NNLO QCD Corrections to the $\bar{B} \to X_s\gamma$
Matrix Elements Using Interpolation in $m_c$

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Abstract

One of the most troublesome contributions to the NNLO QCD corrections to $\bar{B} \to X_s\gamma$ originates from three-loop matrix elements of four-quark operators. A part of this contribution that is proportional to the QCD beta-function coefficient $\beta_0$ was found in 2003 as an expansion in $m_c/m_b$. In the present paper, we evaluate the asymptotic behaviour of the complete contribution for $m_c \gg m_b/2$. The asymptotic form of the $\beta_0$-part matches the small-$m_c$ expansion very well at the threshold $m_c = m_b/2$. For the remaining part, we perform an interpolation down to the measured value of $m_c$, assuming that the $\beta_0$-part is a good approximation at $m_c = 0$. Combining our results with other contributions to the NNLO QCD corrections, we find $\mathcal{B}(\bar{B} \to X_s\gamma) = (3.15 \pm 0.23) \times 10^{-4}$ for $E_\gamma > 1.6$ GeV in the $\bar{B}$-meson rest frame. The indicated error has been obtained by adding in quadrature the following uncertainties: non-perturbative (5%), parametric (3%), higher-order perturbative (3%), and the interpolation ambiguity (3%).
1 Introduction

The decay $\bar{B} \to X_s \gamma$ is a well-known probe of new physics at the electroweak scale. The current world average for its branching ratio with a cut $E_\gamma > 1.6$ GeV in the $\bar{B}$-meson rest frame reads [1]

$$B(\bar{B} \to X_s \gamma)_{E_\gamma > 1.6 \, \text{GeV}} = \left(3.55 \pm 0.24^{+0.09}_{-0.10} \pm 0.03\right) \times 10^{-4},$$

(1.1)

where the first error is combined statistical and systematic. The second one is due to the theory input on the shape function. The third one is caused by the $b \to d \gamma$ contamination.

The total error in Eq. (1.1) amounts to around 7.4%, i.e. it is of the same size as the expected $O(\alpha_s^2)$ corrections to the perturbative transition $b \to X_s^{\text{parton}} \gamma$. On the other hand, the relation

$$\Gamma(\bar{B} \to X_s \gamma) \simeq \Gamma(b \to X_s^{\text{parton}} \gamma)$$

(1.2)

holds up to non-perturbative corrections that turn out to be smaller (see Section 7).

Consequently, evaluating the Next-to-Next-to-Leading Order (NNLO) QCD corrections to $b \to X_s^{\text{parton}} \gamma$ is of crucial importance for deriving constraints on new physics from the measurements of $\bar{B} \to X_s \gamma$.

In the calculation of $b \to X_s^{\text{parton}} \gamma$, resummation of large logarithms $(\alpha_s \ln M_W^2/m_t^2)^n$ is necessary at each order in $\alpha_s$, which is most conveniently performed in the framework of an effective theory that arises from the Standard Model (SM) after decoupling the heavy electroweak bosons and the top quark. The explicit form of the relevant effective Lagrangian is given in the next section. The Wilson coefficients $C_i(\mu)$ play the role of coupling constants at the flavour-changing vertices (operators) $Q_i$.

The perturbative calculations are performed in three steps:

(i) Matching: Evaluating $C_i(\mu_0)$ at the renormalization scale $\mu_0 \sim M_W, m_t$ by requiring equality of the SM and effective theory Green’s functions at the leading order in (external momenta)/(M_W, m_t).

(ii) Mixing: Calculating the operator mixing under renormalization, deriving the effective theory Renormalization Group Equations (RGE) and evolving $C_i(\mu)$ from $\mu_0$ down to the low-energy scale $\mu_b \sim m_b$.

(iii) Matrix elements: Evaluating the on-shell $b \to X_s^{\text{parton}} \gamma$ amplitudes at $\mu_b \sim m_b$.

In the NNLO analysis of the considered decay, the four-quark operators $Q_1, \ldots, Q_6$ and the dipole operators $Q_7$ and $Q_8$ must be matched at the two- and three-loop level, respectively. Three-point amplitudes with four-quark vertices need to be renormalized up to the four-loop level, while “only” three-loop mixing is necessary in the remaining cases. The matrix elements are needed up to two loops for the dipole operators, and up to three loops for the four-quark operators.

The NNLO matching was calculated in Refs. [2, 3]. The three-loop renormalization in the $\{Q_1, \ldots, Q_6\}$ and $\{Q_7, Q_8\}$ sectors was found in Refs. [4, 5]. The results from Ref. [6] on the four-loop mixing of $Q_1, \ldots, Q_6$ into $Q_7$ will be used in our numerical analysis.\footnote{The small effect (-0.35% in the branching ratio) of the four-loop mixing [6] of $Q_1, \ldots, Q_6$ into $Q_8$ is neglected here. It was not yet known in September 2006 when the current paper was being completed.}
As far as the matrix elements are concerned, contributions to the decay rate that are proportional to $|C_7(\mu_t)|^2$ are completely known at the NNLO thanks to the calculations in Refs. [7,8]. These two-loop results have recently been confirmed by an independent group [9,10]. Two- and three-loop matrix elements in the so-called large-$\beta_0$ approximation were found in Ref. [11] as expansions in the quark mass ratio $m_c/m_b$. Such expansions are adequate when $m_c < m_b/2$, which is satisfied by the measured quark masses. Finding all the remaining (“beyond-$\beta_0$”) contributions to the matrix elements is a very difficult task because hundreds of massive three-loop on-shell vertex diagrams need to be calculated.

In the present work, we evaluate the asymptotic form of the $m_c$-dependent NNLO matrix elements in the limit $m_c \gg m_b/2$ using the same decoupling technique as in our three-loop Wilson coefficient calculation [3]. We find that the asymptotic form of the $\beta_0$-part matches the small-$m_c$ expansion very well at the $c\bar{c}$ production threshold $m_c = m_b/2$. The same is true for the Next-to-Leading Order (NLO) matrix elements. Motivated by this observation, we interpolate the beyond-$\beta_0$ part to smaller values of $m_c$ assuming that the $\beta_0$-part is a good approximation at $m_c = 0$. Combining our results with other contributions to the NNLO QCD corrections, we find an estimate for the branching ratio at $O(\alpha_s^2)$.

Our paper is organized as follows. In Section 2, we introduce the effective theory and collect the relevant formulae for the $\bar{B} \to X_s \gamma$ branching ratio. The contributions that are known exactly in $m_c$ are described in Section 3. Expressions for the NNLO matrix elements in the large-$\beta_0$ approximation and in the $m_c \gg m_b/2$ limit are presented in Sections 4 and 5, respectively. Section 6 is devoted to discussing the interpolation in $m_c$. Section 7 contains the analysis of uncertainties. We conclude in Section 8. Our numerical input parameters are collected in Appendix A. Appendix B contains a discussion of the $c\bar{c}$ production treatment in the interpolation.

2 The effective theory

Following Section 3 of Ref. [12], the $\bar{B} \to X_s \gamma$ branching ratio can be expressed as follows:

$$B[\bar{B} \to X_s \gamma]_{E_{\gamma} > E_0} = B[\bar{B} \to X_c e\bar{\nu}] \exp \left[ \frac{V_{ts}^* V_{tb}}{V_{cb}} \right]^2 \frac{6\alpha_{em}}{\pi} \left[ P(E_0) + N(E_0) \right],$$

(2.1)

where $\alpha_{em} = \alpha_{em}(0) \simeq 1/137.036$ and $N(E_0)$ denotes the non-perturbative correction. The $m_c$-dependence of $\bar{B} \to X_c e\bar{\nu}$ is accounted for by

$$C = \left| \frac{V_{ub}}{V_{cb}} \right|^2 \frac{\Gamma[\bar{B} \to X_c e\bar{\nu}]}{\Gamma[\bar{B} \to X_u e\bar{\nu}]},$$

(2.2)

with neglected spectator annihilation. $P(E_0)$ is given by the perturbative ratio

$$\frac{\Gamma[b \to X_s \gamma]_{E_{\gamma} > E_0}}{|V_{cb}/V_{ub}|^2 \Gamma[b \to X_u e\bar{\nu}]} = \left| \frac{V_{ts}^* V_{tb}}{V_{cb}} \right|^2 \frac{6\alpha_{em}}{\pi} P(E_0).$$

(2.3)

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2 See Eqs. (3.10) and (4.7) of Ref. [12]. The corrections found in Eqs. (3.9) and (3.14) of Ref. [13] as well as Eq. (28) of Ref. [14] should be included in $N(E_0)$, too.
Our goal is to calculate the NNLO QCD corrections to the quantity \( P(E_0) \). The denominator on the l.h.s. of Eq. (2.3) is already known at the NNLO level from Refs. [15, 16].

