

# Penguin contribution to width difference and CP asymmetry in $B_q - \bar{B}_q$ mixing at order $\alpha_s^2 N_f$

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We present new contributions to the decay matrix element  $\Gamma_{12}^q$  of the  $B_q - \bar{B}_q$  mixing complex, where  $q = d$  or  $s$ . Our new results constitute the order  $\alpha_s^2 N_f$  corrections to the penguin contributions to the Wilson coefficients entering  $\Gamma_{12}^q$  with full dependence on the charm quark mass. This is the first step towards the prediction of the CP asymmetry  $a_{\text{fs}}^q$  quantifying CP violation in mixing at next-to-next-to-leading logarithmic order (NNLO) in quantum chromodynamics (QCD) and further improves the prediction of the width difference  $\Delta\Gamma_q$  between the two neutral-meson eigenstates. We find a sizable effect from the non-zero charm mass and our partial NNLO result decreases the NLO penguin corrections to  $a_{\text{fs}}^q$  by 37% and those to  $\Delta\Gamma_q$  by 16%. We further update the Standard-Model NLO predictions for  $a_{\text{fs}}^q$  and the ratio of the width and mass differences of the  $B_q$  eigenstates: If we express the results in terms of the pole mass of the bottom quark we find  $a_{\text{fs}}^s = (2.07 \pm 0.10) \cdot 10^{-5}$ ,  $a_{\text{fs}}^d = (-4.71 \pm 0.24) \cdot 10^{-4}$ ,  $\Delta\Gamma_s/\Delta M_s = (4.33 \pm 1.26) \cdot 10^{-3}$ , and  $\Delta\Gamma_d/\Delta M_d = (4.48 \pm 1.19) \cdot 10^{-3}$ . In the  $\overline{\text{MS}}$  scheme these numbers read  $a_{\text{fs}}^s = (2.04 \pm 0.11) \cdot 10^{-5}$ ,  $a_{\text{fs}}^d = (-4.64 \pm 0.25) \cdot 10^{-4}$ ,  $\Delta\Gamma_s/\Delta M_s = (4.97 \pm 1.02) \cdot 10^{-3}$ , and  $\Delta\Gamma_d/\Delta M_d = (5.07 \pm 0.96) \cdot 10^{-3}$ .

## I. INTRODUCTION

Flavor-changing neutral current (FCNC) processes probe new physics with masses far beyond the reach of future particle colliders. This justifies the experimental effort at dedicated experiments like LHCb [1] and Belle II [2]. The  $B_d - \bar{B}_d$  and  $B_s - \bar{B}_s$  mixing amplitudes are sensitive to tree-level exchanges of potential new particles with masses above 100 TeV. The oscillations between the flavor eigenstates  $B_q$  and  $\bar{B}_q$ , where  $q = d$  or  $s$ , are governed by two  $2 \times 2$  matrices, the mass matrix  $M$  and the decay matrix  $\Gamma$ . The inclusive, i.e. process-independent quantities entering all oscillation phenomena are  $|M_{12}^q|$ ,  $|\Gamma_{12}^q|$ , and  $\arg(-M_{12}^q/\Gamma_{12}^q)$ . Diagonalizing  $M^q - i\Gamma^q/2$  gives the mass eigenstates  $B_L^q$  and  $B_H^q$  with the subscripts denoting “light” and “heavy”, respectively. The eigenvalues  $M_L^q - i\Gamma_L^q/2$  and  $M_H^q - i\Gamma_H^q/2$  define masses and decay widths of  $B_L^q$  and  $B_H^q$ , which obey exponential decay laws. The above-mentioned three fundamental physical quantities of  $B_q - \bar{B}_q$  mixing can be found by measuring  $\Delta M_q = M_H^q - M_L^q$  (coinciding with the  $B_q - \bar{B}_q$  mixing

oscillation frequency),  $\Delta\Gamma_q = \Gamma_L^q - \Gamma_H^q$ , and [3]

$$a_{\text{fs}}^q = \text{Im} \frac{\Gamma_{12}^q}{M_{12}^q}. \quad (1)$$

The standard way to measure  $a_{\text{fs}}^q$  involves the semileptonic CP asymmetry

$$a_{\text{sl}}^q = \frac{\Gamma(\bar{B}_q(t) \rightarrow X\ell^+\nu_\ell) - \Gamma(B_q(t) \rightarrow \bar{X}\ell^-\bar{\nu}_\ell)}{\Gamma(\bar{B}_q(t) \rightarrow X\ell^+\nu_\ell) + \Gamma(B_q(t) \rightarrow \bar{X}\ell^-\bar{\nu}_\ell)}. \quad (2)$$

In the absence of direct CP violation in the semileptonic decay amplitude one has  $a_{\text{fs}}^q = a_{\text{sl}}^q$ . Direct CP violation in  $B \rightarrow X\ell^+\nu_\ell$  is extremely suppressed in the Standard Model (SM), so that this identification is justified. (In all plausible models of new physics this statement holds as well for  $B \rightarrow D\ell^+\nu_\ell$ , because the needed CP-conserving phase comes from QED corrections only.) The ratio  $\Delta\Gamma_q/\Delta M_q$  is given by

$$\frac{\Delta\Gamma_q}{\Delta M_q} = -\text{Re} \frac{\Gamma_{12}^q}{M_{12}^q}. \quad (3)$$

In this paper we report on new contributions to  $\Gamma_{12}^q/M_{12}^q$  which constitute a portion of the next-to-next-to-leading order (NNLO) QCD corrections to  $a_{\text{fs}}^q$  in Eq. (1) and  $\Delta\Gamma_q/\Delta M_q$  in Eq. (3).

