/0207315.

[5] A. H. Hoang et al., Eur. Phys. J. directC 2 (2000) 1 arXiv:hep-ph/0001286.

[6] B. A. Kniehl, A. A. Penin, V. A. Smirnov and M. Steinhauser, Nucl. Phys. B 635 (2002) 357 arXiv:hep-ph/0203166.

[7] A. A. Penin and M. Steinhauser, Phys. Lett. B 538 (2002) 335 arXiv:hep-ph/0204290.

[8] A. A. Penin, V. A. Smirnov and M. Steinhauser, Nucl. Phys. B 716 (2005) 303 arXiv:hep-ph/0501042.

[9] M. Beneke, Y. Kiyo and K. Schuller, Nucl. Phys. B 714 (2005) 67 arXiv:hep-ph/0501289.

[10] A. Pineda, Phys. Rev. D 65 (2002) 074007 arXiv:hep-ph/0109117.

[11] A. Pineda, Phys. Rev. D 66 (2002) 054022 arXiv:hep-ph/0110216.

[12] A. H. Hoang, Phys. Rev. D 69 (2004) 034009 arXiv:hep-ph/0307376.

[13] A. A. Penin, A. Pineda, V. A. Smirnov and M. Steinhauser, Nucl. Phys. B 699 (2004) 183 arXiv:hep-ph/0406175.

[14] A. H. Hoang and C. J. Reisser, Phys. Rev. D 71 (2005) 074022 arXiv:hep-ph/0412258.

[15] D. Eiras and M. Steinhauser, arXiv:hep-ph/0605227.

[16] M. Beneke and V. A. Smirnov, Nucl. Phys. B 522 (1998) 321 arXiv:hep-ph/9711391.

[17] V. A. Smirnov, “Applied asymptotic expansions in momenta and masses,” Springer (2002).

[18] P. Nogueira, J. Comput. Phys. 105 (1993) 279.

[19] R. Harlander, T. Seidensticker and M. Steinhauser, Phys. Lett. B 426 (1998) 125 hep-ph/9712228.

[20] T. Seidensticker, hep-ph/9905298.

[21] S. Laporta and E. Remiddi, Phys. Lett. B 379 (1996) 283 arXiv:hep-ph/9602417.

[22] S. Laporta, Int. J. Mod. Phys. A 15 (2000) 5087 arXiv:hep-ph/0102033.
[23] P. A. Baikov, Phys. Lett. B 385 (1996) 404 [arXiv:hep-ph/9603267].
[24] P. A. Baikov, Nucl. Instrum. Meth. A 389 (1997) 347 [arXiv:hep-ph/9611449].
[25] V. A. Smirnov and M. Steinhauser, Nucl. Phys. B 672 (2003) 199 [arXiv:hep-ph/0307088].
[26] K. G. Chetyrkin, M. Faisst, C. Sturm and M. Tentyukov, Nucl. Phys. B 742 (2006) 208 [arXiv:hep-ph/0601165].
[27] K. G. Chetyrkin and F. V. Tkachov, Nucl. Phys. B 192 (1981) 159.
[28] C. Anastasiou and A. Lazopoulos, JHEP 0407 (2004) 046 [arXiv:hep-ph/0404258].
[29] P. Marquard and D. Seidel, unpublished.
[30] C. Bauer, A. Frink and R. Kreckel, arXiv:cs.sc/0004015.
[31] R. H. Lewis, Fermat’s User Guide, http://www.bway.net/~lewis.
[32] M. Tentyukov and J. A. M. Vermaseren, arXiv:cs.sc/0604052.
[33] J. A. M. Vermaseren, arXiv:math-ph/0010025.
[34] D. J. Broadhurst, N. Gray and K. Schilcher, Z. Phys. C 52 (1991) 111.
[35] K. Melnikov and T. van Ritbergen, Nucl. Phys. B 591 (2000) 515 [arXiv:hep-ph/0005131].
[36] G. Källen and A. Sarby, K. Dan. Vidensk. Selsk. Mat.-Fis. Medd. 29, N17 (1955) 1.
[37] A. Czarnecki and K. Melnikov, Phys. Rev. Lett. 80 (1998) 2531 [arXiv:hep-ph/9712222].
[38] M. Beneke, A. Signer and V. A. Smirnov, Phys. Rev. Lett. 80 (1998) 2535 [arXiv:hep-ph/9712302].
[39] B. A. Kniehl, A. Onishchenko, J. H. Piclum and M. Steinhauser, Phys. Lett. B 638 (2006) 209 [arXiv:hep-ph/0604072].
[40] B. A. Kniehl, A. A. Penin, M. Steinhauser and V. A. Smirnov, Phys. Rev. Lett. 90 (2003) 212001 [Erratum-ibid. 91 (2003) 139903(E)] [arXiv:hep-ph/0210161].
[41] J. H. Kühn, A. A. Penin and A. A. Pivovarov, Nucl. Phys. B 534 (1998) 356 [arXiv:hep-ph/9801356].
[42] A. A. Penin and A. A. Pivovarov, Phys. Lett. B 435 (1998) 413 [arXiv:hep-ph/9803363].
[43] A. A. Penin and A. A. Pivovarov, Nucl. Phys. B 549 (1999) 217 [arXiv:hep-ph/9807421].

[44] A. A. Penin and A. A. Pivovarov, Nucl. Phys. B 550 (1999) 375 [arXiv:hep-ph/9810496].

[45] K. Melnikov and A. Yelkhovsky, Phys. Rev. D 59 (1999) 114009 [arXiv:hep-ph/9805270].

[46] B. A. Kniehl and A. A. Penin, Nucl. Phys. B 577 (2000) 197 [arXiv:hep-ph/9911414].

[47] A. V. Manohar and I. W. Stewart, Phys. Rev. D 63 (2001) 054004 [arXiv:hep-ph/9911414].

[48] K. G. Chetyrkin, J. H. K"uhn and M. Steinhauser, Comput. Phys. Commun. 133 (2000) 43 [arXiv:hep-ph/0003107].

[49] V. S. Fadin and V. A. Khoze, JETP Lett. 46 (1987) 525 [Pisma Zh. Eksp. Teor. Fiz. 46 (1987) 417].

[50] D. Binosi and L. Theussl, Comput. Phys. Commun. 161 (2004) 76 [arXiv:hep-ph/0309015].

[51] S. Moch and P. Uwer, Comput. Phys. Commun. 174 (2006) 759 [arXiv:math-ph/0508008].

[52] V. A. Smirnov, Phys. Lett. B 460 (1999) 397 [arXiv:hep-ph/9905323].

[53] J. B. Tausk, Phys. Lett. B 469 (1999) 225 [arXiv:hep-ph/9905323].

[54] S. Groote, J. G. Körner and A. A. Pivovarov, Eur. Phys. J. C 36 (2004) 471 [arXiv:hep-ph/0403122].

[55] M. Czakon, [arXiv:hep-ph/0511200]