The relevant effective Lagrangian reads

\[
\mathcal{L}_{\text{eff}} = \mathcal{L}_{\text{QCD+QED}}(u, d, s, c, b) + \frac{4G_F}{\sqrt{2}} \left[ V_{ts}^* V_{tb} \sum_{i=1}^{8} C_i Q_i + V_{us}^* V_{ub} \sum_{i=1}^{2} C_i^\nu (Q_i^\nu - Q_i) \right],
\]

(2.4)

where

\[
\begin{align*}
Q_1^u &= (\bar{s} L \gamma_i T^a u_L) (\bar{u} L \gamma^\mu T^a b_L), \\
Q_2^u &= (\bar{s} L \gamma_i u_L) (\bar{u} L \gamma^\mu b_L), \\
Q_1 &= (\bar{s} L \gamma_i T^a c_L) (\bar{c} L \gamma^\mu T^a b_L), \\
Q_2 &= (\bar{s} L \gamma_i c_L) (\bar{c} L \gamma^\mu b_L), \\
Q_3 &= (\bar{s} L \gamma_i b_L) \sum_q (\bar{q} \gamma^\mu q), \\
Q_4 &= (\bar{s} L \gamma_i T^a b_L) \sum_q (\bar{q} \gamma^\mu T^a q), \\
Q_5 &= (\bar{s} L \gamma_i \gamma_{i_1} \gamma_{i_2} \gamma_{i_3} b_L) \sum_q (\bar{q} \gamma_{i_1} \gamma_{i_2} \gamma_{i_3} \gamma^\mu q), \\
Q_6 &= (\bar{s} L \gamma_i \gamma_{i_1} \gamma_{i_2} \gamma_{i_3} T^a b_L) \sum_q (\bar{q} \gamma_{i_1} \gamma_{i_2} \gamma_{i_3} T^a \gamma^\mu q), \\
Q_7 &= \frac{e}{16\pi^2} m_b (\bar{s} L \gamma_{i_1} T^a b_R) F_{\mu\nu}, \\
Q_8 &= \frac{2}{16\pi^2} m_b (\bar{s} L \gamma_{i_1} T^a b_R) C_{\mu\nu}^a.
\end{align*}
\]

(2.5)

The last term in the square bracket of Eq. (2.4) gives no contribution at the Leading Order (LO) and only a small contribution at the NLO (around +1% in the branching ratio — see Eq. (3.7) of Ref. [12]). Consequently, we shall neglect its effect on the NNLO QCD correction and omit terms proportional to \( V_{ub} \) in the analytical formulae below. However, our numerical results will include the \( V_{ub} \) terms at the NLO. The same refers to the electroweak corrections that amount to around \(-3.7\% \) in \( P(E_0) \) [12, 17].

The quantity \( P(E_0) \) depends quadratically on the Wilson coefficients\(^3\)

\[
P(E_0) = \sum_{i,j=1}^{8} C_{ij}^\text{eff}(\mu_b) C_{ij}^\text{eff}(\mu_b) K_{ij}(E_0, \mu_b),
\]

(2.6)

where the “effective coefficients” are defined by

\[
C_{ij}^\text{eff}(\mu) = \begin{cases} 
C_i(\mu), & \text{for } i = 1, \ldots, 6, \\
C_7(\mu) + \sum_{j=1}^{6} y_j C_j(\mu), & \text{for } i = 7, \\
C_8(\mu) + \sum_{j=1}^{6} z_j C_j(\mu), & \text{for } i = 8.
\end{cases}
\]

(2.7)

The numbers \( y_j \) and \( z_j \) are defined so that the leading-order \( b \rightarrow s \gamma \) and \( b \rightarrow sg \) matrix elements of the effective Hamiltonian are proportional to the leading-order terms in \( C_7^\text{eff} \) and \( C_8^\text{eff} \), respectively [18]. This means, in particular, that \( K_{ij} = \delta_{ij} \delta_{7j} + \mathcal{O}(\alpha_s) \). In the \( \overline{\text{MS}} \) scheme with fully anticommuting \( \gamma_5 \), \( \vec{y} = (0, 0, -\frac{1}{3}, -\frac{4}{9}, -\frac{20}{3}, -\frac{80}{9}) \) and \( \vec{z} = (0, 0, 1, -\frac{1}{6}, 20, -\frac{19}{3}) \) [19].

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\(^3\) In Eq. (30) of Ref. [7], \( K_{ij} \) was denoted by \( \widetilde{G}_{ij}/G_u \).
In Eq. (2.23), we have assumed that all the Wilson coefficients are real, as it is the case in the SM. Consequently, $K_{ij}$ is a real symmetric matrix.

Once the MS-renormalized coefficients $C_i^{\text{eff}}(\mu)$ are perturbatively expanded

$$C_i^{\text{eff}}(\mu) = C_i^{(0)\text{eff}}(\mu) + \tilde{\alpha}_s(\mu)C_i^{(1)\text{eff}}(\mu) + \tilde{\alpha}_s^2(\mu)C_i^{(2)\text{eff}}(\mu) + \mathcal{O}\left(\tilde{\alpha}_s^3(\mu)\right),$$  

(2.8)

we have assumed that all the Wilson coefficients are real, as it is the case in the SM. Consequently, $K_{ij}$ is a real symmetric matrix.

the expression for $P(E_0)$ can be cast in the following form:

$$P(E_0) = \left[ P^{(0)}(\mu_b) + \tilde{\alpha}_s(\mu_b) \left[P_{1}^{(1)}(\mu_b) + P_{2}^{(1)}(E_0, \mu_b)\right] \right] + \tilde{\alpha}_s^2(\mu_b) \left[P_{1}^{(2)}(\mu_b) + P_{2}^{(2)}(E_0, \mu_b) + P_{3}^{(2)}(E_0, \mu_b)\right] + \mathcal{O}\left(\tilde{\alpha}_s^3(\mu_b)\right).$$

(2.10)

Here, $P^{(0)}$ and $P_{1}^{(k)}$ originate from the tree-level matrix element of $Q_7$

$$P^{(0)}(\mu_b) = \left(C_{7}^{(0)\text{eff}}(\mu_b)\right)^2,$$

$$P_{1}^{(1)}(\mu_b) = 2C_{7}^{(0)\text{eff}}(\mu_b)C_{7}^{(1)\text{eff}}(\mu_b),$$

$$P_{1}^{(2)}(\mu_b) = \left(C_{7}^{(1)\text{eff}}(\mu_b)\right)^2 + 2C_{7}^{(0)\text{eff}}(\mu_b)C_{7}^{(2)\text{eff}}(\mu_b),$$

(2.11)

while $P_{2}^{(k)}$ depend only on the LO Wilson coefficients $C_i^{(0)\text{eff}}$. The NNLO correction $P_{3}^{(2)}$ is defined by requiring that it is proportional to products of the LO and NLO Wilson coefficients only ($C_i^{(0)\text{eff}}C_j^{(1)\text{eff}}$).

3 The corrections $P_{2}^{(1)}$ and $P_{3}^{(2)}$

The corrections $P_{2}^{(1)}$ and $P_{3}^{(2)}$ are known exactly in $m_c$. In order to describe their content, we expand $K_{ij}(E_0, \mu_b)$ in $\tilde{\alpha}_s(\mu_b)$

$$K_{ij} = \delta_{i7}\delta_{j7} + \tilde{\alpha}_s(\mu_b)K_{ij}^{(1)} + \tilde{\alpha}_s^2(\mu_b)K_{ij}^{(2)} + \mathcal{O}\left(\tilde{\alpha}_s^3(\mu_b)\right).$$

(3.1)

The coefficients $K_{ij}^{(1)}$ are easily derived from the known NLO results

$$K_{i7}^{(1)} = \Re\Re\xi_{i}^{(1)} - \frac{1}{2}\gamma_{i7}^{(0)\text{eff}} L_b + 2\phi_{i7}^{(1)}(\delta),$$

for $i \leq 6$,  

(3.2)

$$K_{77}^{(1)} = -\frac{182}{9} + \frac{8}{9}\pi^2 - \gamma_{77}^{(0)\text{eff}} L_b + 4\phi_{77}^{(1)}(\delta),$$

(3.3)

$$K_{78}^{(1)} = \frac{44}{9} - \frac{8}{27}\pi^2 - \frac{1}{2}\gamma_{87}^{(0)\text{eff}} L_b + 2\phi_{78}^{(1)}(\delta),$$

(3.4)

$$K_{ij}^{(1)} = 2(1 + \delta_{ij})\phi_{ij}^{(1)}(\delta),$$

for $i,j \neq 7$,  

(3.5)

The evanescent operators are as in Eqs. (23)–(25) of Ref. [4].
where
\[ L_b = \ln \left( \frac{\mu_b}{m_b^{1S}} \right)^2. \] (3.6)

The matrix \( \hat{\gamma}^{(0)\text{eff}} \) and the quantities \( r_i^{(1)} \) as functions of
\[ z = \left( \frac{m_c(\mu_c)}{m_b^{1S}} \right)^2 \] (3.7)
can be found respectively in Eqs. (6.3) and (3.1) of Ref. [20]. The bottom mass is renormalized in the 1S scheme [21] throughout the paper. The charm mass \( \overline{\text{MS}} \) renormalization scale \( \mu_c \) is chosen to be independent from \( \mu_b \). For future convenience, we quote \( r_{1,2}^{(1)} \):
\[ r_2^{(1)}(z) = -6 r_1^{(1)}(z) = -\frac{1666}{243} + 2[a(z) + b(z)] - \frac{80}{81}i\pi. \] (3.8)