The mass differences  $\Delta M_s = (17.757 \pm 0.021) \text{ ps}^{-1}$  and  $\Delta M_d = (0.5064 \pm 0.0019) \text{ ps}^{-1}$  [4, 5] have been determined very precisely by the CDF [6] and LHCb [7] experiments from the  $B_q - \bar{B}_q$  oscillation frequencies. The experimental values of the width differences [4, 5],

$$\Delta\Gamma_s^{\text{exp}} = (8.9 \pm 0.6) \cdot 10^{-2} \text{ ps}^{-1} \quad (4)$$

$$\Delta\Gamma_d^{\text{exp}} = (-1.32 \pm 6.58) \cdot 10^{-3} \text{ ps}^{-1} \quad (5)$$

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are based on measurements by LHCb [8, 9], ATLAS [10], CMS [11], and CDF [12]. The current experimental world averages for the semileptonic asymmetries are [4, 5]

$$a_{\text{sl}}^{s,\text{exp}} = (60 \pm 280) \cdot 10^{-5}, \quad (6)$$

$$a_{\text{sl}}^{d,\text{exp}} = (-21 \pm 17) \cdot 10^{-4}. \quad (7)$$

Clearly,  $\Delta\Gamma_s$  is a precision observable, while the three other quantities are still far from giving precise information on fundamental parameters. For  $a_{\text{fs}}^d$  and  $\Delta\Gamma_d$  it is worthwhile to study the clean sample of  $B \rightarrow J/\psi K_s$  decays [13]. While new physics will primarily enter  $M_{12}^q$  scenarios in which  $\Gamma_{12}^q$  is affected have been studied as well [14, 15], especially the doubly Cabibbo-suppressed  $\Gamma_{12}^d$  could play a role in new-physics studies.

The state-of-the-art of the theory predictions of  $a_{\text{fs}}^d$  and  $\Delta\Gamma_d$  is next-to-leading logarithmic order (NLO) QCD for the leading-power contribution [16–19] and LO QCD for the  $\mathcal{O}(\Lambda_{\text{QCD}}/m_b)$  power-suppressed corrections [19, 20]. The accuracy of  $\Delta\Gamma_s^{\text{exp}}$  in Eq. (5) calls for an NNLO calculation, which is a formidable project. First steps in this direction have been made in Ref. [21], in which terms of order  $\alpha_s^2 N_f$  to  $\Gamma_{12}$ , where  $N_f = 5$  is the number of active quark flavors, have been calculated up to order  $m_c/m_b$ . This calculation has permitted a better assessment of  $\Delta\Gamma_q$ , but not of  $a_{\text{fs}}^q$ , which is proportional to  $m_c^2/m_b^2$ .

The purpose of the present paper is to do the next step in the calculation of NNLO QCD corrections to  $\Gamma_{12}$ . We calculate the penguin contributions with full dependence on the charm quark mass. These terms constitute an improvement for the prediction of  $\Delta\Gamma_q$  compared to Ref. [21], and, more importantly, are the first step towards the prediction of  $a_{\text{fs}}^q$  at NNLO accuracy.

Penguin contributions are small in the Standard Model, because the Wilson coefficients of the corresponding operators are small, of order 0.05 or smaller. However, this makes these coefficients sensitive to contributions of new physics, which can easily be of the same size [22] as the SM coefficients. Thus in order to study such effects beyond the SM a precise knowledge of the penguin contributions to  $\Gamma_{12}^q$  is desirable.

This paper is organized as follows: In the following section we summarize the theoretical framework of the calculation. In Section III we present our analytical results and subsequently perform a phenomenological analysis in Section IV. Finally we conclude. Results for matrix elements needed for the calculation are relegated to the appendix.

## II. THEORETICAL FRAMEWORK

The effective  $\Delta B = 1$  weak Hamiltonian, relevant for  $b \rightarrow s$  transition, reads [25]

$$H_{\text{eff}}^{\Delta B=1} = -\frac{G_F}{\sqrt{2}} \left\{ \lambda_t^s \left[ \sum_{i=1}^6 C_i O_i + C_8 O_8 \right] - \lambda_u^s \sum_{i=1}^2 C_i (O_i^u - O_i) \right\}, \quad (8)$$

where

$$\lambda_t^s = V_{ts}^* V_{tb}, \quad \lambda_u^s = V_{us}^* V_{ub} \quad (9)$$

comprises the elements of the Cabibbo-Kobayashi-Maskawa (CKM) matrix. The dimension-six effective operators in Eq. (8) are

$$\begin{aligned} O_1^u &= (\bar{s}_i u_j)_{V-A} (\bar{u}_j b_i)_{V-A}, O_2^u = (\bar{s}_i u_i)_{V-A} (\bar{u}_j b_j)_{V-A}, \\ O_1 &= (\bar{s}_i c_j)_{V-A} (\bar{c}_j b_i)_{V-A}, O_2 = (\bar{s}_i c_i)_{V-A} (\bar{c}_j b_j)_{V-A}, \\ O_3 &= (\bar{s}_i b_i)_{V-A} (\bar{q}_j q_j)_{V-A}, O_4 = (\bar{s}_i b_j)_{V-A} (\bar{q}_j q_i)_{V-A}, \\ O_5 &= (\bar{s}_i b_i)_{V-A} (\bar{q}_j q_j)_{V+A}, O_6 = (\bar{s}_i b_j)_{V-A} (\bar{q}_j q_i)_{V+A}, \\ O_8 &= \frac{g_s}{8\pi^2} m_b \bar{s}_i \sigma^{\mu\nu} (1 - \gamma_5) T_{ij}^a b_j G_{\mu\nu}^a. \end{aligned} \quad (10)$$

Here  $i, j$  are color indices and summation over  $q = u, d, s, c, b$  is understood.  $V \pm A$  denote  $\gamma_\mu(1 \pm \gamma_5)$  and  $S \pm P$  (needed below) represents  $(1 \pm \gamma_5)$ .  $C_1, \dots, C_6$  and  $C_8$  are the corresponding Wilson coefficients, which are functions of the top mass  $m_t$  and the  $W$  mass  $M_W$ .  $G_F$  is the Fermi constant. The corresponding formulae for  $b \rightarrow d$  transitions can be obtained from Eqs. (8)-(10) by replacing  $s$  with  $d$ .

