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Large-m_c Asymptotic Behaviour of the $\mathcal{O}(\alpha_s^2)$ Corrections to $\bar{B} \to X_s\gamma$

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Abstract

We present details of our evaluation of the NNLO QCD corrections to $\mathcal{B}(\bar{B} \to X_s\gamma)$ in the heavy charm limit ($m_c \gg \frac{m_b}{2}$). Results of this calculation have been essential for estimating $\mathcal{O}(\alpha_s^2)$ effects in this branching ratio via interpolation in m_c.

1 Introduction

The inclusive branching ratio $\mathcal{B}(\bar{B} \to X_s\gamma)$ is well-known to provide important constraints on extensions of the SM [1]. Its evaluation is based on an approximate equality of the hadronic and and partonic decay widths[1]

$$\Gamma(\bar{B} \to X_s\gamma)_{E_\gamma > E_0} \;\simeq\; \Gamma(b \to X_s^p\gamma)_{E_\gamma > E_0}, \tag{1.1}$$

where X_s^p stands for s, sg, sgg, $sq\bar{q}$, etc. This approximation works well only in a certain range of E_0, namely when E_0 is large ($E_0 \sim \frac{m_b}{2}$) but not too close to the endpoint ($m_b - 2E_0 \gg \Lambda_{\rm QCD}$). It has become customary to use $E_0 = 1.6$ GeV $\simeq \frac{m_b}{3}$ for comparing theory with experiment. Calculations including the $\mathcal{O}(\alpha_s^2)$ and $\mathcal{O}(\alpha_{\rm em})$ effects in the SM give [4, 5]

$$\mathcal{B}(\bar{B} \to X_s\gamma)_{E_\gamma > 1.6\,{\rm GeV}} = (3.15 \pm 0.23) \times 10^{-4}, \tag{1.2}$$

where the uncertainty is dominated by $\mathcal{O}(\alpha_s\Lambda_{\rm QCD}/m_b)$ non-perturbative effects [2].

The currently available experimental world averages read

$$\mathcal{B}(\bar{B} \to X_s\gamma)_{E_\gamma > 1.6\,{\rm GeV}} = \begin{cases} (3.55 \pm 0.24_{\rm exp} \pm 0.09_{\rm model}) \times 10^{-4} & [6], \\ (3.50 \pm 0.14_{\rm exp} \pm 0.10_{\rm model}) \times 10^{-4} & [7]. \end{cases} \tag{1.3}$$

They have been obtained from the measurements of CLEO [8], BABAR [9] and BELLE [10,11] by extrapolation in E_0 according to various photon energy spectrum models, whose parameters have been fit to data.[2] The SM prediction (1.2) and the averages (1.3) are consistent at the 1.2σ level.

The $\mathcal{O}(\alpha_s^2)$ contributions to the branching ratio amount to around 10%, which exceeds the experimental errors and theoretical non-perturbative uncertainties. However, these corrections have not been included in a complete manner in Eq. (1.2) because their charm-mass dependence remains unknown beyond the BLM-approximation [12]. Instead, we have calculated all the m_c-dependent non-BLM corrections in the $m_c \gg \frac{m_b}{2}$ limit, and performed their interpolation in m_c down to the measured value $m_c \simeq \frac{m_b}{4}$, assuming that they vanish at $m_c = 0$. Our previous paper [5] contains only the final analytic expressions for the large-m_c results together with a description of the interpolation. Presenting details of the large-m_c calculation is the purpose of the present article.

The paper is organized as follows. Sec. 2 is devoted to recalling the relevant definitions from Ref [5]. Sec. 3 contains an explanation why we did not use asymptotic expansions of three-loop on-shell Feynman diagrams. Our actual method that involved charm decoupling at the Lagrangian level is described in Secs. 4 and 5. We conclude in Sec. 6. Expressions for the relevant functions $\phi_{ij}^{(1)}$ that originate from $b \to s\gamma g$ are collected in the Appendix.

[1] Corrections to Eq. (1.1) of various origin have been widely discussed in the literature, most recently in Ref. [2]. A compact overview of previous results can be found in Ref. [3].

[2] Ref. [6] gives a larger error than [7] because it includes results at $E_0 \geq 1.8$ GeV from the older measurements [8, 9] only, ignoring the more precise ones from Ref. [11].

2 Notation

We shall strictly follow the notation of Ref. [5]. The present section collects the most important definitions only. The effective Lagrangian that matters for evaluating QCD corrections to $b \to X_s^p \gamma$ reads[3]

$$\mathcal{L}_{\rm eff} \;=\; \mathcal{L}_{\rm QCD\times QED}(u,d,s,c,b) \;+\; \frac{4G_F}{\sqrt{2}} V_{ts}^* V_{tb} \sum_{i=1}^{8} C_i Q_i, \tag{2.1}$$

where the local flavour-changing operators Q_i arise from decoupling of the W boson and all the heavier particles. We shall need explicit expressions for the following ones:

$$\begin{array}{rclrcl} Q_1 &=& (\bar{s}_L \gamma_\mu T^a c_L)(\bar{c}_L \gamma^\mu T^a b_L), & Q_2 &=& (\bar{s}_L \gamma_\mu c_L)(\bar{c}_L \gamma^\mu b_L), \\ && Q_4 \;=\; (\bar{s}_L \gamma_\mu T^a b_L) \sum_q (\bar{q}\gamma^\mu T^a q), &&& \\ Q_7 &=& \frac{e}{16\pi^2} m_b (\bar{s}_L \sigma^{\mu\nu} b_R) F_{\mu\nu}, & Q_8 &=& \frac{g}{16\pi^2} m_b (\bar{s}_L \sigma^{\mu\nu} T^a b_R) G^a_{\mu\nu}. \end{array} \tag{2.2}$$

The remaining three (Q_3, Q_5 and Q_6) are similar to Q_4 but involve different Dirac and color structures. The sum over q in Q_4 runs over all the active flavours (u,d,s,c,b). Masses of the light quarks (u,d,s) are neglected throughout the paper, except for the collinear logarithm in Eq. (A.3) of the Appendix.