The exact expressions for \( a(z) \) and \( b(z) \) in terms of Feynman parameter integrals can be found in Eqs. (3.3) and (3.4) of Ref. [20]. Their small-\( m_c \) expansions up to \( \mathcal{O}(z^4) \) read [22, 23]
\[
a(z) = \frac{16}{9} \left\{ \left[ \frac{5}{2} - \frac{\pi^2}{3} - 3\zeta(3) + \left( \frac{5}{2} - \frac{3\pi^2}{4} \right)L_z + \frac{1}{4}L_z^2 + \frac{1}{12}L_z^3 \right] z + \left( \frac{7}{4} + \frac{2\pi^2}{3} - \frac{\pi^2}{2}L_z \right) \right. \\
\left. - \frac{1}{4}L_z^2 + \frac{1}{12}L_z^3 \right\} z^2 + \left[ -\frac{7}{6} - \frac{\pi^2}{6} + \frac{1}{2}L_z \right] z^3 + \left( \frac{457}{216} - \frac{5\pi^2}{18} - \frac{1}{72}L_z - \frac{5}{6}L_z^2 \right) z^4 \\
+ i\pi \left[ \left( 4 - \frac{\pi^2}{3} + L_z + L_z^2 \right) \frac{z}{2} + \left( \frac{1}{2} - \frac{\pi^2}{6} - L_z + \frac{1}{2}L_z^2 \right) z^2 + \frac{5}{9}z^4 \right] \right) + \mathcal{O}(z^5L_z^2), \tag{3.9}
\]
\[
b(z) = -\frac{8}{9} \left\{ \left[ -3 + \frac{\pi^2}{6} - L_z \right] z - 2\pi^2 z^{3/2} + \left( \frac{1}{2} + \pi^2 - 2L_z - \frac{1}{2}L_z^2 \right) z^2 \\
+ \left( \frac{25}{12} - \frac{1}{9}\pi^2 - \frac{19}{18}L_z + 2L_z^2 \right) z^3 + \left( \frac{-1376}{225} + \frac{137}{30}L_z + 2L_z^2 + \frac{2\pi^2}{3} \right) z^4 \\
+ i\pi \left[ -z + (1 - 2L_z) z^2 + \left( \frac{-10}{9} + \frac{4}{3}L_z \right) z^3 + z^4 \right] \right) \right\} + \mathcal{O}(z^5L_z^2), \tag{3.10}
\]
where
\[ L_z = \ln z. \tag{3.11} \]

The functions \( \phi_{ij}^{(1)}(\delta = 1 - 2E_0/m_b^{1S}) \) with \( i, j \in \{1, 2, 7, 8\} \) can be found in Appendix E of Ref. [12]. The remaining ones (that affect \( P(1.6 \text{ GeV}) \) by \( \sim 0.1\% \) only) can be read out from the results of Ref. [24]. In particular,
\[
\phi_{47}^{(1)}(\delta) = -\frac{1}{54} \delta \left( 1 - \delta + \frac{1}{3} \delta^2 \right) + \frac{1}{12} \lim_{m_c \to m_b} \phi_{27}^{(1)}(\delta), \tag{3.12}
\]
\[
\phi_{48}^{(1)}(\delta) = \frac{1}{3} \phi_{47}^{(1)}(\delta). \tag{3.13}
\]
Once all the ingredients of \( K_{ij}^{(1)} \) have been specified, \( P_2^{(1)} \) and \( P_3^{(2)} \) are evaluated by simple substitutions to Eq. \((2.6)\)

\[
P_2^{(1)} = \sum_{i,j=1}^{8} C_i^{(0)\text{eff}} C_j^{(0)\text{eff}} K_{ij}^{(1)},
\]

\[
P_3^{(2)} = 2 \sum_{i,j=1}^{8} C_i^{(0)\text{eff}} C_j^{(1)\text{eff}} K_{ij}^{(1)}.
\]

\[(3.14)\]

\[(3.15)\]

### 4 The \( \beta_0 \)-part of \( P_2^{(2)} \)

The only NNLO correction to \( P(E_0) \) in Eq. \((2.10)\) that has not yet been given is \( P_2^{(2)} \). For this contribution, we shall neglect the tiny LO Wilson coefficients of \( Q_3, \ldots, Q_6 \). The NLO matrix elements of these operators affect the branching ratio by only around 1\% \[20\]. Thus, neglecting the corresponding NNLO ones has practically no influence on the final accuracy.

Let us split \( K_{ij}^{(2)} \) into the \( \beta_0 \)-parts \( K_{ij}^{(2)\beta_0} \) and the remaining parts \( K_{ij}^{(2)\text{rem}} \)

\[
K_{ij}^{(2)} = A_{ij} n_f + B_{ij} = K_{ij}^{(2)\beta_0} + K_{ij}^{(2)\text{rem}},
\]

\[(4.1)\]

where \( n_f \) stands for the number of massless flavours in the effective theory, and

\[
K_{ij}^{(2)\beta_0} = -\frac{3}{2} \beta_0 A_{ij} = -\frac{3}{2} \left( 11 - \frac{2}{3} n_f \right) A_{ij}, \quad K_{ij}^{(2)\text{rem}} = \frac{33}{2} A_{ij} + B_{ij}.
\]

\[(4.2)\]

Following Ref. \[11\], we shall take \( n_f = 5 \). Effects related to the absence of real \( \bar{c}c \) production in \( b \to X_s^{\text{parton}} \gamma \) and to non-zero masses in quark loops on gluon propagators are relegated to \( K_{ij}^{(2)\text{rem}} \). Thus, the only \( m_c \)-dependent contributions to \( K_{ij}^{(2)\beta_0} \) originate from charm loops containing the four-quark vertices \( Q_1 \) and \( Q_2 \).

The explicit \( K_{ij}^{(2)\beta_0} \) that we derive from the results of Refs. \[7,8,11,15,20\] read

\[
K_{27}^{(2)\beta_0} = \beta_0 \Re \left\{ -\frac{3}{2} r_2^{(2)}(z) + 2 \left[ a(z) + b(z) - \frac{290}{81} \right] \left( L_b - \frac{100}{81} L_b^2 \right) \right\} + 2 \phi_{27}^{(2)\beta_0}(\delta),
\]

\[(4.3)\]

\[
K_{17}^{(2)\beta_0} = -\frac{1}{6} K_{27}^{(2)\beta_0},
\]

\[(4.4)\]

\[
K_{77}^{(2)\beta_0} = \beta_0 \left\{ -\frac{3803}{54} - \frac{46}{27} \pi^2 + \frac{80}{3} \zeta(3) + \left( \frac{8}{9} \pi^2 - \frac{98}{3} \right) L_b - \frac{16}{3} L_b^2 \right\} + 4 \phi_{77}^{(2)\beta_0}(\delta),
\]

\[(4.5)\]

\[
K_{78}^{(2)\beta_0} = \beta_0 \left\{ -\frac{1256}{81} - \frac{64}{81} \pi^2 - \frac{32}{9} \zeta(3) + \left( \frac{188}{27} - \frac{8}{27} \pi^2 \right) L_b + \frac{8}{9} L_b^2 \right\} + 2 \phi_{78}^{(2)\beta_0}(\delta),
\]

\[(4.6)\]

\[
K_{ij}^{(2)\beta_0} = 2(1 + \delta_{ij}) \phi_{ij}^{(2)\beta_0}(\delta), \quad \text{for } i, j \neq 7.
\]

\[(4.7)\]

The small-\( m_c \) expansion of \( \Re r_2^{(2)}(z) \) up to \( \mathcal{O}(z^4) \) was calculated by Bieri et al. \[11\]

\[
\Re r_2^{(2)}(z) = \frac{67454}{6561} - \frac{124 \pi^2}{729} - \frac{4}{1215} \left( 11280 - 1520 \pi^2 - 171 \pi^4 - 5760 \zeta(3) + 6840 L_z \right).
\]
\[ -1440\pi^2 L_z - 2520\zeta(3) L_z + 120 L_z^2 + 100 L_z^3 - 30 L_z^4 \bigg) z \]
\[ - \frac{64\pi^2}{243} (43 - 12 \ln 2 - 3L_z) z^{3/2} - \frac{2}{1215} \left( 11475 - 380\pi^2 + 96\pi^4 + 7200\zeta(3) \right) \]
\[ - 1110 L_z - 1560\pi^2 L_z + 1440\zeta(3) L_z + 990 L_z^2 + 260 L_z^3 - 60 L_z^4 \bigg) z^2 \]
\[ + \frac{2240\pi^2}{243} z^{5/2} - \frac{2}{2187} \left( 62471 - 2424\pi^2 - 33264\zeta(3) - 19494 L_z - 504\pi^2 L_z \right) \]
\[ - \frac{5184 L_z^2 + 2160 L_z^3}{243} z^3 - \frac{2464}{6075} \pi^2 z^{7/2} + \left( -\frac{15103841}{546750} + \frac{7912}{3645} \pi^2 + \frac{2368}{81} \zeta(3) \right) \]
\[ + \frac{147038}{6075} L_z + \frac{352}{243} \pi^2 L_z + \frac{88}{243} L_z^2 - \frac{512}{243} L_z^3 \bigg) z^4 + \mathcal{O}(z^{9/2} L_z^4). \quad (4.8) \]

The function \( \phi^{(2)\beta_0}_{77}(\delta) \) reads
\[
\phi^{(2)\beta_0}_{77}(\delta) = \beta_0 \left[ \phi^{(1)}_{77}(\delta) L_b + 4 \int_0^{1-\delta} dx \, F^{(2,nf)} \right], \quad (4.9)
\]
where \( F^{(2,nf)} \) as a function of \( x = 2E_\gamma / m_b \) is given in Eq. (9) of Ref. [8].