To find  $\Delta\Gamma \simeq 2|\Gamma_{12}|$  we must calculate

$$\Gamma_{12} = \text{Abs} \langle B_s | i \int d^4x T \mathcal{H}_{\text{eff}}^{\Delta B=1}(x) \mathcal{H}_{\text{eff}}^{\Delta B=1}(0) | \bar{B}_s \rangle, \quad (11)$$

where ‘Abs’ denotes the absorptive part of the matrix element and  $T$  is the time ordering operator. Following [17] we write  $\Gamma_{12}$  as

$$\begin{aligned} \Gamma_{12} &= - \left[ \lambda_c^2 \Gamma_{12}^{cc} + 2\lambda_c \lambda_u \Gamma_{12}^{uc} + \lambda_u^2 \Gamma_{12}^{uu} \right] \\ &= -\lambda_t^2 \left[ \Gamma_{12}^{cc} + 2\frac{\lambda_u}{\lambda_t} (\Gamma_{12}^{cc} - \Gamma_{12}^{uc}) \right. \\ &\quad \left. + \frac{\lambda_u^2}{\lambda_t^2} (\Gamma_{12}^{uu} + \Gamma_{12}^{cc} - 2\Gamma_{12}^{uc}) \right], \end{aligned} \quad (12)$$

where the coefficients  $\Gamma_{12}^{ab}$ ,  $a, b = u, c$  are positive. The Heavy Quark Expansion (HQE) expresses Eq. (11) in terms of matrix elements of local operators. The leading term (in powers of  $\Lambda_{\text{QCD}}/m_b$ ) reads

$$\Gamma_{12}^{ab} = \frac{G_F^2 m_b^2}{24\pi M_{B_s}} [G^{ab} \langle B_s | Q | \bar{B}_s \rangle - G_S^{ab} \langle B_s | Q_S | \bar{B}_s \rangle]. \quad (13)$$

The two  $|\Delta B| = 2$  operators ( $B$  denotes the beauty quantum number) are

$$Q = (\bar{s}_i b_i)_{V-A} (\bar{s}_j b_j)_{V-A}, \quad (14)$$

$$\tilde{Q}_S = (\bar{s}_i b_j)_{S-P} (\bar{s}_j b_i)_{S-P}. \quad (15)$$

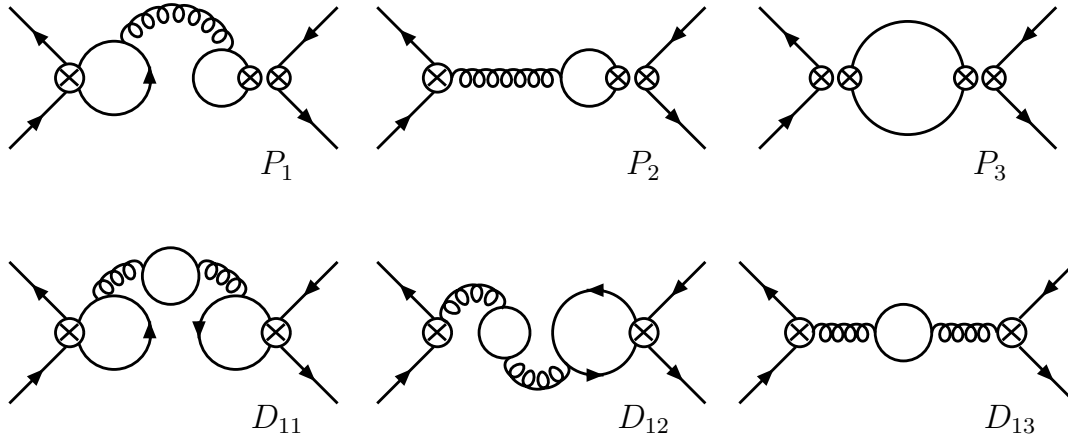


FIG. 1. Diagrams for the penguin contribution at  $\mathcal{O}(\alpha_s^2 N_f)$ . The small Wilson coefficients  $C_{3-6}$  are counted as  $\mathcal{O}(\alpha_s)$ .  $P_1, P_2$  are diagrams with one insertion of a penguin operator  $O_3, \dots, O_6$ , depicted as two circles with crosses, and one insertion of  $O_2^{u,c}$  or  $O_8$ , shown as a single circle with cross.  $P_3$  denotes a one-loop diagram with two insertions of penguin operators  $O_3, \dots, O_6$ .  $D_{11}, D_{12}$  and  $D_{13}$  are diagrams with insertions of operators  $O_2^{u,c}$  or  $O_8$ . (The notation follows Ref. [21].)

The hadronic matrix elements, which are calculated with non-perturbative methods like lattice QCD, are usually expressed in term of the “bag” parameters  $B_{B_q}, B'_{S,B_q}$  as

$$\begin{aligned} \langle B_q | Q(\mu_2) | \bar{B}_q \rangle &= \frac{8}{3} M_{B_q}^2 f_{B_q}^2 B_{B_q}(\mu_2), \\ \langle B_q | \tilde{Q}_S(\mu_2) | \bar{B}_q \rangle &= \frac{1}{3} M_{B_q}^2 f_{B_q}^2 \tilde{B}'_{S,B_q}(\mu_2). \end{aligned} \quad (16)$$

Here  $f_{B_q}$  is the  $B_q$  decay constant and  $\mu_2 = \mathcal{O}(m_b)$  is the renormalization scale at which the matrix elements are calculated. In a lattice-QCD calculation  $\mu_2$  is the scale of lattice-continuum matching. In the expression for  $\Gamma_{12}$  the matrix elements of Eq. (16) are multiplied by perturbative Wilson coefficients depending on  $\mu_2$  as well, resulting in a cancellation of the unphysical scale  $\mu_2$  from  $\Gamma_{12}$ . Analogously, the dependence on the renormalization scheme cancels between the Wilson coefficients and  $B(\mu_2), \tilde{B}'_S(\mu_2)$ . In this paper we use the renormalization scheme of Ref. [16].

Using the notation of Refs. [16, 17, 19], we decompose  $G^{ab}$  and  $G_S^{ab}$  further as

$$G^{ab} = F^{ab} + P^{ab}, \quad G_S^{ab} = -F_S^{ab} - P_S^{ab}. \quad (17)$$

Here  $F^{ab}$  and  $F_S^{ab}$  are the contributions from the current-current operators  $O_{1,2}$ , while  $P^{ab}$  and  $P_S^{ab}$  stem from the penguin operators  $O_{3-6}$  and  $O_8$ . The coefficients  $G^{ab}, G_S^{ab}$  are found by applying an operator product expansion (resulting in the HQE) to the bilocal matrix elements (“full theory”)

$$\text{Abs} \langle i \int d^4x T O_i(x) O_j(0) \rangle. \quad (18)$$

The HQE expresses these bilocal matrix elements in terms of the local matrix elements  $\langle Q \rangle, \langle Q_S \rangle$  (“effective

theory”), the coefficients of the latter are the perturbative short-distance objects studied in this paper. This matching calculation can be done order-by-order in the strong coupling  $\alpha_s$ , with quarks instead of mesons in the external states in Eq. (18). The NLO result of Refs. [16–19] contains the result of Eq. (18) at the two-loop level for  $i, j = 1, 2$ . The chromomagnetic operator  $O_8$  is proportional to the strong coupling  $g_s$ , so that for  $i = 8$  or  $j = 8$  NLO accuracy means one loop only. One further counts the small penguin Wilson coefficients  $C_{3-6}$  as  $\mathcal{O}(\alpha_s)$  and considers only one-loop diagrams for  $i \geq 3$  or  $j \geq 3$ .