The Wilson Coefficients (WCs) C_i are assumed to be $\overline{\rm MS}$-renormalized at the scale $\mu_b \sim \frac{m_b}{2}$. To avoid scheme-dependence at the Leading Order (LO) in QCD, one usually works with certain linear combinations called "effective coefficients"

$$C_i^{\rm eff} = \begin{cases} C_i, & \text{for } i = 1,...,6, \\ C_7 + \sum_{j=1}^{6} y_j C_j, & \text{for } i = 7, \\ C_8 + \sum_{j=1}^{6} z_j C_j, & \text{for } i = 8, \end{cases} \tag{2.3}$$

where $y_j = (0,0,-\frac{1}{3},-\frac{4}{9},-\frac{20}{3},-\frac{80}{9})_j$ and $z_j = (0,0,1,-\frac{1}{6},20,-\frac{10}{3})_j$ in dimensional regularization with fully anticommuting γ_5. In the SM, all the $C_i^{\rm eff}(\mu_b)$ are known up to $\mathcal{O}(\alpha_s^2)$ [13–15].

We are interested in evaluating the Next-to-Next-to-Leading Order (NNLO) QCD corrections to the ratio of partonic radiative and charmless semileptonic decay rates

$$\frac{\Gamma[b \to X_s \gamma]_{E_\gamma > E_0}}{\Gamma[b \to X_u e \bar{\nu}]} = \left| \frac{V_{ts}^* V_{tb}}{V_{ub}} \right|^2 \frac{6\alpha_{\rm em}}{\pi} \sum_{i,j=1}^{8} C_i^{\rm eff}(\mu_b)\, C_j^{\rm eff}(\mu_b)\, K_{ij}, \tag{2.4}$$

where the symmetric matrix K_{ij} is perturbatively expanded as

$$K_{ij} = \delta_{i7}\delta_{j7} + \tilde{\alpha}_{\rm s} K_{ij}^{(1)} + \tilde{\alpha}_{\rm s}^2 K_{ij}^{(2)} + \mathcal{O}\left(\tilde{\alpha}_{\rm s}^3\right) \qquad \text{with} \qquad \tilde{\alpha}_{\rm s} \equiv \frac{\alpha_s^{(5)}(\mu_b)}{4\pi}. \tag{2.5}$$

Splitting $K_{ij}^{(2)}$ into the BLM ($K_{ij}^{(2)\beta_0}$) and non-BLM ($K_{ij}^{(2){\rm rem}}$) pieces is done in a standard manner:

$$K_{ij}^{(2)} \;=\; A_{ij}\, n_f + B_{ij} \;=\; K_{ij}^{(2)\beta_0} + K_{ij}^{(2){\rm rem}}, \tag{2.6}$$

[3] Including the electroweak or CKM-suppressed corrections would require adding more terms to Eq. (2.1).

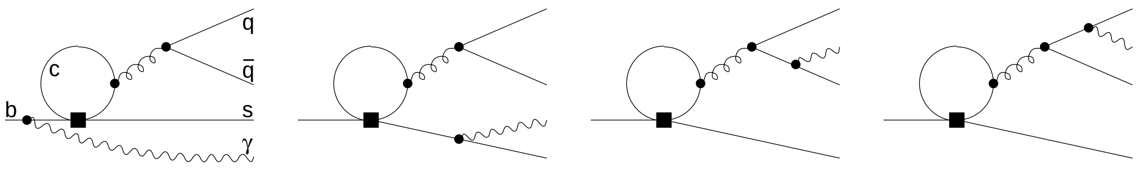

Figure 1: $b \to s\gamma q\bar{q}$ $(q = u, d, s)$ diagrams with $Q_{1,2}$ vertices that survive in the large-m_c limit.

where n_f stands for the number of quark flavours in the effective theory (2.1), and

$$K_{ij}^{(2)\beta_0} \equiv -\frac{3}{2}\beta_0 A_{ij} = -\frac{3}{2}\left(11 - \frac{2}{3}n_f\right) A_{ij}, \qquad\qquad K_{ij}^{(2)\text{rem}} \equiv \frac{33}{2}A_{ij} + B_{ij}. \tag{2.7}$$

In the $\mathcal{O}(\tilde{\alpha}_\mathrm{s}^2)$ correction, one can safely ignore the small $C_{3,4,5,6}^{(0)\text{eff}}(\mu_b)$. Thus, it is sufficient to consider $K_{ij}^{(2)}$ with $i, j \in \{1, 2, 7, 8\}$ only. As far as $K_{ij}^{(2)\beta_0}$ with such indices are concerned, all of them except $K_{18}^{(2)\beta_0}$ and $K_{28}^{(2)\beta_0}$ are known [16–19] for the measured value of m_c. A calculation of $K_{18}^{(2)\beta_0}$ and $K_{28}^{(2)\beta_0}$ is underway [20].

Effects related to the absence of real $c\bar{c}$ production in $b \to X_s^p\gamma$ and to non-zero masses of b and c quarks in loops on gluon propagators belong to $K_{ij}^{(2)\text{rem}}$. They are presently known for all the $i, j \in \{1, 2, 7, 8\}$, either for arbitrary m_c or at least in the vicinity of its measured value [17, 21]. In fact, charm quark loops on gluon propagators are the only source of m_c-dependent terms in $K_{77}^{(2)}$, $K_{78}^{(2)}$ and $K_{88}^{(2)}$. Therefore, the only quantities for which the m_c-interpolation still needs to be performed are $K_{ij}^{(2)\text{rem}}$ for $i \in \{1, 2\}$ and $j \in \{1, 2, 7, 8\}$. In the following, we shall restrict our considerations to those cases only.

Before closing this section, let us remark that our large-m_c calculation is not 100% complete. There exist certain simple though yet uncalculated contributions to $K_{ij}^{(2)\text{rem}}$ with $i \in \{1, 2\}$ and $j \in \{1, 2, 7, 8\}$ that survive in the large-m_c limit. They originate from the four diagrams in Fig. 1 that may interfere either with $b \to s\gamma q\bar{q}$ contributions of $Q_{7,8}$ or just with themselves. Their effect on the decay rate is of order $\tilde{\alpha}_\mathrm{s}^2$, and it is expected to be numerically very small due to limited four-body phase space left out by the high photon energy cutoff $E_0 \sim \frac{m_b}{3}$. A convention advocated in Ref. [18], which we follow here, is to exclude those uncalculated terms from the BLM contribution, even though some of them are proportional to the number of massless flavours. We shall comment on this issue again in Sec. 5.