The remaining functions \( \phi^{(2)\beta_0}_{ij}(\delta) \) will be neglected in our numerical analysis. It should not cause any significant uncertainty for \( E_0 = 1.6 \) GeV. For this particular cut, the NLO functions \( \phi^{(1)}_{ij}(\delta) \) affect the branching ratio by around \(-4\%\) only, which is partly due to a certain convention in their definitions (\( \phi^{(1)}_{ij}(0) = 0 \) for \((ij) \neq (77)\), and \( \phi^{(1)}_{77}(1) = 0 \)). An analogous convention is used for \( \phi^{(2)\beta_0}_{ij}(\delta) \). The known \( \phi^{(2)\beta_0}_{77}(\delta) \) affects the branching ratio by around \(-0.4\%\) only. If the NLO pattern is repeated, an effect of similar magnitude is expected from the other \( \phi^{(2)\beta_0}_{ij}(\delta) \).

As in Eq. (4.11), we can split \( P_2^{(2)} = P_2^{(2)\beta_0} + P_2^{(2)\text{rem}} \) and express \( P_2^{(2)\beta_0} \) in terms of \( K_{ij}^{(2)\beta_0} \), by analogy to Eq. (3.11).

\[
P_2^{(2)\beta_0} \simeq \sum_{i,j=1,2,7,8} C_i^{(0)\text{eff}} C_j^{(0)\text{eff}} K_{ij}^{(2)\beta_0}. \quad (4.10)
\]

The “\( \simeq \)” sign is used above only because we skip \( i,j = 3,4,5,6 \) in the sum.

5 The full correction \( P_2^{(2)} \) in the limit \( m_c \gg m_b/2 \)

The present section contains the main new result of our paper, namely the asymptotic form of \( P_2^{(2)} \) in the limit \( m_c \gg m_b/2 \). It has been evaluated by performing a formal three-loop decoupling of the charm quark in the effective theory, using the method that has been previously applied by us to the calculation of the three-loop matching at the electroweak scale [3,25]. Once the charm decoupling scale is set equal to \( \mu_s \), one recovers the asymptotic form of the matrix elements in the large \( m_c \) limit. Details of this calculation will be presented elsewhere [26].

---

5 The original calculation of \( F^{(2,nf)} \) and several other contributions to the photon spectrum was performed in Ref. [27].
The $m_c$-dependence of $P(E_0)$ at the NLO is dominated by $\text{Re}[a(z) + b(z)]$. At the two-loop level, we find the following asymptotic form of the functions $a(z)$ and $b(z)$

$$\text{Re} a(z) = \frac{4}{3}L_z + \frac{34}{9} + \frac{1}{z} \left( \frac{5}{27}L_z + \frac{101}{486} \right) + \frac{1}{z^2} \left( \frac{1}{15}L_z + \frac{1393}{24300} \right) + O\left( \frac{1}{z^3} \right),$$

$$\text{Re} b(z) = -\frac{4}{81}L_z + \frac{8}{81} - \frac{1}{z} \left( \frac{2}{45}L_z + \frac{76}{2025} \right) - \frac{1}{z^2} \left( \frac{4}{189}L_z + \frac{487}{33075} \right) + O\left( \frac{1}{z^3} \right).$$

(5.1)

(5.2)

The small-$m_c$ expansion of this function has been given in Eq. (4.8).

For the real part of the three-loop function $r_2^{(2)}(z)$ introduced in Eq. (4.3), we find

$$\text{Re} r_2^{(2)}(z) = \frac{8}{9}L_z^2 + \frac{112}{243}L_z + \frac{27650}{6561} + \frac{1}{z} \left( \frac{38}{405}L_z^2 - \frac{572}{18225}L_z + \frac{10427}{30375} - \frac{8}{135}\pi^2 \right)$$

$$+ \frac{1}{z^2} \left( \frac{86}{2835}L_z^2 - \frac{1628}{893025}L_z + \frac{198999293}{125023500} - \frac{8}{405}\pi^2 \right) + O\left( \frac{1}{z^3} \right).$$

(5.3)

The expressions that we have found for the leading terms in the large-$m_c$ expansion of $K_{ij}^{(2)\text{rem}}$ are presented below. The necessary leading terms of $K_{ij}^{(1)}$ are easily derived from Eqs. (5.1).
and (5.2), taking into account that only $\phi^{(1)}_{ij}$ with $i, j > 2$ do not vanish at large $z$, and that $\phi^{(1)}_{ij}$ are $z$-independent for $i, j = 4, 7, 8$.

$$K_{22}^{(2)\text{rem}} = 36 K_{11}^{(2)\text{rem}} + \mathcal{O}\left(\frac{1}{z}\right) = -6 K_{12}^{(2)\text{rem}} + \mathcal{O}\left(\frac{1}{z}\right) = \left(K_{27}^{(1)\text{rem}}\right)^2 + \mathcal{O}\left(\frac{1}{z}\right), \quad (5.4)$$

$$K_{27}^{(2)\text{rem}} = K_{27}^{(1)\text{rem}} + \left(\frac{127}{324} - \frac{35}{27}L_D\right) K_{78}^{(1)\text{rem}} + \frac{2}{3}(1 - L_D) K_{47}^{(1)\text{rem}} - \frac{4736}{729} L_D^2 + \frac{1150}{729} L_D - \frac{1617980}{19683} + \frac{20060}{243}\zeta(3) + \frac{1664}{81} L_c + \mathcal{O}\left(\frac{1}{z}\right), \quad (5.5)$$

$$K_{28}^{(2)\text{rem}} = K_{27}^{(1)\text{rem}} + \left(\frac{127}{324} - \frac{35}{27}L_D\right) K_{88}^{(1)\text{rem}} + \frac{2}{3}(1 - L_D) K_{48}^{(1)\text{rem}} + \mathcal{O}\left(\frac{1}{z}\right), \quad (5.6)$$

$$K_{17}^{(2)\text{rem}} = -\frac{5}{6} K_{27}^{(2)\text{rem}} + \left(\frac{5}{16} - \frac{3}{4}L_D\right) K_{78}^{(1)\text{rem}} - \frac{1237}{729} + \frac{232}{27}\zeta(3) + \frac{70}{27} L_D^2 - \frac{20}{27} L_D + \mathcal{O}\left(\frac{1}{z}\right), \quad (5.7)$$

$$K_{18}^{(2)\text{rem}} = -\frac{5}{6} K_{28}^{(2)\text{rem}} + \left(\frac{5}{16} - \frac{3}{4}L_D\right) K_{88}^{(1)\text{rem}} + \mathcal{O}\left(\frac{1}{z}\right), \quad (5.8)$$

$$K_{77}^{(2)\text{rem}} = \left(K_{77}^{(1)\text{rem}} - 4\phi_{77}^{(1)}(\delta) + \frac{2}{3}L_z\right) K_{77}^{(1)\text{rem}} - \frac{32}{9} L_D^2 + \frac{224}{27} L_D - \frac{628487}{729} - \frac{628}{405}\pi^4 + \frac{31823}{729}\pi^2 + \frac{428}{27}\pi^2 \ln 2 + \frac{26590}{81}\zeta(3) - \frac{160}{3} L_b^2 - \frac{2720}{9} L_b + \frac{256}{27}\pi^2 L_b + \frac{512}{27}\pi\alpha_T + 4\phi_{77}^{(2)\text{rem}}(\delta) + \mathcal{O}\left(\frac{1}{z}\right), \quad (5.9)$$

$$K_{78}^{(2)\text{rem}} = \left(-\frac{50}{3} + \frac{8}{3}\pi^2 - \frac{2}{3}L_D\right) K_{78}^{(1)\text{rem}} + \frac{16}{27} L_D^2 - \frac{112}{81} L_D + \frac{364}{243} + X_{78}^{(2)\text{rem}} + \mathcal{O}\left(\frac{1}{z}\right), \quad (5.10)$$

$$K_{88}^{(2)\text{rem}} = \left(-\frac{50}{3} + \frac{8}{3}\pi^2 - \frac{2}{3}L_D\right) K_{88}^{(1)\text{rem}} + X_{88}^{(2)\text{rem}} + \mathcal{O}\left(\frac{1}{z}\right), \quad (5.11)$$

where

$$K_{47}^{(1)\text{rem}} = K_{47}^{(1)\text{rem}} - \beta_0 \left(\frac{26}{81} - \frac{4}{27}L_b\right), \quad (5.12)$$

$$L_c = \ln\left(\frac{\mu_c}{m_c(\mu_c)}\right)^2, \quad (5.13)$$

and the "decoupling logarithm"

$$L_D \equiv L_b - L_z = \ln\left(\frac{\mu_b}{m_c(\mu_c)}\right)^2. \quad (5.14)$$
The function $\phi_{T7}^{(2)\text{rem}}(\delta)$ reads

$$
\phi_{T7}^{(2)\text{rem}}(\delta) = -4 \int_0^{1-\delta} dx \left[ \frac{16}{9} F^{(2,a)} + 4 F^{(2,na)} + \frac{29}{3} F^{(2,nf)} \right] - \frac{8\pi \alpha_T}{27 \delta} \left[ 2\delta \ln^2 \delta + (4 + 7\delta - 2\delta^2 + 3\delta^3) \ln \delta + 7 - \frac{8}{3} \delta - 7\delta^2 + 4\delta^3 - \frac{4}{3}\delta^4 \right],
$$