### III. RESULTS FOR THE PENGUIN COEFFICIENTS $P, P_S$ AT ORDER $\alpha_s^2 N_f$

For the contributions of penguin diagrams and penguin operators in Eq. (17) we write

$$\begin{aligned} P^{ab}(z) &= P^{ab,(1)}(z) + P^{ab,(2)}(z), \\ P_S^{ab}(z) &= P_S^{ab,(1)}(z) + P_S^{ab,(2)}(z), \end{aligned} \quad (19)$$

where  $P^{ab,(1)}(z)$  and  $P_S^{ab,(1)}(z)$  denote the NLO results of Ref. [16], while  $P^{ab,(2)}(z)$  and  $P_S^{ab,(2)}(z)$  are the NNLO corrections studied in this paper. Since we treat  $C_{3-6}$  as  $\mathcal{O}(\alpha_s)$ ,  $P_{(S)}^{ab,(2)}(z)$  contain terms of order  $C_{3-6}C_{3-6}$ ,  $\alpha_s C_2 C_{3-6}$ , and  $\alpha_s^2 C_2^2$ . The large- $N_f$  part of  $P^{ab,(2)}(z)$  is decomposed as

$$\begin{aligned} P^{ab,(2),N_f}(z) &= N_H P^{ab,(2),N_H}(1, z) \\ &+ N_V P^{ab,(2),N_V}(z_i, z) + N_L P^{ab,(2),N_L}(0, z) \end{aligned} \quad (20)$$

with an analogous formula for  $P_S^{ab,(2)}(z)$ . Here,  $N_H = 1$ ,  $N_V = 1$  and  $N_L = 3$  denote the number of heavy ( $b$ -quark), intermediate-mass ( $c$ -quark) and light ( $u, d, s$ )

quark flavors, with the total number of quark flavors  $N_f = N_H + N_V + N_L = 5$ . In the penguin contributions, as well as in charm loops, we keep the charm mass non-zero, i.e. equal to its physical value. This improves our results over those in Ref. [21], where the charm mass on all lines touching  $O_2$  was set to zero. This affects all loops in the diagrams in Fig. 1 (see also Figure 1 of [21]). The diagrams  $P_{1-2}$  are not only needed for the contributions involving  $C_{3-6,8}$ , but also appear in counter-term contributions to  $D_{11-13}$ , in which the charm mass must be treated in the same way as in the diagrams which they renormalize.

We introduce the abbreviation  $z_i \equiv m_i^2/m_b^2$ , where  $m_i$  denotes the quark in all closed fermion loops, in which all  $N_f = 5$  quarks can run. Thus  $z_i = 1$ ,  $z_i = m_c^2/m_b^2$ , or  $z_i = 0$  in  $P^{ab,(2),N_H}(z_i, z)$ ,  $P^{ab,(2),N_V}(z_i, z)$ , or  $P^{ab,(2),N_L}(z_i, z)$ , respectively. The second argument  $z = m_c^2/m_b^2$  of the loop functions involves the charm mass originating from  $O_{1,2}$  operators.

Our results are:

$$P^{cc,(2),N_H}(1, z) = \frac{\alpha_s(\mu_1)}{4\pi} G_p^{cc,(1),N_H}(1, z) M_4'(\mu_1) + \frac{\alpha_s^2(\mu_1)}{(4\pi)^2} G_p^{cc,(2),N_H}(1, z) C_2^2(\mu_1), \quad (21)$$

$$P_S^{cc,(2),N_H}(1, z) = -\frac{\alpha_s(\mu_1)}{4\pi} 8G_p^{cc,(1),N_H}(1, z) M_4'(\mu_1) - \frac{\alpha_s^2(\mu_1)}{(4\pi)^2} 8G_p^{cc,(2),N_H}(1, z) C_2^2(\mu_1), \quad (22)$$

$$P^{cc,(2),N_V}(z_i, z) = \sqrt{1-4z_i} \left( (1-z_i) M_1'(\mu_1) + \frac{1}{2}(1-4z_i) M_2'(\mu_1) + 3z_i M_3'(\mu_1) \right) + \frac{\alpha_s(\mu_1)}{4\pi} G_p^{cc,(1),N_V}(z_i, z) M_4'(\mu_1) + \frac{\alpha_s^2(\mu_1)}{(4\pi)^2} G_p^{cc,(2),N_V}(z_i, z) C_2^2(\mu_1), \quad (23)$$

$$P_S^{cc,(2),N_V}(z_i, z) = \sqrt{1-4z_i} (1+2z_i) (M_1'(\mu_1) - M_2'(\mu_1)) - \frac{\alpha_s(\mu_1)}{4\pi} 8G_p^{cc,(1),N_V}(z_i, z) M_4'(\mu_1) - \frac{\alpha_s^2(\mu_1)}{(4\pi)^2} 8G_p^{cc,(2),N_V}(z_i, z) C_2^2(\mu_1), \quad (24)$$

with

$$G_p^{cc,(1),N_H}(1, z) = -\frac{1}{54} \left( 6 \log \left( \frac{\mu_1}{m_b} \right) - 3\sqrt{3}\pi + 17 \right) \times \sqrt{1-4z}(2z+1), \quad (25)$$

$$G_p^{cc,(2),N_H}(1, z) = \frac{2}{81} \left( 6 \log \left( \frac{\mu_1}{m_b} \right) - 3\sqrt{3}\pi + 17 \right) \times \sqrt{1-4z}(2z+1) \left[ 2 \log \left( \frac{\mu_1}{m_b} \right) + \frac{2}{3} + 4z - \log(z) + \sqrt{1-4z}(2z+1) \log(\sigma) + \frac{3C_8(\mu_1)}{C_2(\mu_1)} \right], \quad (26)$$