3 Choice of the method

Our goal amounts to evaluating $K_{ij}^{(2)\text{rem}}$ for $i \in \{1, 2\}$ and $j \in \{1, 2, 7, 8\}$ in the $m_c \gg \frac{m_b}{2}$ limit, at the leading order in $\frac{m_b^2}{m_c^2}$. On general grounds, one expects results of the form

$$K_{ij}^{(2)\text{rem}} = X_{ij}^{(0)} + X_{ij}^{(1)} \ln z + X_{ij}^{(2)} \ln^2 z + \mathcal{O}\left(\frac{1}{z}\right) \qquad \text{with} \qquad z = \frac{m_c^2}{m_b^2}, \tag{3.1}$$

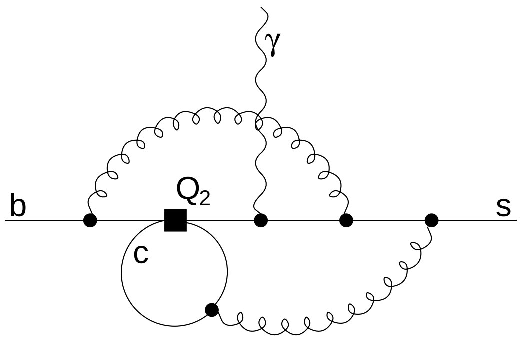

Figure 2: One of the on-shell non-planar diagrams contributing to $K_{27}^{(2)\mathrm{rem}}$.

where $X_{ij}^{(k)}$ are m_c-independent. A straightforward method to perform such a computation via asymptotic expansions [22] would involve three-loop on-shell vertex diagrams like the one shown in Fig. 2 in the heavy-charm limit. Application of the so-called hard-mass procedure to such diagrams leads to one-, two- and three-loop vacuum integrals with mass scale m_c, as well as one- and two-loop on-shell vertex integrals with external momenta $p_b^2 = m_b^2$, $p_s^2 = 0$ and $p_\gamma^2 = 0$. Internal lines of the vertex diagrams are either massless or carry mass m_b. At the two-loop order many different cases occur since up to four bottom quark lines can be present, and the photon can couple in all possible ways to the charm or bottom quark. In 2006, i.e. at the time when our actual calculation [5] was performed, some of the relevant two-loop on-shell massive vertex integrals remained unknown. Furthermore, in addition to the virtual corrections, also contributions from real gluon radiation had to be considered, which involved phase-space integrals in parallel to the loop ones.

Although technical challenges related to the asymptotic expansion method are certainly manageable, we decided to follow a field theory based approach, as already mentioned in the Introduction. This method takes advantage of the fact that charm decoupling at the Lagrangian level can be facilitated with the help of Equations of Motion (EOM). In effect, all the necessary two-loop on-shell vertex integrals could be reduced to the (planar) ones that are already known from the Next-to-Leading Order (NLO) calculations of $b \to s\gamma$ [23].

Before discussing in more detail the charm quark decoupling in the next section, let us recall the large-m_c results for $K_{ij}^{(2)\beta_0}$ with $i \in \{1,2\}$ and $j \in \{1,2,7,8\}$. Contributions to them from the two-body channel $b \to s\gamma$ have been evaluated with the help of asymptotic expansions using the program `exp` [24, 25]. Vacuum integrals were treated with `MATAD` [26], and the reduction of two-loop vertex contributions to master integrals, which can, e.g., be found in Ref. [27], was performed with the help of `AIR` [28]. `AIR` is written in `MAPLE` and is based on the Laporta algorithm [29]. A more flexible and more powerful alternative, which is available since 2008, would be the program `FIRE` [30].

Following Ref. [5], we write

$$K_{27}^{(2)\beta_0} = -6K_{17}^{(2)\beta_0} = \beta_0 \,\mathrm{Re}\left\{-\tfrac{3}{2} r_2^{(2)}(z) + 2\left[a(z) + b(z) - \tfrac{290}{81}\right] L_b - \tfrac{100}{81} L_b^2\right\} + 2\phi_{27}^{(2)\beta_0}(\delta), \tag{3.2}$$

$$K_{ij}^{(2)\beta_0} = 2\,(1+\delta_{ij})\,\phi_{ij}^{(2)\beta_0}(\delta), \qquad \text{for } i,j \neq 7, \tag{3.3}$$

where $L_b = \ln \frac{\mu_b^2}{m_b^2}$ and $\delta = 1 - \frac{2E_0}{m_b}$. Our results for the first three terms of the large-z expansion of $\mathrm{Re}\, r_2^{(2)}(z)$, $\mathrm{Re}\, a(z)$ and $\mathrm{Re}\, b(z)$ read

$$\begin{aligned}
\mathrm{Re}\, r_2^{(2)}(z) &= \tfrac{8}{9}\ln^2 z + \tfrac{112}{243}\ln z + \tfrac{27650}{6561} + \tfrac{1}{z}\left(\tfrac{38}{405}\ln^2 z - \tfrac{572}{18225}\ln z + \tfrac{10427}{30375} - \tfrac{8}{135}\pi^2\right)\\
&+ \tfrac{1}{z^2}\left(\tfrac{86}{2835}\ln^2 z - \tfrac{1628}{893025}\ln z + \tfrac{19899293}{125023500} - \tfrac{8}{405}\pi^2\right) + \mathcal{O}\left(\tfrac{1}{z^3}\right),\\
\mathrm{Re}\, a(z) &= \tfrac{4}{3}\ln z + \tfrac{34}{9} + \tfrac{1}{z}\left(\tfrac{5}{27}\ln z + \tfrac{101}{486}\right) + \tfrac{1}{z^2}\left(\tfrac{1}{15}\ln z + \tfrac{1393}{24300}\right) + \mathcal{O}\left(\tfrac{1}{z^3}\right),\\
\mathrm{Re}\, b(z) &= -\tfrac{4}{81}\ln z + \tfrac{8}{81} - \tfrac{1}{z}\left(\tfrac{2}{45}\ln z + \tfrac{76}{2025}\right) - \tfrac{1}{z^2}\left(\tfrac{4}{189}\ln z + \tfrac{487}{33075}\right) + \mathcal{O}\left(\tfrac{1}{z^3}\right),
\end{aligned} \tag{3.4}$$

which has been confirmed in Ref. [17] using a numerical evaluation of the coefficients at $z^{-k}\ln^n z$ $(k, n = 0, 1, 2)$. The above functions are also known in the small-z expansion [16, 31] – see Eqs. (3.9)–(3.10), (4.8) and Fig. 1 of Ref. [5].