(5.15)

where $F^{(2,a)}$, $F^{(2,na)}$ and $F^{(2,nf)}$ as functions of $x = 2E_r/m_b$ are given in Eqs. (7)–(9) of Ref. [8]. The terms proportional to $\alpha_T \equiv \alpha_s^{(4)}(\mu = m_b^{1S})$ occur in Eqs. (5.9) and (5.15) because the so-called Upsilon expansion prescription [28] is followed here, which means that $m_b^{\text{pole}}$ is expressed in terms of $m_b^{1S}$, and $\alpha_T$ in the ratio

$$
\frac{m_b^{1S}}{m_b^{\text{pole}}} = 1 - \frac{8\pi}{9} \tilde{\alpha}_s(\mu_b) \alpha_T + \ldots
$$

(5.16)

is treated as independent from $\tilde{\alpha}_s(\mu_b)$, i.e. it is not included in the order-counting when the $\mathcal{O}(\tilde{\alpha}_s^3(\mu_b))$ terms are neglected. A reader who wants to bypass this prescription and use another kinetic scheme for $m_b$ should set $\alpha_T$ to zero in Eqs. (5.9) and (5.15) and at the same time replace $m_b^{1S}$ by $m_b^{\text{pole}}$. Next, the latter mass should be perturbatively re-expressed in terms of the chosen $m_b^{\text{kinetic}}$ to get rid of the renormalon ambiguity. We have verified that the $\sim 0.4\%$ effect of the $\alpha_T$-terms on the branching ratio can be reproduced by using $m_b^{\text{pole}} = 4.74$ GeV at the considered order.

The $m_c$-independent quantities $X_{78}^{(2)\text{rem}}$ and $X_{88}^{(2)\text{rem}}$ in Eqs. (5.10) and (5.11) stand for the unknown non-$\beta_0$ contributions from the two-loop matrix element of $Q_8$ in the theory with decoupled charm (together with the corresponding bremsstrahlung). They will be set to zero in the numerical analysis. Neglecting them can be justified by arguing that the contribution of $K_{78}^{(2)}$ to $P(E_0)$ is suppressed relative to that of $K_{17}^{(2)}$ by $|Q_6 C_8^{\text{eff}} / C_7^{\text{eff}}| \approx \frac{1}{6}$. In effect, $K_{78}^{(2)\beta_0}$ in Eq. (4.6) affects $P(E_0)$ by around $0.1\%$ only. The suppression factor gets squared for $K_{88}^{(2)}$. Thus, neglecting $X_{78}^{(2)\text{rem}}$ and $X_{88}^{(2)\text{rem}}$ is not expected to cause any significant uncertainty.

Using the results of Refs. [7,8], one easily derives an expression for the $m_c \to 0$ limit of $K_{77}^{(2)\text{rem}}$ that differs from $K_{77}^{(2)\text{rem}}$ by inclusion of the real $c\bar{c}$ production contributions (see Appendix B)

$$
\tilde{K}_{77}^{(2)\text{rem}}(z = 0) = (K_{77}^{(1)} - 4\phi_{77}^{(1)}(\delta) + \frac{2}{3} L_b) K_{77}^{(1)} - \frac{587708}{729} + \frac{32651}{729} \pi^2 - \frac{628}{405} \pi^4
$$

$$
+ \frac{428}{27} \pi^2 \ln 2 + \frac{25150}{81} \zeta(3) - \frac{448}{9} L_b^2 + \left( \frac{80}{9} \pi^2 - \frac{2524}{9} \right) L_b
$$

$$
+ \frac{512}{27} \pi \alpha_T + 4 \phi_{77}^{(2)\text{rem}}(\delta) - \frac{8 \phi_{77}^{(2)\beta_0}}{3 \beta_0}.
$$

(5.17)

We are going to use this formula for testing the $m_c$-interpolation prescription in the next section.

By analogy to Eqs. (3.14) and (4.10), we can write $P_2^{(2)\text{rem}}$ as

$$
P_2^{(2)\text{rem}} \simeq \sum_{i,j=1,2,7,8} C_i^{(0)\text{eff}} C_j^{(0)\text{eff}} K_{ij}^{(2)\text{rem}}.
$$

(5.18)

The “$\simeq$” sign is used above only because $i, j = 3, 4, 5, 6$ are skipped in the sum.
6 Interpolation in $m_c$

In the present section, we are going to estimate $P^{(2)\text{rem}}_2$ for $m_c < m_b/2$ by performing a certain interpolation between its large-$m_c$ asymptotic form and an assumed value at $m_c = 0$. In particular, we shall assume that the large-$\beta_0$ approximation is accurate at $m_c = 0$, which may be argued for by recalling that no charm mass renormalization effects arise at that point. Since such an assumption is obviously a weak point of the calculation, two alternative forms of it will be considered:

(a) \[ P^{(2)\text{rem}}_2 \xrightarrow{z \to 0} 0, \]  
(b) \[ P^{(2)}_1 + P^{(2)}_2 + P^{(2)}_3 \xrightarrow{z \to 0} P^{(2)\beta_0}_2. \]

The difference between these two cases will serve as a basis to estimate the interpolation uncertainty. As a cross-check, we shall also consider the case

(c) \[ P^{(2)\text{rem}}_2 \xrightarrow{z \to 0} \left( C^{(0)\text{eff}}_7 \right)^2 \tilde{K}^{(2)\text{rem}}_{77} (z = 0), \]

which does not rely on the large-$\beta_0$ approximation but rather on assuming that the “77” term dominates at $m_c = 0$. In Appendix B, issues related to the $c\bar{c}$ production are discussed.

The functional form of $P^{(2)\text{rem}}_2(z)$ that we are going to use for the interpolation is a linear combination

\[ P^{(2)\text{rem}}_2 = x_1 |r^{(1)}_2(z)|^2 + x_2 \text{Re} r^{(2)}_2(z) + x_3 \text{Re} r^{(1)}_2(z) + x_4 z \frac{d}{dz} \text{Re} r^{(1)}_2(z) + x_5. \]  

If $P^{(2)\text{rem}}_2$ was dominated by renormalization effects, the last three terms would be sufficient. The first two terms are included because otherwise no $\ln^2 z$ would be reproduced at large $z$. The function $|r^{(1)}_2|^2$ is non-analytic at $m_c = m_b/2$ and takes into account the pure four-quark operator contribution to the squared amplitude. The function $\text{Re} r^{(2)}_2(z)$ matches the remaining $\ln^2 z$ in the large-$m_c$ asymptotics. We use this function because it is the only genuine NNLO four-quark operator matrix element that is known for small $z$.

The determination of the coefficients $x_i$ is most easily explained in a specific numerical example. Let us choose the renormalization scales as follows: $\mu_0 = 2M_W$, $\mu_b = m_b^{1S}/2$ and $\mu_c = m_c(m_c)$. When the central values of the input parameters from Appendix A are used but only $m_c$ is retained arbitrary, Eq. (5.18) yields

\[ P^{(2)\text{rem}}_2 \simeq (9.57 + 7.12) \ln^2 z + 50.52 \ln z + 47.44 + \mathcal{O} \left( \frac{1}{z} \right), \]  

where the contribution from Eq. (5.3) has been singled out in the coefficient at $\ln^2 z$ (the first term). This first term is assumed to determine $x_1$. Then the second term in the coefficient at $\ln^2 z$ determines $x_2$. Next, $x_3$ is determined from the coefficient at $\ln z$. Finally, by adjusting $x_4$ and $x_5$, one can simultaneously match the constant term in Eq. (6.5) and satisfy.
one of the requirements (6.1), (6.2) or (6.3). In our example, the results are

(a) \( P_2^{(2)\text{rem}}(z) \approx 1.45 \left[ |r_2^{(1)}(z)|^2 - |r_2^{(1)}(0)|^2 \right] + 8.01 \text{Re} \left[ r_2^{(2)}(z) - r_2^{(2)}(0) \right] \\
+ 15.63 \text{Re} \left[ r_2^{(1)}(z) - r_2^{(1)}(0) \right] + 16.52 z \frac{d}{dz} \text{Re} r_2^{(1)}(z), \quad (6.6)

(b) \( P_2^{(2)\text{rem}}(z) \approx 1.45 \left[ |r_2^{(1)}(z)|^2 - |r_2^{(1)}(0)|^2 \right] + 8.01 \text{Re} \left[ r_2^{(2)}(z) - r_2^{(2)}(0) \right] \\
+ 15.63 \text{Re} \left[ r_2^{(1)}(z) - r_2^{(1)}(0) \right] + 0.89 z \frac{d}{dz} \text{Re} r_2^{(1)}(z) + 40.15, \quad (6.7)

(c) \( P_2^{(2)\text{rem}}(z) \approx 1.45 \left[ |r_2^{(1)}(z)|^2 - |r_2^{(1)}(0)|^2 \right] + 8.01 \text{Re} \left[ r_2^{(2)}(z) - r_2^{(2)}(0) \right] \\
+ 15.63 \text{Re} \left[ r_2^{(1)}(z) - r_2^{(1)}(0) \right] + 8.14 z \frac{d}{dz} \text{Re} r_2^{(1)}(z) + 21.53, \quad (6.8)

where \( P_1^{(2)} + P_3^{(2)}(z = 0) \approx -40.15 \) determines the very last term in the (b) case.