$$G_p^{cc,(1),N_V}(z_i, z) = -\frac{1}{54} \left[ \sqrt{1-4z_i}(1+2z_i) \times \left( 6 \log \left( \frac{\mu_1}{m_b} \right) - 3 \log(z) + 2 + 12z \right) + \sqrt{1-4z}(1+2z) \times \left( 6 \log \left( \frac{\mu_1}{m_b} \right) - 3 \log(z_i) + 5 + 12z_i \right) + 3\sqrt{1-4z}(1+2z)\sqrt{1-4z_i}(1+2z_i) \times (\log(\sigma) + \log(\sigma_i)) + \frac{9C_8(\mu_1)}{C_2(\mu_1)} \sqrt{1-4z_i}(1+2z_i) \right], \quad (27)$$

$$G_p^{cc,(2),N_V}(z_i, z) = \frac{1}{81} \left\{ 2\sqrt{1-4z}(2z+1)\sqrt{1-4z_i} \times (2z_i+1)(\log(\sigma) + \log(\sigma_i)) \times \left( 6 \log \left( \frac{\mu_1}{m_b} \right) + 12z - 3 \log(z) + 2 \right) + \frac{2}{3}\sqrt{1-4z}(2z+1) \times \left( 6 \log \left( \frac{\mu_1}{m_b} \right) + 5 + 12z_i - 3 \log(z_i) \right) \times \left( 6 \log \left( \frac{\mu_1}{m_b} \right) + 2 + 12z - 3 \log(z) + 3\sqrt{1-4z}(2z+1) \log(\sigma) \right) + \frac{1}{3}\sqrt{1-4z_i}(2z_i+1) \times \left[ \left( 6 \log \left( \frac{\mu_1}{m_b} \right) + 2 + 12z - 3 \log(z) \right)^2 + 9(1-4z)(2z+1)^2 \times \left( 2 \log(\sigma) \log(\sigma_i) + \log^2(\sigma) - \pi^2 \right) \right] + \frac{6C_8(\mu_1)}{C_2(\mu_1)} \left[ \sqrt{1-4z}(2z+1) \times \left( 6 \log \left( \frac{\mu_1}{m_b} \right) - 3 \log(z_i) + 5 + 12z_i \right) + \sqrt{1-4z_i}(2z_i+1) \times \left( 6 \log \left( \frac{\mu_1}{m_b} \right) + 2 + 12z - 3 \log(z) \right) + 3\sqrt{1-4z}(2z+1)\sqrt{1-4z_i}(2z_i+1) \times \left( \log(\sigma) + \log(\sigma_i) \right) + \frac{9C_8(\mu_1)}{2C_2(\mu_1)} \sqrt{1-4z_i}(2z_i+1) \right] \right\}, \quad (28)$$

where we have defined

$$\begin{aligned} M_1' &= 3C_3^2 + 2C_3C_4 + 3C_5^2 + 2C_5C_6 \\ M_2' &= C_4^2 + C_6^2, \\ M_3' &= 2(3C_3C_5 + C_3C_6 + C_4C_5 + C_4C_6), \\ M_4' &= 2(C_2C_4 + C_2C_6) \end{aligned} \quad (29)$$

and

$$\sigma = \frac{1 - \sqrt{1 - 4z}}{1 + \sqrt{1 - 4z}}, \quad (30)$$

while  $\sigma_i$  is defined by replacing  $z$  with  $z_i$  in (30). Then  $P^{uu,(2),NA}(z_i, 0) = P^{cc,(2),NA}(z_i, 0)$  (with  $A = H, V, L$ ) and

$$P^{uc,(2),NA}(z_i, z) = \frac{P^{cc,(2),NA}(z_i, z) + P^{cc,(2),NA}(z_i, 0)}{2} + \Delta P^{uc,(2),NA}, \quad (31)$$

$$P_S^{uc,(2),NA}(z_i, z) = \frac{P_S^{cc,(2),NA}(z_i, z) + P_S^{cc,(2),NA}(z_i, 0)}{2} - 8\Delta P^{uc,(2),NA}, \quad (32)$$

where

$$\begin{aligned} \Delta P^{uc,(2),NH} = & -\frac{\alpha_s^2(\mu_1)}{(4\pi)^2} C_2^2(\mu_1) \frac{1 - \sqrt{1 - 4z}(1 + 2z)}{81} \\ & \times \left( 6 \log\left(\frac{\mu_1}{m_b}\right) - 3\sqrt{3}\pi + 17 \right) \\ & \times \left[ \log(z) - \sqrt{1 - 4z}(1 + 2z) \log(\sigma) - 4z \right], \quad (33) \end{aligned}$$

$$\begin{aligned} \Delta P^{uc,(2),NV} = & \frac{\alpha_s^2(\mu_1)}{(4\pi)^2} C_2^2(\mu_1) \\ & \times \frac{1}{162} \left\{ \left( 1 - \sqrt{1 - 4z}(1 + 2z) \right) \right. \\ & \times \left[ 3\sqrt{1 - 4z_i}(1 + 2z_i) \left[ \pi^2 \left( 1 - \sqrt{1 - 4z}(1 + 2z) \right) \right. \right. \\ & \quad \left. \left. + \left( \sqrt{1 - 4z}(1 + 2z) + 1 \right) \log^2(\sigma) \right. \right. \\ & \quad \left. \left. + 2(4z - \log(z)) \log(\sigma) \right] \right. \\ & \left. - 2 \left( \log(z) - \sqrt{1 - 4z}(1 + 2z) \log(\sigma) - 4z \right) \right. \\ & \quad \left. \times \left( 6 \log\left(\frac{\mu_1}{m_b}\right) + 3\sqrt{1 - 4z_i}(1 + 2z_i) \log(\sigma_i) \right. \right. \\ & \quad \left. \left. + 12z_i - 3 \log(z_i) + 5 \right) \right] \\ & \left. - 3\sqrt{1 - 4z_i}(1 + 2z_i) \left( 16z^2 \right. \right. \\ & \quad \left. \left. + (\log(z) - \log(\sigma)) (\log(z) - \log(\sigma) - 8z) \right) \right\}. \quad (34) \end{aligned}$$

$P^{ab,(2),NL}(0, z)$  can be obtained from the expressions presented above by setting  $z_i$  to 0, i.e.  $P^{ab,(2),NL}(0, z) = P^{ab,(2),NV}(0, z)$ .

Taking the limit  $z \rightarrow 0$  in the results presented in this section (with the replacement  $z_i \rightarrow z$ ) reproduces the results in Eqs. (4.15)-(4.22) of Ref. [21].