The functions $\phi_{ij}^{(2)\beta_0}(\delta)$ originate from the bremsstrahlung $b \to s\gamma g$ and $b \to s\gamma q\bar{q}$ channels (but excluding the diagrams in Fig. 1). Their numerical importance for $b \to X_s^p \gamma$ is mild due to the relatively high photon energy cutoff $E_0 \sim \frac{m_b}{3}$. At large z, all the $\phi_{ij}^{(2)\beta_0}(\delta)$ with $i \in \{1, 2\}$ and $j \in \{1, 2, 7, 8\}$ behave as $\mathcal{O}(\frac{1}{z})$. Consequently, they can be ignored in the next section where only the leading terms of the large-z expansion of $K_{ij}^{(2)}$ are considered.

4 Charm decoupling: evaluation of the WCs

The matrices $X_{ij}^{(n)}$ in Eq. (3.1) can be obtained by charm decoupling in the limit $m_c \gg \frac{m_b}{2}$. In the first step, we perform three-loop matching of the 5-flavour theory (2.1) onto the 4-flavour one given by

$$\mathcal{L}'_{\rm eff} = \mathcal{L}_{\rm QCD\times QED}(u, d, s, b) + \tfrac{4G_F}{\sqrt{2}} V_{ts}^* V_{tb} \sum_{i=3}^{8} C'_i Q'_i. \tag{4.1}$$

Here, Q'_i differ from Q_i in Eq. (2.2) only by the absence of charm-quark currents in $Q_{3,4,5,6}$. Additional terms containing non-physical (evanescent and/or EOM-vanishing) operators on the r.h.s. of Eqs. (2.1) and (4.1) are implicitly assumed. A complete list of such terms can be found in Sec. 3 of Ref. [14]. Here, we just quote three examples of gauge-invariant EOM-vanishing operators

$$(\bar{s}_L\gamma^\mu T^a b_L) D^\nu G^a_{\mu\nu} + g Q_4^{(\prime)}, \qquad \bar{s}_L \not{D}\not{D}\not{D} b_L, \qquad \frac{ie}{16\pi^2}\left[\bar{s}_L \overleftarrow{\not{D}}\, \sigma^{\mu\nu} b_L F_{\mu\nu} - F_{\mu\nu}\bar{s}_L\sigma^{\mu\nu}\not{D} b_L\right] + Q_7^{(\prime)}. \tag{4.2}$$

We proceed by analogy to our NNLO electroweak-scale matching for $b \to s\gamma$ and $b \to sg$ [13]. Requiring equality of appropriately renormalized off-shell Green functions in both theories leads to relations that allow to express C'_i in terms of C_i. Expansion in external momenta is performed prior to loop integration. No IR regulators are introduced. All the particles except for the decoupled charm are treated as massless, although linear terms in m_b from bottom propagators and operator vertices are retained. Diagrams like the one in Fig. 2 still enter our calculation, but going off-shell and expanding in external momenta makes their evaluation much easier. The necessary three-loop integrals are found with the help of `MATAD` [26].

As well known, spurious IR divergences that appear in such a procedure (regulated dimensionally) cancel out in the final expressions for C'_i in terms of C_i. All the loop diagrams that contain no charm quark are scaleless, so they vanish in dimensional regularization. Thus, $1/\epsilon^n$ poles on the 4-flavour theory side originate from the UV-renormalization constants only, while the 5-flavour theory poles come from loop diagrams, too.

We identify the renormalization scale at which the matching is performed with the previously introduced scale μ_b. However, the charm mass m_c is assumed to be $\overline{\rm MS}$-renormalized at another scale called μ_c. The coefficients $C_i^{\rm eff}(\mu_b)$ and $C_i'^{\rm eff}(\mu_b)$ are expanded in terms of $\widetilde{\alpha}_{\rm s}$ and $\widetilde{\alpha}'_{\rm s} = \frac{\alpha_s^{(4)}(\mu_b)}{4\pi}$, respectively, as follows:

$$
\begin{aligned}
C_i^{\rm eff} &= C_i^{(0)\rm eff} + \widetilde{\alpha}_{\rm s} C_i^{(1)\rm eff} + \widetilde{\alpha}_{\rm s}^2 C_i^{(2)\rm eff} + \mathcal{O}\left(\widetilde{\alpha}_{\rm s}^3\right), \\
C_i'^{\rm eff} &= C_i'^{(0)\rm eff} + \widetilde{\alpha}'_{\rm s} C_i'^{(1)\rm eff} + \widetilde{\alpha}_{\rm s}'^2 C_i'^{(2)\rm eff} + \mathcal{O}\left(\widetilde{\alpha}_{\rm s}'^3\right),
\end{aligned} \tag{4.3}
$$

while $C_i'^{\rm eff}$ are related to C'_i precisely as in Eq. (2.3), with the same numbers y_i and z_i.

Once the r.h.s. of Eq. (2.4) is perturbatively expanded up to $\mathcal{O}(\widetilde{\alpha}_{\rm s}^2)$, the sought $K_{ij}^{(2)}$ are multiplied by $C_{1,2,7,8}^{(0)\rm eff}$ only. All the other unprimed WCs will be set to zero everywhere in the following. After such a simplification, our results for $C_i'^{\rm eff}$ take the form

$$
C_i'^{(0)\rm eff} = C_i'^{(0)} = \begin{cases} 0, & \text{for} \quad i = 3,4,5,6, \\ C_i^{(0)\rm eff}, & \text{for} \quad i = 7,8. \end{cases} \tag{4.4}
$$

$$
C_i'^{(1)\rm eff} = \begin{cases} 0, & \text{for} \quad i = 3,5,6, \\ \frac{2}{3}\left(1 - L_D\right)\left(C_2^{(0)} - \frac{1}{6} C_1^{(0)}\right), & \text{for} \quad i = 4, \\ \left(\frac{218}{243} - \frac{208}{81} L_D\right)\left(C_2^{(0)} - \frac{1}{6} C_1^{(0)}\right), & \text{for} \quad i = 7, \\ \left(\frac{961}{3888} - \frac{173}{324} L_D\right) C_1^{(0)} + \left(\frac{127}{324} - \frac{35}{27} L_D\right) C_2^{(0)}, & \text{for} \quad i = 8. \end{cases} \tag{4.5}
$$