Substituting the central value of \( m_c(m_c) \) from Appendix A sets \( z \) to \( z_0 \approx (0.262)^2 \approx 0.0684 \). Then, \( P_2^{(2)\beta_0}(z_0) \approx 3.86 \) and

(a) \( P_2^{(2)\text{rem}}(z_0) \approx -3.00 \Rightarrow P_2^{(2)}(z_0) \approx 0.87, \quad (6.9)\)

(b) \( P_2^{(2)\text{rem}}(z_0) \approx 10.98 \Rightarrow P_2^{(2)}(z_0) \approx 14.85, \quad (6.10)\)

(c) \( P_2^{(2)\text{rem}}(z_0) \approx 4.50 \Rightarrow P_2^{(2)}(z_0) \approx 8.36. \quad (6.11)\)

The corrections \( P_2^{(2)\text{rem}} \) from Eqs. (6.6), (6.7) and (6.8) are shown in the left plot of Fig. 2 as functions of \( \sqrt{z} = m_c/m_b \). The other NNLO corrections \( P_1^{(2)}, P_2^{(2)\beta_0} \) and \( P_3^{(2)} \) are shown in

Figure 2: \( P_2^{(2)\text{rem}}, P_2^{(2)\beta_0}, P_1^{(2)} \) and \( P_3^{(2)} \) as functions of \( m_c/m_b = \sqrt{z} \) for \( \mu_0 = 2M_W, \mu_b = m_b/S/2 \) and \( \mu_c = m_c(m_c) \). The other input parameters are set to their central values from Appendix A. See the text below Eq. (6.14).
the right plot. For the same parameters, one finds:

\[ P_1^{(2)} \approx -8.45, \]  
\[ P_2^{(2)\beta_0}(z) \approx 10.35 \text{Re} \left[ \frac{r_2^{(2)}(z) - r_2^{(2)}(0)}{z} \right] + 9.57 \text{Re} \left[ \frac{r_2^{(1)}(z) - r_2^{(1)}(0)}{z} \right] + 0.71 \Rightarrow P_2^{(2)\beta_0}(z_0) \approx 3.86, \]  
\[ P_3^{(2)}(z) \approx 17.00 \text{Re} a(z) + 16.83 \text{Re} b(z) - 31.04 \Rightarrow P_3^{(2)}(z_0) \approx -10.64. \]

The solid lines in Fig. 2 show the small-\(m_c\) expansions up to \(O(z^4)\). The dashed lines describe the leading terms in the large-\(m_c\) expansions. The dotted lines correspond to exact expressions. The (a), (b) and (c) cases of the interpolated \(P_2^{(2)\text{rem}}\) are indicated in the plot. The two vertical dash-dotted lines mark the 1\(\sigma\) range for \(m_c(m_c)/m_b^{1S}\).

As in Fig. 1, the large- and small-\(m_c\) expansions nicely match at \(m_c = m_b/2\). It is only a consequence of the properties of \(r_2^{(1)}\) and \(\text{Re} r_2^{(2)}\) that determine the \(z\)-dependence of all the considered functions.

It should be stressed that the shape of the curves in Fig. 2 is quite sensitive to the choice of renormalization scales. For instance, when the charm mass renormalization scale \(\mu_c\) is shifted from its default value \(\mu_c = m_c(m_c)\) to twice this value, the coefficients at \(z \frac{d}{dz} \text{Re} r_2^{(1)}(z)\) in Eqs. (6.6), (6.7) and (6.8) change quite dramatically (to 3.30, -12.34 and -5.09, respectively). However, the resulting effect on the decay rate is partly compensated by a correlated change of \(m_c(\mu_c)\) in the NLO correction \(P_2^{(1)}\). The numerical relevance of \(P_2^{(2)\beta_0}\) is very much \(\mu_b\)-dependent, which compensates the \(\mu_b\)-dependence of \(\alpha_s(\mu_b)\) in the NLO correction. The relatively small value in Eq. (6.13) indicates that \(\mu_b = m_b^{1S}/2\) that is used in this section is in the vicinity of the so-called BLM scale [29]. The renormalization scale dependence of our results will be discussed in more detail at the level of the branching ratio in the next section.

From the above results for \(P_k^{(2)}\) and

\[ P^{(0)} \approx 0.1396, \]  
\[ P_1^{(1)} \approx -1.515, \]  
\[ P_2^{(1)}(z) \approx 3.347 - 1.826 \text{Re} a(z) - 1.652 \text{Re} b(z) \Rightarrow P_2^{(1)}(z_0) \approx 1.151, \]

that are calculated using the same parameters, we obtain

(a) \( P(E_0) \approx 0.1226 + O(\alpha_{em}, \alpha_s V_{ub}) \approx 0.1192, \)  
(b) \( P(E_0) \approx 0.1295 + O(\alpha_{em}, \alpha_s V_{ub}) \approx 0.1261, \)  
(c) \( P(E_0) \approx 0.1263 + O(\alpha_{em}, \alpha_s V_{ub}) \approx 0.1229. \)

In the second step above, the electroweak and \(O(V_{ub})\) corrections are added according to Eq. (3.10) of Ref. [17] and Eq. (3.7) of Ref. [12], respectively.

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6 In \(P_2^{(2)}(z)\) (6.14) and \(P_2^{(1)}(z)\) (6.17), we display only the \(z\)-dependence that is due to \(a(z)\) and \(b(z)\). Other \(z\)-dependent effects that originate from \(\phi_2^{(1)}(\sigma)\) are very small.

7 We are grateful to the authors of Ref. [17] for providing us with their results in an extended version that allows for arbitrarily varying \(\mu_0\) and \(\mu_b\).
Figure 3: Renormalization scale dependence of $\mathcal{B}(\bar{B} \to X_s\gamma)$ in units $10^{-4}$ at the LO (dotted lines), NLO (dashed lines) and NNLO (solid lines). The upper-left, upper-right and lower plots describe the dependence on $\mu_c$, $\mu_b$ and $\mu_0$ [GeV], respectively.

Next, using Eq. (2.1) with $N(E_0) \approx 0.0031$, one finds

(a) $\mathcal{B}[\bar{B} \to X_s\gamma]|_{E_\gamma>1.6\text{ GeV}} \approx 3.02 \times 10^{-4}$,

(b) $\mathcal{B}[\bar{B} \to X_s\gamma]|_{E_\gamma>1.6\text{ GeV}} \approx 3.19 \times 10^{-4}$,

(c) $\mathcal{B}[\bar{B} \to X_s\gamma]|_{E_\gamma>1.6\text{ GeV}} \approx 3.11 \times 10^{-4}$.

7 Estimating the uncertainties

The results (a) and (b) given at the end of the previous section are within the range of around $\pm 3\%$ from their average, and the result (c) is in between them. The spread of the three solutions decreases for higher scales $\mu_b$. Moreover, the left plot in Fig. 2 seems reasonable even as a description of an extrapolation rather than an “interpolation with an assumption”.

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Table 1: $B(B \rightarrow X_s \gamma) \times 10^4$ in various cases for several choices of $\mu_b$ and $\mu_c$. The matching scale $\mu_0$ is set to 160 GeV, and the remaining parameters are as in Appendix A.

| $\mu_b$ [GeV] | 2   | 2.5 | 5   | 2.5 |
|----------------|-----|-----|-----|-----|
| $\mu_c$ [GeV] |     |     |     |     |
| (a)            | 3.01| 3.06| 3.14| 3.03| 3.10 |
| (b)            | 3.23| 3.24| 3.26| 3.19| 3.33 |
| (c)            | 3.16| 3.15| 3.18| 3.10| 3.21 |
| $[(a)+(b)]/2$  | 3.12| 3.15| 3.20| 3.11| 3.22 |

Therefore, we shall assign a fixed ±3% to the interpolation ambiguity. Unfortunately, such a rough way of determining this error may need to remain in the $B \rightarrow X_s \gamma$ analysis until a complete evaluation of the three-loop matrix elements is performed. Calculating them just in the $m_c = 0$ case would help a lot.