#### IV. PHENOMENOLOGY OF $\Delta\Gamma_q$ AND $a_{\text{fs}}^q$

In this section we first show the impact of a non-zero charm quark mass in the  $\alpha_s^2 N_f$  corrections to  $\Delta\Gamma_s$  and  $a_{\text{fs}}^q$ , which is the novel analytic result of this paper. Subsequently we present updated predictions for  $\Delta\Gamma_q/\Delta M_q$

and  $a_{\text{fs}}^q$ , reflecting the progress in the determination of hadronic parameters, quark masses, CKM elements, and other parameters entering these quantities.

We may express  $\Delta\Gamma_q$  and  $a_{\text{fs}}^q$  in terms of  $m_b$  and  $z = m_c^2/m_b^2$ . As shown in Ref. [26], trading  $z$  for  $\bar{z} = (\bar{m}_c(\bar{m}_b)/\bar{m}_b(\bar{m}_b))^2$  (with the appropriate changes in the expressions for the radiative corrections) resums the  $z \log z$  terms to all orders, i.e. there are no  $\bar{z} \log \bar{z}$  terms. In the numerics presented below we will always use  $\bar{z}$ . This still leaves (at least) two natural possibilities to define  $m_b$ , two powers of which appear in the prefactor of  $\Delta\Gamma_s$  and  $a_{\text{fs}}^q$ , namely the  $\overline{\text{MS}}$  mass  $\bar{m}_b(\bar{m}_b)$  and the pole mass  $m_b^{\text{pole}}$ . In our numerics we use  $\bar{m}_b(\bar{m}_b) = (4.18 \pm 0.03)$  GeV as input in both schemes and calculate  $m_b^{\text{pole}} = (4.58 \pm 0.03)$  GeV at NLO and  $m_b^{\text{pole}} = (4.84 \pm 0.03)$  GeV at NNLO.

In our partial NNLO results we further use the complete NNLO  $\Delta B = 1$  Wilson coefficients  $C_1, C_2$  [28, 29] and the complete NLO expressions for  $C_{3-6}, C_8$  (see Ref. [21] for details). From the values of  $\sin(2\beta)$  and  $R_t$  listed in Tab. I we obtain

$$\begin{aligned} \frac{\lambda_u^d}{\lambda_t^d} &= (0.0122 \pm 0.0097) - (0.4203 \pm 0.0090)i, \quad (35) \\ \frac{\lambda_u^s}{\lambda_t^s} &= -(0.00865 \pm 0.00042) \\ &+ (0.01832 \pm 0.00039)i. \quad (36) \end{aligned}$$

For all central values quoted in the following we took  $\mu_1 = m_b^{\text{pole}}$  and  $\mu_1 = \bar{m}_b$  for the pole and  $\overline{\text{MS}}$  schemes, respectively. For the contribution to the width differences  $\Delta\Gamma_s$  that originates from the penguin sector and is proportional to  $\alpha_s^2 N_f$  (neglecting  $\lambda_u$  part) we find

$$\frac{\delta\Delta\Gamma_s^{(2),N_f,P}(z)}{\delta\Delta\Gamma_s^{(2),N_f,P}(0)} = 1.14. \quad (37)$$

Eq. (37) shows that the effect of a non-zero charm quark mass on the lines touching  $O_2$  are important for the penguin contribution, leading to an about 14% increase of the  $\alpha_s^2 N_f$  contribution to the latter in comparison to the case in which the charm quark mass on all lines touching  $O_2$  is set to zero.

The penguin contribution at order  $\alpha_s$  [16] evaluates to

$$\begin{aligned} \frac{\delta\Delta\Gamma_s^{(1),P}(z)}{\Delta\Gamma_s^{\text{NLO}}(z)} &= -14.5\% \quad (\text{pole}), \\ \frac{\delta\Delta\Gamma_s^{(1),P}(z)}{\Delta\Gamma_s^{\text{NLO}}(z)} &= -11.2\% \quad (\overline{\text{MS}}), \quad (38) \end{aligned}$$

and the new  $\alpha_s^2 N_f$  corrections are

$$\begin{aligned} \frac{\delta\Delta\Gamma_s^{(2),N_f,P}(z)}{\Delta\Gamma_s^{\text{NLO}}(z)} &= 2.4\%, \quad (\text{pole}), \\ \frac{\delta\Delta\Gamma_s^{(2),N_f,P}(z)}{\Delta\Gamma_s^{\text{NLO}}(z)} &= 1.8\%, \quad (\overline{\text{MS}}), \quad (39) \end{aligned}$$

$\bar{m}_b(\bar{m}_b) = (4.18 \pm 0.03) \text{ GeV}$	[32]	$\bar{m}_c(\bar{m}_c) = (1.2982 \pm 0.0013_{\text{stat}} \pm 0.0120_{\text{sys}}) \text{ GeV}$	[30, 33, 34]
$\bar{m}_s(\bar{m}_b) = (0.0786 \pm 0.0006) \text{ GeV}$	[27]	$\bar{m}_t(m_t) = (165.26 \pm 0.11_{\text{stat}} \pm 0.30_{\text{sys}}) \text{ GeV}$	[30]
$m_b^{\text{pow}} = 4.7 \text{ GeV}$	[19]	$\alpha_s(M_Z) = 0.1181(11)$	[35]
$M_{B_s} = 5366.88 \text{ MeV}$	[35]	$M_{B_d} = 5279.64 \text{ MeV}$	[35]
$B_{B_s} = 0.813 \pm 0.034$	[36]	$B_{B_d} = 0.806 \pm 0.041$	[36]
$\tilde{B}'_{S,B_s} = 1.31 \pm 0.09$	[36]	$\tilde{B}'_{S,B_d} = 1.20 \pm 0.09$	[36]
$B_{R_0}^s = 1.27 \pm 0.52$	[36]	$B_{R_0}^d = 1.02 \pm 0.55$	[36]
$B_{\tilde{R}_2}^s = 0.89 \pm 0.35$	[37]	$B_{\tilde{R}_2}^d = B_{\tilde{R}_2}^s$	
$B_{\tilde{R}_3}^s = 1.14 \pm 0.39$	[37]	$B_{\tilde{R}_3}^d = B_{\tilde{R}_3}^s$	
$B_{R_2}^q = -B_{\tilde{R}_2}^q$	[20]	$B_{R_3}^q = \frac{5}{7}B_{\tilde{R}_3}^q + \frac{2}{7}B_{\tilde{R}_2}^q$	[20]
$f_{B_s} = (0.2307 \pm 0.0013) \text{ GeV}$	[38]	$f_{B_d} = (0.1905 \pm 0.0013) \text{ GeV}$	[38]
$\sin(2\beta) = 0.7083_{-0.0098}^{+0.0127}$	[30]	$R_t = 0.9124_{-0.0100}^{+0.0064}$	[30]
$ V_{us}  = 0.22483_{-0.00006}^{+0.00025}$	[30]		