$$
\begin{aligned}
C_7'^{(2)\rm eff} &= \left[\frac{2661293}{118098} - \frac{14293}{19683} n_\ell - \frac{3766}{729}\zeta_3 - \left(\frac{1877}{729} - \frac{220}{2187} n_\ell\right) L_D + \left(\frac{13384}{2187} - \frac{4}{27} n_\ell\right) L_D^2 - \frac{832}{243} L_c\right] C_1^{(0)} \\
&+ \left[-\frac{2861687}{19683} + \frac{28586}{6561} n_\ell + \frac{20060}{243}\zeta_3 + \left(\frac{2674}{243} - \frac{440}{729} n_\ell\right) L_D - \left(\frac{15428}{729} - \frac{8}{9} n_\ell\right) L_D^2 + \frac{1664}{81} L_c\right] C_2^{(0)} \\
&+ \left(-\frac{364}{81} + \frac{112}{27} L_D - \frac{16}{9} L_D^2\right) C_7^{(0)\rm eff} + \left(\frac{364}{243} - \frac{112}{81} L_D + \frac{16}{27} L_D^2\right) C_8^{(0)\rm eff}.
\end{aligned} \tag{4.6}
$$

where $L_D = \ln \frac{\mu_b^2}{m_c^2}$, $L_c = \ln \frac{\mu_c^2}{m_c^2}$, and $n_\ell = 3$ denotes the number of flavours that are kept massless throughout the calculation. Retaining n_ℓ as a symbol is convenient for cross-checking the BLM-part subtraction later on.

The above results have been obtained by matching $b \to s\gamma$, $b \to sg$ and $b \to sq\bar{q}$ off-shell Green functions in both theories. As a by-product, we have also obtained WCs of EOM-vanishing operators like the ones in Eq. (4.2). However, since on-shell matrix elements of such operators vanish [32], there is no need to consider them further. This is precisely the point where the Lagrangian-level decoupling is advantageous with respect to the purely diagrammatic approach. In the latter case, complicated on-shell integrals may occur in contributions that are due to EOM-vanishing operators alone, but this fact is not visible before reduction to truly independent master integrals. An additional advantage in our particular case is that we can use (in the next section) the known two-loop on-shell $b \to s\gamma$ matrix element of Q_4 that has been evaluated without reduction to master integrals [23].

In the remainder of this section, let us recall several important points concerning renormalization in off-shell matching calculations. First, the external fields must be renormalized in an identical manner on both sides of each matching equation. One possibility is to renormalize all the fields on shell. More conveniently, one can shift from the on-shell to the $\overline{\rm MS}$ scheme on the 4-flavour theory side, and perform an identical shift on the 5-flavour side. Second, one adjusts the gauge coupling renormalization on the 5-flavour theory side in such a way that the renormalized coupling equals to $\widetilde{\alpha}'_{\rm s}$ exactly in $\epsilon = (4-D)/2$. At one loop, the necessary renormalization of $\widetilde{\alpha}'_{\rm s}$ in the 5-flavour theory is given by $\widetilde{\alpha}'^{\rm BARE}_{\rm s} = Z_g^2 \widetilde{\alpha}'_{\rm s}$ with

$$Z_g = 1 \;+\; \widetilde{\alpha}'_{\rm s} \left[-\frac{25}{6}\left(\frac{1}{\epsilon} - \gamma + \ln 4\pi\right) \;+\; \frac{\Gamma(1+\epsilon)}{3\epsilon}\left(\frac{4\pi\mu_b}{m_c^2}\right)^{\epsilon} \right] \;+\; \mathcal{O}(\widetilde{\alpha}'^2_{\rm s}), \tag{4.7}$$

in full analogy to Sec. 4 of Ref. [13] where more explanations can be found.[4] Explicit expressions for shifts in the quark mass and wave function renormalization can be found there, too.

As far as the WC renormalization is concerned ($C_i^{(\prime)\rm BARE} = \sum_j C_j^{(\prime)} Z_{ji}^{(\prime)}$), we begin with the $\overline{\rm MS}$ scheme in both theories, and never redefine the $Z_{ji}^{(\prime)}$. However, we re-express them on the 5-flavour side in terms of $\widetilde{\alpha}'_{\rm s}$ that is renormalized according to Eq. (4.7). This leads to appearance of UV-finite terms in Z_{ij} because the relation between $\widetilde{\alpha}'_{\rm s}$ and $\widetilde{\alpha}_{\rm s}$ contains $\mathcal{O}(\epsilon)$ terms. Application of D-dimensional rather than 4-dimensional relations between the gauge couplings has been essential for successful tests of our expressions (4.4)–(4.6) against results derived with the help of asymptotic expansions in the off-shell case. These tests involved direct three-loop $b \to s\gamma$ matching between the full SM and the 4-flavour effective theory (4.1) for $m_c \ll M_W$,

5 On–shell amplitudes

We can now proceed to evaluating on-shell $b \to X_s\gamma$ amplitudes in the 4-flavour theory using $C_i'^{(k)}$ as they stand in Eqs. (4.4)–(4.6). With all the gauge couplings factorized out and the overall factor of $\frac{4G_F}{\sqrt{2}} V_{ts}^* V_{tb}$ omitted, the relevant expressions read

$$\begin{aligned} A(b \to s\gamma) \;&=\; C_7'^{(0)} \langle Q_7' \rangle^{(0)} \;+\; \widetilde{\alpha}'_{\rm s} \left[C_7'^{(1)\rm eff} \langle Q_7' \rangle^{(0)} + C_7'^{(0)} \langle Q_7' \rangle^{(1)} + C_8'^{(0)} \langle Q_8' \rangle^{(1)} \right] \\ &+\; \widetilde{\alpha}'^2_{\rm s} \left[C_7'^{(2)\rm eff} \langle Q_7' \rangle^{(0)} + C_7'^{(1)\rm eff} \langle Q_7' \rangle^{(1)} + C_7'^{(0)} \langle Q_7' \rangle^{(2)} + C_8'^{(1)\rm eff} \langle Q_8' \rangle^{(1)} \right. \end{aligned}$$

[4] Terms containing $(-\gamma + \ln 4\pi)$ are often skipped in Ref. [13]. For more details about decoupling relations see Ref. [33] and Eq. (12) of Ref. [34].