As far as the higher-order ($O(\alpha_s^3)$) perturbative uncertainties are concerned, renormalization-scale dependence is usually used to place lower bounds on their size. The three plots in Fig. 3 show the branching ratio dependence on each of the three scales, once the remaining two are fixed at the values that were used in the previous section ($\mu_0 = 2M_W$, $\mu_b = m_b^S/2$ and $\mu_c = m_c(m_c)$). Dotted, dashed and solid lines describe the LO, NLO and NNLO results. The NNLO branching ratio is defined as the average of the (a) and (b) cases. Stabilization of the scale dependence with growing order in $\alpha_s$ is clearly seen. It is especially encouraging in the case of $\mu_b$ because the interpolation assumptions (6.1) and (6.2) violate the analytic $\mu_b$-dependence cancellation even at $O(\alpha_s^2)$. The $\mu_c$-stabilization is more obvious because it is built into our interpolation prescription by construction. The perfect $\mu_0$-stabilization arises both due to the smaller value of $\alpha_s$ at the matching scale and to the fact that the NNLO matching conditions are complete.

By studying plots like those in Fig. 3 for various choices of the fixed scales, we have convinced ourselves that ±3% is a reasonable estimate of the higher order perturbative uncertainty. At the same time, we find that $3.15 \times 10^{-4}$ is a good central value. It is reproduced (as an average of the (a) and (b) cases), e.g., for $\mu_0 = 160$ GeV, $\mu_b = 2.5$ GeV and $\mu_c = 1.5$ GeV. Table 1 contains our results for the branching ratio in various cases and for several particular choices of the renormalization scales.

The parametric uncertainty is the most straightforward one. Our input parameters and their uncertainties are listed in Appendix A. The correlation between $C$ and $m_c(m_c)$ is taken into account. The remaining errors that are quoted in the right columns of Tables 2, 3 and 4 in Appendix A are treated as uncorrelated. This way we find the overall parametric uncertainty of ±3.0%.

Finally, the non-perturbative uncertainties need to be considered. It has been customary for a long time to quote the known $O(\Lambda^2/m_b^2)$ and $O(\Lambda^2/m_c^2)$ non-perturbative corrections as the

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8 Various uncertainties will be added in quadrature later. Thus, each of them should be understood as a “theoretical 1σ” rather than a strict range. Of course, such statements concerning theoretical uncertainties are never well-defined, but one can hardly improve on this point.
dominant ones (see Section VI of Ref. [30] for discussion and references). The subdominant $\mathcal{O}(\Lambda^2/m_b^2)$ and $\mathcal{O}(\Lambda^2/(m_b^2 m_c^2))$ ones are known, too [13]. More recently, the $\mathcal{O}(\alpha_s \Lambda^2/(m_b - 2E_0)^2)$ correction was evaluated [14]. All these corrections are included in $N(E_0)$ in Eq. (2.1) and cause around 2.4% enhancement of the branching ratio. However, the non-perturbative corrections that arise in the matrix elements of $Q_1, Q_2$ in the presence of one gluon that is not soft remain unknown. They scale like $\alpha_s \Lambda/m_b$ in the limit $m_c \ll m_b/2$ and like $\alpha_s \Lambda^2/m_c^2$ in the limit $m_c \gg m_b/2$.

Since $m_c < m_b/2$ in reality, we consider $\alpha_s \Lambda/m_b$ as the quantity that sets the size of such effects. In consequence, we assign a $\pm 5\%$ non-perturbative uncertainty to our result. This is the dominant uncertainty at the moment. The very recent estimates [31] of similar corrections to the $Q_7$-$Q_8$ interference term are neglected here. They are smaller than the overall uncertainty of $\pm 5\%$ that both the authors of Ref. [31] and us assign to all the unknown $\mathcal{O}(\alpha_s \Lambda/m_b)$ effects.

8 Conclusions

Our final NNLO result
\[
B[\bar{B} \rightarrow X_s \gamma]_{E_\gamma > 1.6 \text{ GeV}} \simeq (3.15 \pm 0.23) \times 10^{-4}
\] (8.1)
is obtained for the input parameters listed in Appendix A and for the renormalization scales $\mu_0 = 160 \text{ GeV}$, $\mu_b = 2.5 \text{ GeV}$ and $\mu_c = 1.5 \text{ GeV}$. The total uncertainty is found by combining in quadrature the ones discussed in Section 7. As it is clearly seen in Fig. 3, the NNLO corrections significantly improve the stability of the prediction with respect to the renormalization scale variation and, in consequence, reduce the total error. Comparing the NLO and NNLO $\mu_c$-dependence in Fig. 3, one realizes why all the previously published NLO predictions had significantly higher central values than the current NNLO one.

In order to relate our result with $E_0 = 1.6 \text{ GeV}$ to the measurements with cuts at 1.8 GeV (Belle [32]) and 1.9 GeV (BaBar [33]), one needs to compute ratios of the decay rates with different cuts (see, e.g., Ref. [34]). This is a non-trivial issue because new perturbative and non-perturbative effects become important in the endpoint region. A new calculation of such effects has recently been completed [35] but its numerical results were not yet available when the average in Eq. (1.1) was being evaluated.

We have chosen $E_0 = 1.6 \text{ GeV}$ as default here assuming that it is low enough for the cutoff-enhanced perturbative corrections [14,35] to become negligible. If this turns out not to be the case, one should use our results with lower $E_0$. For this purpose, we give

\[
B[\bar{B} \rightarrow X_s \gamma]_{E_\gamma > 1.5 \text{ GeV}} \simeq (3.18 \pm 0.23) \times 10^{-4},
\] (8.2)
\[
B[\bar{B} \rightarrow X_s \gamma]_{E_\gamma > 1.4 \text{ GeV}} \simeq (3.20 \pm 0.23) \times 10^{-4},
\] (8.3)
\[
B[\bar{B} \rightarrow X_s \gamma]_{E_\gamma > 1.3 \text{ GeV}} \simeq (3.22 \pm 0.23) \times 10^{-4},
\] (8.4)

9 We thank M. Beneke for a clarifying discussion on this point.

10 These results do not include contributions from tree-level diagrams with four quark operator insertions that are suppressed either by $|V_{ub}|^2$ or by squares of the small Wilson coefficients $C_3, \ldots, C_6$ [27].
\begin{align}
B[\bar{B} \to X_s \gamma ; E_\gamma > 1.2 \text{ GeV}] & \simeq (3.24 \pm 0.23) \times 10^{-4}, \\
B[\bar{B} \to X_s \gamma ; E_\gamma > 1.1 \text{ GeV}] & \simeq (3.25 \pm 0.23) \times 10^{-4}, \\
B[\bar{B} \to X_s \gamma ; E_\gamma > 1.0 \text{ GeV}] & \simeq (3.27 \pm 0.23) \times 10^{-4}.
\end{align}
(8.5)

Note added

A numerical analysis of cutoff-related perturbative corrections (see Section 8) became available [36] when the current paper was being refereed. The authors of Ref. [36] use our result given in Eq. (8.7) and combine it with their cutoff-related corrections that turn out to suppress the branching ratio at $E_0 = 1.6$ GeV by around 3% with respect to Eq. (8.1). Such an effect is of the same size as our higher-order uncertainty, which means that the unknown $O(\alpha_s^3)$ non-logarithmic effects can be as important at $E_0 = 1.6$ GeV as the logarithmic ones calculated in Ref. [36]. Therefore, we leave the results of the current paper unaltered, yet not excluding the possibility of taking the correction from Ref. [36] into account in future upgrades of the phenomenological analysis, once other effects of potentially the same size are collected (see Section 1 of Ref. [37]).

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Appendix A: Numerical inputs

In this appendix, we collect numerical parameters that are used in Sections 6 and 7. The default value of the photon energy cut is $E_0 = 1.6$ GeV. In Section 6, the renormalization scales were $\mu_0 = 2M_W$, $\mu_b = m_b^S/2$ and $\mu_c = m_c(m_c)$. The final central value of the branching ratio in Eq. (8.1) is reproduced e.g. for $\mu_0 = 160$ GeV, $\mu_b = 2.5$ GeV and $\mu_c = 1.5$ GeV.

The other parameters are displayed in the tables below. Errors are indicated only if varying a given parameter within its 1σ range causes a larger than ±0.1% effect on the branching ratio (8.1). In such cases, the effects in percent are given in the right column of the corresponding table.

Table 2 contains the four quantities that determine the overall normalization factor multiplying $P(E_0)$ in the expression (2.1) for the branching ratio.

17
\[ B(B \to X_c e\bar{\nu})_{\exp} = 0.1061 \pm 0.0017 \text{ [42]} \pm 1.6\% \]
\[ C = 0.580 \pm 0.016 \text{ [39, 41]} \pm 2.8\% \]
\[ |V_{ts}^* V_{tb}/V_{cb}|^2 = 0.9676 \pm 0.0033 \text{ [43, 44]} \pm 0.4\% \]
\[ \alpha_{em}(0) = 1/137.036 \text{ [45]} \]

Table 2: Parameters that determine the overall normalization factor in Eq. \((8.1)\).

\[ M_Z = 91.1876 \text{ GeV [45]} \]
\[ \alpha_s(M_Z) = 0.1189 \pm 0.0020 \text{ [45, 46]} \pm 2.0\% \]
\[ m_{t, \text{pole}} = (171.4 \pm 2.1) \text{ GeV [47]} \pm 0.5\% \]
\[ M_W = 80.403 \text{ GeV [45]} \]
\[ m_b^{\text{LS}} = (4.68 \pm 0.03) \text{ GeV [39]} \pm 0.2\% \]
\[ m_c(m_c) = (1.224 \pm 0.017 \pm 0.054) \text{ GeV [40]} \pm 2.8\% \]

Table 3: Experimental inputs that are necessary in the calculation of \(P(E_0)\) before including the electroweak and \(\mathcal{O}(V_{ub})\) corrections.