TABLE I. Input parameters used in Sec. IV.  $\bar{m}_s(\bar{m}_b)$  is calculated from  $\bar{m}_s(2 \text{ GeV}) = 0.09344 \pm 0.00068 \text{ GeV}$  [27]. The listed values for  $B_{B_q}$  and  $\tilde{B}'_{S,B_q}$  are found by rescaling the numbers in Table V of Ref. [36] by 8/3 and 3, respectively (see Eq. (16)).  $m_B^{\text{pow}}$  is a redundant parameter calibrating the overall size of the hadronic parameters  $B_{R_i}$  which quantify the matrix elements at order  $\Lambda_{\text{QCD}}/m_b$ .  $B_{R_0}^q$  is calculated from  $\langle B_s | R_0 | \bar{B}_s \rangle = -(0.66 \pm 0.27) \text{ GeV}^4$  and  $\langle B_d | R_0 | \bar{B}_d \rangle = -(0.36 \pm 0.20) \text{ GeV}^4$  [36] (with  $\langle R_0 \rangle$  defined as in Ref. [19, 20]) with the central values of  $f_{B_q}$  and the quark and meson masses listed above, so that the error quoted for  $B_{R_0}^q$  correctly reflects the error of only the matrix element (and not the uncertainty of the artificial conversion factor from matrix elements to bag parameters). In the same way  $B_{\tilde{R}_{2,3}}^s$  is calculated from  $\langle B_s | \tilde{R}_2 | \bar{B}_s \rangle = (0.28 \pm 0.11) \text{ GeV}^4$  and  $\langle B_s | \tilde{R}_3 | \bar{B}_s \rangle = (0.44 \pm 0.15) \text{ GeV}^4$  [37]. The expressions for  $B_{\tilde{R}_2}^q$  and  $B_{\tilde{R}_3}^q$  hold up to  $\Lambda_{\text{QCD}}/m_b$  corrections.  $B_{R_1}^q = 1.5$  and  $B_{\tilde{R}_1}^q = 1.2$  [37] are phenomenologically irrelevant. The charm and bottom masses imply  $z = m_c^2(m_c)/m_b^2(m_b) = 0.096$  leading to  $\bar{z} = m_c^2(m_b)/m_b^2(m_b) = 0.052 \pm 0.002$  at NLO and we use the same value at NNLO.

where  $\delta\Delta\Gamma_s^{(1),p}(z)$  denotes the contribution to  $\Delta\Gamma_s$  from the penguin sector at order  $\alpha_s$  and  $\delta\Delta\Gamma_s^{(2),N_f,p}(z)$  is the corresponding contribution at order  $\alpha_s^2 N_f$ .

The analogous contributions to the CP asymmetries at NLO [17] are

$$\begin{aligned} \frac{\delta a_{\text{fs}}^{q(1),p}}{a_{\text{fs}}^{q,\text{NLO}}} &= 3.0\%, \quad (\text{pole}), \\ \frac{\delta a_{\text{fs}}^{q(1),p}}{a_{\text{fs}}^{q,\text{NLO}}} &= 2.7\%, \quad (\overline{\text{MS}}), \end{aligned} \quad (40)$$

with  $q = s, d$ , while at order  $\alpha_s^2 N_f$  we obtain

$$\begin{aligned} \frac{\delta a_{\text{fs}}^{q(2),N_f,p}}{a_{\text{fs}}^{q,\text{NLO}}} &= -1.2\% \quad (\text{pole}), \\ \frac{\delta a_{\text{fs}}^{q(2),N_f,p}}{a_{\text{fs}}^{q,\text{NLO}}} &= -1.0\%. \quad (\overline{\text{MS}}), \end{aligned} \quad (41)$$

Judging from the numbers presented above, we see that the penguin contributions at order  $\alpha_s^2 N_f$  have opposite sign compared to the  $\mathcal{O}(\alpha_s)$  penguin corrections and decrease the latter by approximately 37%. This nurtures the expectation that the full  $\alpha_s^2$  corrections may also be large and a reliable assessment of the penguin contribution calls for a complete NNLO calculation. For the SM contribution considered here the overall contributions to  $\Delta\Gamma_q$  and  $a_{\text{fs}}^q$  is small (see Eqs. (39) and (41)), but in BSM models with enhanced penguin coefficients these corrections are relevant to constrain these coefficients from the data.

Until the full NNLO calculation is available, we recommend to use the following updated NLO SM values for  $\Delta\Gamma_q/\Delta M_q$ :

$$\begin{aligned} \frac{\Delta\Gamma_s}{\Delta M_s} &= (4.33 \pm 0.83_{\text{scale}} \pm 0.11_{B,\tilde{B}_s} \pm 0.94_{\Lambda_{\text{QCD}}/m_b}) \\ &\times 10^{-3} \quad (\text{pole}), \\ \frac{\Delta\Gamma_s}{\Delta M_s} &= (4.97 \pm 0.62_{\text{scale}} \pm 0.13_{B,\tilde{B}_s} \pm 0.80_{\Lambda_{\text{QCD}}/m_b}) \\ &\times 10^{-3} \quad (\overline{\text{MS}}), \end{aligned} \quad (42)$$

$$\begin{aligned} \frac{\Delta\Gamma_d}{\Delta M_d} &= (4.48 \pm 0.82_{\text{scale}} \pm 0.12_{B,\tilde{B}_s} \pm 0.86_{\Lambda_{\text{QCD}}/m_b}) \\ &\times 10^{-3} \quad (\text{pole}), \\ \frac{\Delta\Gamma_d}{\Delta M_d} &= (5.07 \pm 0.61_{\text{scale}} \pm 0.14_{B,\tilde{B}_s} \pm 0.73_{\Lambda_{\text{QCD}}/m_b}) \\ &\times 10^{-3} \quad (\overline{\text{MS}}) \end{aligned} \quad (43)$$

and  $a_{\text{fs}}^q$ :