$$+ \quad C_8'^{(0)} \langle Q_8' \rangle^{(2)} + C_4'^{(1)} \langle Q_4' \rangle^{(2)}_{\rm eff} \Big] \;+\; \mathcal{O}\left(\widetilde{\alpha}_{\rm s}'^{3}\right), \tag{5.1}$$

$$A(b \to s\gamma g) \;=\; g_s' \left[C_7'^{(0)} \langle Q_7' \rangle^{(0)} + C_8'^{(0)} \langle Q_8' \rangle^{(0)} \right] \;+\; g_s' \widetilde{\alpha}_{\rm s}' \Big[C_7'^{(1){\rm eff}} \langle Q_7' \rangle^{(0)} + C_7'^{(0)} \langle Q_7' \rangle^{(1)}$$

$$+ \quad C_8'^{(1){\rm eff}} \langle Q_8' \rangle^{(0)} + C_8'^{(0)} \langle Q_8' \rangle^{(1)} + C_4'^{(1)} \langle Q_4' \rangle^{(1)}_{\rm eff} \Big] \;+\; \mathcal{O}\left(g_s' \widetilde{\alpha}_{\rm s}'^{2}\right), \tag{5.2}$$

$$A(b \to s\gamma gg) \;=\; \widetilde{\alpha}_{\rm s}' \left[C_7'^{(0)} \langle Q_7' \rangle^{(0)} + C_8'^{(0)} \langle Q_8' \rangle^{(0)} \right] \;+\; \mathcal{O}\left(\widetilde{\alpha}_{\rm s}'^{2}\right), \tag{5.3}$$

$$A(b \to s\gamma q\bar{q}) \;=\; \widetilde{\alpha}_{\rm s}' \left[C_7'^{(0)} \langle Q_7' \rangle^{(0)} + C_8'^{(0)} \langle Q_8' \rangle^{(0)} + C_4'^{(1)} \langle Q_4' \rangle^{(0)} \right] \;+\; \mathcal{O}\left(\widetilde{\alpha}_{\rm s}'^{2}\right), \tag{5.4}$$

where $\langle Q_j' \rangle^{(n)}$ denotes the n-loop renormalized matrix element of Q_j' between the considered external states, and $C_i'^{(k)}$ are used only when $C_i'^{(k)} = C_i'^{(k){\rm eff}}$.

For the penguin operators (j=3,4,5,6) we have $\langle Q_j^{(\prime)} \rangle^{(n)}_{\rm eff} \equiv \langle Q_j^{(\prime)} \rangle^{(n)} - y_j \langle Q_7^{(\prime)} \rangle^{(n-1)} - z_j \langle Q_8^{(\prime)} \rangle^{(n-1)}$ with the same numbers y_j and z_j as in Eq. (2.3). In fact, those numbers are determined by the requirement $\langle s\gamma | Q_j^{(\prime)} | b \rangle^{(1)}_{\rm eff} = 0 = \langle sg | Q_j^{(\prime)} | b \rangle^{(1)}_{\rm eff}$. Expressing amplitudes in terms of $\langle Q_j^{(\prime)} \rangle^{(n)}_{\rm eff}$ is convenient in other cases, too. For instance, the bremsstrahlung matrix elements $\langle s\gamma g | Q_j^{(\prime)} | b \rangle^{(1)}_{\rm eff}$ are given by subsets of diagrams contributing to $\langle s\gamma g | Q_j^{(\prime)} | b \rangle^{(1)}$, namely those where both the photon and the gluon are attached to the quark loop [35]. At two loops, $\langle s\gamma | Q_j^{(\prime)} | b \rangle^{(2)}_{\rm eff}$ contain no IR divergences, contrary to $\langle s\gamma | Q_j^{(\prime)} | b \rangle^{(2)}$ [23].

In Eq. (5.1), we need

$$\langle s\gamma | Q_4' \, | b \rangle^{(2)}_{\rm eff} \;=\; \langle s\gamma | Q_7' \, | b \rangle^{(0)} \left[r_4' + \left(-\frac{20}{243} + \frac{8}{81} n_\ell \right) L_b \right], \tag{5.5}$$

where

$$\mathrm{Re}\, r_4' \;=\; -\frac{137}{729} - \frac{52}{243} n_\ell - \frac{4\pi}{9\sqrt{3}} - \frac{16}{27} X_b + \frac{1}{6} \mathrm{Re}\, a(1) + \frac{5}{3} \mathrm{Re}\, b(1), \tag{5.6}$$

and

$$X_b \;=\; \int_0^1 dx \int_0^1 dy \int_0^1 dv \; xy \ln \left[v + x(1-x)(1-v)(1-v+vy) \right] \;\simeq\; -0.1684,$$

$$\mathrm{Re}\, a(1) \;=\; \tfrac{43}{9} + \tfrac{8}{9} \int_0^1 dx \int_0^1 dy \int_0^1 dv \, \{ [2 - v + xy(2v-3)] \ln[v + x(1-x)(1-v)(1-v+vy)]$$

$$+ \quad [1 - v + xy(2v-1)] \ln[1 - x(1-x)yv] \} \;\simeq\; 4.0859,$$

$$\mathrm{Re}\, b(1) \;=\; \frac{320}{81} - \frac{4\pi}{3\sqrt{3}} + \frac{632}{1215}\pi^2 - \frac{8}{45} \left[\frac{d^2 \ln \Gamma(x)}{dx^2} \right]_{x=\frac{1}{6}} \;\simeq\; 0.0316. \tag{5.7}$$

The result in Eq. (5.5) has been extracted from Eqs. (3.1) and (6.21) of Ref. [23] after reintroducing explicit n_ℓ-dependence there. More precisely, setting $z = 0$ in the quoted equations of Ref. [23] gives the same number for $r_4 + \gamma_{47}^{(0){\rm eff}} \ln(m_b/\mu_b)$ there as setting $n_\ell = 4$ in the square bracket of Eq. (5.5) here. However, here we need $n_\ell = 3$.

The next steps to perform are as follows:

- Calculate moduli squared of the amplitudes in Eqs. (5.1)–(5.4), sum over polarizations and integrate over the phase space.
- Re-expand everything in terms of $\tilde{\alpha}_s$ using $\tilde{\alpha}'_s = \tilde{\alpha}_s\left(1 - \frac{2}{3}\tilde{\alpha}_s L_D + \mathcal{O}(\tilde{\alpha}_s^2)\right)$, and take into account normalization to the semileptonic rate in Eq. (2.4).
- Pick up only those $\mathcal{O}(\tilde{\alpha}_s^2)$ terms that contain at least a single $C_{1,2}^{(0)}$, and read out the corresponding $K_{ij}^{(2)}$.
- Subtract the BLM contributions (leading terms in the large-z expansion only) using Eqs. (3.2)–(3.3) with $\beta_0 = 11 - \frac{2}{3}(n_\ell + 2)$, and check that all the n_ℓ-terms cancel out.

A brief look at Eqs. (4.4)–(4.5) and (5.1)–(5.4) ensures that the matrix element in Eq. (5.5) is actually the only two-loop on-shell one that we need. Let us stress again that this is the case only thanks to identifying the EOM-vanishing operators at the Lagrangian level.