Table \(\text{3}\) contains the experimental inputs that are necessary in the calculation of \(P(E_0)\), before including the electroweak and \(\mathcal{O}(V_{ub})\) corrections. For \(\alpha_s(M_Z)\), we adopt the central value from Ref. \([46]\) but conservatively use a twice larger error which then overlaps with the one given by the PDG \([45]\). One should take into account that the phase space factor \(C\) in Table \(\text{2}\) and \(m_c(m_c)\) in Table \(\text{3}\) are strongly correlated. For this reason, we take both parameters as determined in the same global fit to the semileptonic \(B\)-decay spectra \([38–40]\) instead of adopting \(m_c(m_c)\) from Ref. \([48]\). The normalized correlation coefficient amounts to \([41]\)

\[ F \equiv \frac{\langle C m_c \rangle - \langle C \rangle \langle m_c \rangle}{\sigma_C \sigma_{m_c}} \simeq \begin{cases} -0.97, & \text{method A}, \\ -0.92, & \text{method B}, \end{cases} \tag{A.1} \]

where the meaning of the two methods is explained in Section III of Ref. \([40]\). Denoting the uncertainties in the right columns of Tables \(\text{2}\) and \(\text{3}\) by \(\Delta x\), where \(x\) is the relevant variable, one finds that the combined uncertainty due to \(C\) and \(m_c\) is given by

\[ \Delta_{C,m_c} = \sqrt{\Delta_C^2 + \Delta_{m_c}^2 + 2F|\Delta_C \Delta_{m_c}|}. \tag{A.2} \]

Since \(\Delta_C\) and \(\Delta_{m_c}\) are very close in size (by coincidence) and \(F\) is close to \(-1\), the combined uncertainty is much smaller than it would be in the absence of the correlation. For our final result, we adopt \(F = -0.92\) that gives larger \(\Delta_{C,m_c}\) (\(\pm 1.1\%\) rather than \(\pm 0.7\%\)).

The dependence of \(m_c(m_c)\) on \(\alpha_s(M_Z)\) in the semileptonic fit can affect \(m_c(m_c)\) by up to \(\sim 10 \text{ MeV [41]}\), which would translate to \(\sim 0.5\%\) in \(\Delta_{\alpha_s}\). We neglect this effect here. An analogous correlation for \(C\) is also neglected, as it turns out to be even smaller \([41]\).
Table 4: Remaining parameters that are necessary for the electroweak, $\mathcal{O}(V_{ub})$ and non-perturbative corrections. Since we treat the phase space factor $C$ as an independent input, $\lambda_1$ is needed only for the small cutoff-related non-perturbative correction [14]. The parameters $\rho_1$ and $\rho_2$ are needed for the $\mathcal{O}(\Lambda^3/m_b^3)$ contributions to $N(E_0)$ that are derived from the formulae of Refs. [13,52]. An important subtlety in this calculation is that the $\mathcal{O}(\Lambda^3/m_b^3)$ corrections to $\Gamma(B \rightarrow X_u\nu)$ logarithmically diverge when $m_u \rightarrow 0$, so long as hard gluon interactions with the spectator quark are neglected. When they are included, one encounters new non-perturbative matrix elements whose values are rather uncertain [53]. Since these effects cancel in the ratio $(P(E_0) + N(E_0))/C$, we follow the approach that has been used in the calculation of $C$ in Ref. [39], namely we neglect the spectator effects and set $\ln m_b/m_u$ to zero. At the same time, we neglect the additional uncertainty in $C$ that is caused by this arbitrary procedure (see the comments below Eq. (25) in Ref. [39]). Our final result (8.1) is the same as if the considered subtlety did not occur at all. In the future, simultaneous

| parameter                                                                 | effect on Eq. (8.1) |
|---------------------------------------------------------------------------|---------------------|
| $\alpha_{em}(M_Z) = 1/128.940$ [49,50]                                   |                     |
| $\sin^2 \theta_W = 0.2324$ [51]                                          |                     |
| $M_{Higgs} \in [114.4,194] \text{ GeV (95\% C.L)}$ [45]                 |                     |
| $\left(V_{us}^*V_{ub}\right) / \left(V_{ts}^*V_{tb}\right) = -0.011 + 0.018 i$ [43,44] |                     |
| $\lambda_1 = (-0.27 \pm 0.04) \text{ GeV}^2$ [39]                       | $0.3\%$            |
| $\lambda_2 \simeq \frac{1}{4} (m_{B^*}^2 - m_B^2) \simeq 0.12 \text{ GeV}^2$ [45] | $\pm 0.4\%$        |
| $\rho_1 = (0.038 \pm 0.028) \text{ GeV}^3$ [39,41]                      | $\pm 0.6\%$        |
| $\rho_2 = (0.0045 \pm 0.035) \text{ GeV}^3$ [39,41]                      |                     |

Table 5: The LO and NLO Wilson coefficients $C_i^{(k)\text{eff}}(\mu_b)$ at $\mu_b = m_{b}^{1S}/2 = 2.34 \text{ GeV}$. The matching scale $\mu_0$ was set to $2M_W$ in their evaluation.

| $i$ | $C_i^{(0)\text{eff}}(\mu_b)$ | $C_i^{(1)\text{eff}}(\mu_b)$ |
|-----|------------------------------|------------------------------|
| 1   | -0.8411                      | 15.278                       |
| 2   | 1.0647                       | -2.124                       |
| 3   | -0.0133                      | 0.096                        |
| 4   | -0.1276                      | -0.463                       |
| 5   | 0.0012                       | -0.021                       |
| 6   | 0.0028                       | -0.013                       |
| 7   | -0.3736                      | 2.027                        |
| 8   | -0.1729                      | -0.614                       |

Table 4 contains the remaining parameters that are necessary for the electroweak, $\mathcal{O}(V_{ub})$ and non-perturbative corrections. Since we treat the phase space factor $C$ as an independent input, $\lambda_1$ is needed only for the small cutoff-related non-perturbative correction [14].
calculations of $C$ and $N(E_0)$ should be performed on the basis of the semileptonic fit results of Ref. [34], which would constitute an independent test of the the current calculation.

Although the Wilson coefficients $C_i^{\text{eff}}(\mu_b)$ are derived quantities, we quote for convenience their values at $\mu_b = m_b^{1S}/2$. The LO and NLO ones are collected in Table 5. From among the NNLO ones, only $C_7^{(2)\text{eff}}(m_b^{1S}/2) \simeq 16.81$ including the four-loop mixing $(Q_1, \ldots, Q_6) \to Q_7$ but neglecting the four-loop mixing $(Q_1, \ldots, Q_6) \to Q_8$.

The analytical solutions to the NNLO RGE for the Wilson coefficients can be found, e.g., in Section 3.3 of Ref. [54]. The resulting explicit expressions for $C_i^{(k)\text{eff}}(\mu_b)$ in terms of $C_i^{(k)\text{eff}}(\mu_0)$ and $\eta = \alpha_s(\mu_0)/\alpha_s(\mu_b)$ are given in Ref. [6]. As far as $\alpha_s(\mu)$ is concerned, we have used the four-loop RGE and applied two independent methods for solving it: a numerical one implemented in RunDec [55] and an iterative analytical one that includes (tiny) QED effects, too [54]. Our final results are independent of which method is used. However, the intermediate quantities, for which more digits are presented, slightly depend on the method.

Appendix B: The $m_c = 0$ case and $c\bar{c}$ production

The $\bar{B} \to X_s\gamma$ branching ratio contains no contribution from $c\bar{c}$ production because events involving charmed hadrons in the final state are not included on the experimental side. Thus, the evaluation of $b \to X_s^{\text{parton}}\gamma$ should be performed accordingly. However, such a definition of $b \to X_s^{\text{parton}}\gamma$ may break down for $m_c \to 0$, since logarithmic divergences containing $\ln m_c$ may arise in $P_{2}^{(2)\text{rem}}$.

No such divergences are present in the NLO contributions to $P(E_0)$, and in the other than $P_{2}^{(2)\text{rem}}$ NNLO ones. There, all the logarithms of $m_c$ get multiplied by positive powers of this mass. If $P_{2}^{(2)\text{rem}}$ turns out to be logarithmically divergent at $m_c \to 0$, it should be redefined to include the $c\bar{c}$ production contributions. The assumptions (6.1)–(6.3) would then refer to the redefined quantity that must be convergent at $m_c \to 0$. At the same time, the large-$m_c$ asymptotics would remain unaltered. After performing the interpolation of the redefined quantity as in Section 6 one should subtract the $c\bar{c}$ production effects at the measured value of $m_c$. At present, possible effects of such a subtraction are understood to be contained in the interpolation ambiguity.

 Actually, Eq. (5.17) does contain the $c\bar{c}$ production contributions in the $m_c \to 0$ case. However, it is used only in the assumption (6.3) that serves just as a cross check, and has no influence on our final numerical result (8.1).

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