Another straightforward observation is that $K_{ij}^{(2)}$ for $i,j \in \{1,2\}$ receive contributions only from the $C_7'^{(1)\text{eff}}\langle Q_7'\rangle^{(0)}$ term in Eq. (5.1) and the $C_4'^{(1)}\langle Q_4'\rangle^{(0)}$ term in Eq. (5.4). As the latter term is not known, we shall neglect it in what follows.[5] With this approximation, everything we need is given by the quantity that multiplies $\left(C_2^{(0)} - \frac{1}{6}C_1^{(0)}\right)$ in $C_7'^{(1)\text{eff}}$ (see Eq. (4.5)). It contains no n_ℓ-piece, and is equal to $K_{27}^{(1)} + \mathcal{O}(1/z)$. Consequently

$$\begin{aligned}
K_{22}^{(2)\text{rem}} &= 36\,K_{11}^{(2)\text{rem}} + \mathcal{O}\left(\tfrac{1}{z}\right) = -6\,K_{12}^{(2)\text{rem}} + \mathcal{O}\left(\tfrac{1}{z}\right) = \left(K_{27}^{(1)}\right)^2 + \mathcal{O}\left(\tfrac{1}{z}\right) \\
&= \left[\tfrac{218}{243} - \tfrac{208}{81}L_D\right]^2 + \mathcal{O}\left(\tfrac{1}{z}\right), \qquad (5.8)
\end{aligned}$$

which is identical to Eq. (5.4) of Ref. [5].

It remains to determine $K_{(12)(78)}^{(2)\text{rem}}$, i.e., $K_{ij}^{(2)\text{rem}}$ for $i \in \{1,2\}$ and $j \in \{7,8\}$. Once $\langle s\gamma q\bar{q}|Q_4'|b\rangle^{(0)}$ has been neglected, the only relevant processes are $b \to s\gamma$ and $b \to s\gamma g$, and we need at least one beyond-LO coefficient $C_i'^{(k)\text{eff}}$, which makes the calculation very similar to the $b \to X_s^p\gamma$ one at the NLO. In fact, all the necessary matrix elements and phase-space integrals come in the same combinations as in the known results for

$$\begin{aligned}
K_{77}'^{(1)} &= K_{77}^{(1)} = -\tfrac{182}{9} + \tfrac{8}{9}\pi^2 - \tfrac{32}{3}L_b + 4\,\phi_{77}^{(1)}(\delta), \\
K_{78}'^{(1)} &= K_{78}^{(1)} = \tfrac{44}{9} - \tfrac{8}{27}\pi^2 + \tfrac{16}{9}L_b + 2\,\phi_{78}^{(1)}(\delta), \\
K_{88}'^{(1)} &= K_{88}^{(1)} = 4\,\phi_{88}^{(1)}(\delta), \\
K_{47}'^{(1)} &= K_{47}^{(1)} - 2\,\mathrm{Re}\,b(z) + \tfrac{52}{243} - \tfrac{8}{81}L_b = \mathrm{Re}\,r_4' + \left(-\tfrac{20}{243} + \tfrac{8}{81}n_\ell\right)L_b + 2\,\phi_{47}^{(1)}(\delta), \\
K_{48}'^{(1)} &= K_{48}^{(1)} = 2\,\phi_{48}^{(1)}(\delta). \qquad (5.9)
\end{aligned}$$

[5] It originates precisely from the diagrams in Fig. 1 that were discussed at the end of Sec. 2. Now it is clear that including their n_ℓ-parts in the BLM approximation would not be mandatory because the $q\bar{q}$ pair emitted from Q_4' has no gluonic counterpart in any other diagram. More precisely, this counterpart occurs only in the first EOM-vanishing operator in Eq. (4.2) that gives no contribution on shell.

For completeness, all the relevant functions $\phi^{(1)}_{ij}(\delta)$ are collected in the Appendix. Normalization to the semileptonic rate is already taken into account in $K^{(1)}_{77}$, and there is no other point where it could matter in the evaluation of $K^{(2)\rm rem}_{(12)(78)}$.

Once the quantities from Eq. (5.9) are used, equations that determine the sought $K^{(2)}_{ij}$ take a simple form

$$\begin{aligned} C_1^{(0)} K^{(2)}_{17} + C_2^{(0)} K^{(2)}_{27} + \mathcal{O}\left(\tfrac{1}{z}\right) &= \widetilde{C}'^{(2)\rm eff}_7 + \left(K^{(1)}_{77} - \tfrac{2}{3} L_D\right) C'^{(1)\rm eff}_7 + K^{(1)}_{78} C'^{(1)\rm eff}_8 + K'^{(1)}_{47} C'^{(1)}_4 \\ C_1^{(0)} K^{(2)}_{18} + C_2^{(0)} K^{(2)}_{28} + \mathcal{O}\left(\tfrac{1}{z}\right) &= K^{(1)}_{78} C'^{(1)\rm eff}_7 + K^{(1)}_{88} C'^{(1)\rm eff}_8 + K^{(1)}_{48} C'^{(1)}_4, \end{aligned} \tag{5.10}$$

where $\widetilde{C}'^{(2)\rm eff}_7$ stands for $C'^{(2)\rm eff}_7$ (4.6) with $C^{(0)\rm eff}_{7,8}$-terms set to zero.

In the last step, as already mentioned above, we need to subtract the BLM parts (3.2)–(3.3) from the calculated $K^{(2)}_{ij}$ to obtain $K^{(2)\rm rem}_{ij}$. At this level, it is convenient to express $K'^{(1)}_{47}$ first in terms of $K^{(1)}_{47}$, and next in terms of

$$\begin{aligned} K^{(1)\rm rem}_{47} &= K^{(1)}_{47} - \beta_0\left(\tfrac{26}{81} - \tfrac{4}{27} L_b\right) \\ &= -\tfrac{2411}{729} - \tfrac{4\pi}{9\sqrt{3}} - \tfrac{16}{27} X_b + \tfrac{1}{6}{\rm Re}\, a(1) + \tfrac{5}{3}{\rm Re}\, b(1) + \tfrac{328}{243} L_b + \tfrac{8}{81} L_D + 2\,\phi^{(1)}_{47}(\delta) + \mathcal{O}\left(\tfrac{1}{z}\right). \end{aligned} \tag{5.11}$$

Our final results for $K^{(2)\rm rem}_{(12)(78)}$ take the form

$$\begin{aligned} K^{(2)\rm rem}_{27} &= K^{(1)}_{27} K^{(1)}_{77} + \left(\tfrac{127}{324} - \tfrac{35}{27} L_D\right) K^{(1)}_{78} + \tfrac{2}{3}(1 - L_D) K^{(1)\rm rem}_{47} \\ &- \tfrac{4736}{729} L_D^2 + \tfrac{1150}{729} L_D - \tfrac{1617980}{19683} + \tfrac{20060}{243}\zeta_3 + \tfrac{1664}{81} L_c + \mathcal{O}\left(\tfrac{1}{z}\right), \end{aligned} \tag{5.12}$$

$$K^{(2)\rm rem}_{28} = K^{(1)}_{27} K^{(1)}_{78} + \left(\tfrac{127}{324} - \tfrac{35}{27} L_D\right) K^{(1)}_{88} + \tfrac{2}{3}(1 - L_D) K^{(1)}_{48} + \mathcal{O}\left(\tfrac{1}{z}\right), \tag{5.13}$$

$$K^{(2)\rm rem}_{17} = -\tfrac{1}{6} K^{(2)\rm rem}_{27} + \left(\tfrac{5}{16} - \tfrac{3}{4} L_D\right) K^{(1)}_{78} - \tfrac{1237}{729} + \tfrac{232}{27}\zeta_3 + \tfrac{70}{27} L_D^2 - \tfrac{20}{27} L_D + \mathcal{O}\left(\tfrac{1}{z}\right), \tag{5.14}$$

$$K^{(2)\rm rem}_{18} = -\tfrac{1}{6} K^{(2)\rm rem}_{28} + \left(\tfrac{5}{16} - \tfrac{3}{4} L_D\right) K^{(1)}_{88} + \mathcal{O}\left(\tfrac{1}{z}\right), \tag{5.15}$$

which is identical to Eqs. (5.5)–(5.8) of Ref. [5].

6 Conclusions

We have presented details of our large-m_c calculation [5] of those NNLO corrections to $\mathcal{B}(\bar{B} \to X_s\gamma)$ that still require interpolation in m_c. Applying Lagrangian-level decoupling rather than the purely diagrammatic asymptotic expansions has led to appreciable simplifications of the analysis.

Our results are going to be useful again in the near future when the calculation of $K^{(2)\rm rem}_{17}$ and $K^{(2)\rm rem}_{27}$ at $m_c = 0$ is completed [36] providing data for an upgraded interpolation in m_c. With those inputs, as well as new results for $K^{(2)\rm rem}_{78}$ [37] and the remaining BLM terms [20], an update of the phenomenological analysis [4, 5] will be mandatory. An ultimate goal is to make the perturbative uncertainties in $\mathcal{B}(\bar{B} \to X_s\gamma)$ negligible with respect to the non-perturbative [2] and experimental [6] ones.

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Appendix

Here, we quote explicit expressions for the relevant functions $\phi_{ij}^{(1)}(\delta)$ [35, 38]:

$$\phi_{77}^{(1)} = -\tfrac{2}{3}\ln^2\delta - \tfrac{7}{3}\ln\delta - \tfrac{31}{9} + \tfrac{10}{3}\delta + \tfrac{1}{3}\delta^2 - \tfrac{2}{9}\delta^3 + \tfrac{1}{3}\delta(\delta-4)\ln\delta, \tag{A.1}$$

$$\phi_{78}^{(1)} = \tfrac{8}{9}\left[\mathrm{Li}_2(1-\delta) - \tfrac{1}{6}\pi^2 - \delta\ln\delta + \tfrac{9}{4}\delta - \tfrac{1}{4}\delta^2 + \tfrac{1}{12}\delta^3\right], \tag{A.2}$$

$$\begin{aligned}\phi_{88}^{(1)} &= \tfrac{1}{27}\Big\{\left[\delta^2 + 2\delta + 4\ln(1-\delta)\right]\ln\frac{m_s^2}{m_b^2} \\ &+ 4\mathrm{Li}_2(1-\delta) - \tfrac{2}{3}\pi^2 - \delta(2+\delta)\ln\delta + 8\ln(1-\delta) - \tfrac{2}{3}\delta^3 + 3\delta^2 + 7\delta\Big\}.\end{aligned} \tag{A.3}$$

$$\begin{aligned}\phi_{47}^{(1)}(\delta) &= -3\phi_{48}^{(1)}(\delta) = -\tfrac{1}{54}\delta\left(1-\delta+\tfrac{1}{3}\delta^2\right) - \tfrac{1}{4}\lim_{m_c\to m_b}\phi_{27}^{(1)}(\delta) \\ &= \tfrac{1}{54}\pi\left(3\sqrt{3}-\pi\right) + \tfrac{1}{81}\delta^3 - \tfrac{25}{108}\delta^2 + \tfrac{5}{54}\delta + \tfrac{2}{9}\left(\delta^2+2\delta+3\right)\arctan^2\sqrt{\frac{1-\delta}{3+\delta}} \\ &- \tfrac{1}{3}\left(\delta^2+4\delta+3\right)\sqrt{\frac{1-\delta}{3+\delta}}\arctan\sqrt{\frac{1-\delta}{3+\delta}}.\end{aligned} \tag{A.4}$$

The functions $\phi_{47}^{(1)}$ and $\phi_{48}^{(1)}$ are exactly the same in the 5-flavour and 4-flavour theories.[6] They are generated by the s- and b-quark loops with no Dirac traces only. Contributions with traces cancel out in the same way as in the QED electron-loop contributions to three-photon interactions (Furry theorem).

Let us note that $\phi_{88}^{(1)}$ in Eq. (A.3), $\phi_{88}^{(2)\beta_0}$, as well as the neglected diagrams in Fig. 1 contain collinear logarithms where $m_q \neq 0$ for $q = u, d, s$ need to be retained at the perturbative level. The actual collinear regulators in reality are of order of the light meson masses (m_π, m_K). Non-perturbative collinear effects in $\bar{B} \to X_s\gamma$ have been discussed in Refs. [2, 39]. Their numerical effect on the branching ratio for $E_0 \sim \frac{m_b}{3}$ is generically small ($\sim 1\%$) thanks to the phase-space suppression, electric charge factors and/or small values of the relevant WCs.

[6] Eq. (3.12) of Ref. [5] contains a misprint in the coefficient at $\lim_{m_c\to m_b}$ which we correct in the first line of Eq. (A.4) here.

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