$$\begin{aligned} a_{\text{fs}}^s &= (2.07 \pm 0.08_{\text{scale}} \pm 0.02_{B,\tilde{B}_s} \pm 0.05_{\Lambda_{\text{QCD}}/m_b} \\ &\pm 0.04_{\text{CKM}}) \times 10^{-5} \quad (\text{pole}), \\ a_{\text{fs}}^s &= (2.04 \pm 0.09_{\text{scale}} \pm 0.02_{B,\tilde{B}_s} \pm 0.04_{\Lambda_{\text{QCD}}/m_b} \\ &\pm 0.04_{\text{CKM}}) \times 10^{-5} \quad (\overline{\text{MS}}), \end{aligned} \quad (44)$$

$$\begin{aligned} a_{\text{fs}}^d &= -(4.71 \pm 0.18_{\text{scale}} \pm 0.04_{B,\tilde{B}_s} \pm 0.11_{\Lambda_{\text{QCD}}/m_b} \\ &\pm 0.10_{\text{CKM}}) \times 10^{-4} \quad (\text{pole}), \\ a_{\text{fs}}^d &= -(4.64 \pm 0.21_{\text{scale}} \pm 0.04_{B,\tilde{B}_s} \pm 0.09_{\Lambda_{\text{QCD}}/m_b} \\ &\pm 0.10_{\text{CKM}}) \times 10^{-4} \quad (\overline{\text{MS}}). \end{aligned} \quad (45)$$

The error indicated with “ $\Lambda_{\text{QCD}}/m_b$ ” comprises the uncertainty from the bag factors of Refs. [36, 37]. The new lattice results for the bag parameters of the  $\Lambda_{\text{QCD}}/m_b$  corrections have errors comparable to those assumed in Ref. [21], but the central value of  $B_{R_0}^s$  has shifted upwards by more than a factor of 2. Furthermore,  $\tilde{B}'_{S,B_s}/B_{B_s}$  decreased by 12%, which also lowered the  $\mu_1$  dependence. Adding the individual errors quoted in Eqs. (42) to (45) in quadrature yields the values quoted in the abstract.

With the input values of Tab. I we reproduce the measured  $\Delta M_s$  in an excellent way. It makes therefore no difference, whether we use the experimental or theoretical value to calculate  $\Delta\Gamma_s$  from the ratios in Eq. (42). The central values for  $\Delta\Gamma_s$  in Ref. [21] are proportional to  $B_{B_s}$ , and the value used in that analysis was larger than the one in Tab. I by 16%, explaining why the  $\Delta\Gamma_s$  values in Ref. [21] were larger by roughly the same amount compared to

$$\begin{aligned}\Delta\Gamma_s^{\text{pole}} &= (0.077 \pm 0.022) \text{ ps}^{-1}, \\ \Delta\Gamma_s^{\overline{\text{MS}}} &= (0.088 \pm 0.018) \text{ ps}^{-1}\end{aligned}\quad (46)$$

inferred from Eq. (42) with  $\Delta M_s^{\text{exp}} = (17.757 \pm 0.021) \text{ ps}^{-1}$ .

In  $a_{\text{fs}}^q$ , however, the lattice results for the  $\Lambda_{\text{QCD}}/m_b$  bag parameters already have an impact on reducing the uncertainty, because unlike  $\Delta\Gamma_q/\Delta M_q$  the CP asymmetry  $a_{\text{fs}}^q$  is very sensitive to  $B_{R_3}^s$ , whose uncertainty of  $\pm 0.39$  is below the  $\pm 0.5$  assumed in older analyses done without the lattice input.

The scale dependence is calculated by varying  $\mu_1$  between  $m_b/2$  and  $2m_b$ . Both this scale dependence and the sizable scheme dependence indicate that the missing perturbative higher-order corrections in  $\Delta\Gamma_q/\Delta M_q$  are not small. However, the  $\mu_1$  dependence might well underestimate this error in the case of  $a_{\text{fs}}^q$ .

The central values of all our  $\overline{\text{MS}}$  scheme results are in excellent agreement with Ref. [39]. Our error estimate of the  $\Lambda_{\text{QCD}}/m_b$  corrections is conservative, as we add the errors of individual bag parameters linearly, leading to overall uncertainties in  $\Delta\Gamma_q/\Delta M_q$  which are larger by roughly a factor of 1.5 compared to those of  $\Delta\Gamma_q$  in Ref. [39]. Our uncertainties for  $a_{\text{fs}}^q$ , though, are smaller compared to Ref. [39], as we find a smaller  $\mu_1$ -dependence and assume a smaller error on  $m_c$ . (Recall that  $a_{\text{fs}}^q \propto m_c^2$ .) In our error budget the 0.9% error in  $m_c$  quoted in Tab. I would contribute another 3% uncertainty to  $a_{\text{fs}}^q$ .

## V. CONCLUSIONS

We have calculated the penguin contributions of order  $\alpha_s^2 N_f$  to the width difference  $\Delta\Gamma_q$  and the CP asymme-

try in flavor-specific decays of  $B_q$  mesons,  $a_{\text{fs}}^q$ . These and the mass difference  $\Delta M_q$  are fundamental quantities characterizing the  $B_q - \bar{B}_q$  mixing complex. The calculation improves over Ref. [21] by taking into account the full dependence on the charm quark mass. In line with the general findings of Ref. [26] we find no enhancement proportional to  $\log(m_b^2/m_c^2)$  in the new terms of order  $\alpha_s^2 N_f m_c^2/m_b^2$ , but we discover a largish coefficient of this term and conclude that the future full NNLO calculation of the penguin pieces should incorporate the full  $m_c$ -dependence. In both  $\Delta\Gamma_q$  and  $a_{\text{fs}}^q$  the  $\alpha_s^2 N_f$  terms have signs opposite to the NLO corrections. The calculated partial NNLO corrections are smaller than the corresponding NLO terms by factors of roughly 6 and 3 for  $\Delta\Gamma_s$  and  $a_{\text{fs}}^q$ , respectively, indicating a good convergence of the perturbative series.

In response to the recent progress in the lattice calculations of the non-perturbative matrix elements [36, 37] we have further presented updated NLO values for  $\Delta\Gamma_q$  and  $a_{\text{fs}}^q$  in Eqs. (42) to (45).

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## Appendix A: Full-theory matrix elements

In this section we collect the needed unrenormalized LO and NLO matrix elements to order  $\epsilon^2$  and  $\epsilon$ , respectively, where  $\epsilon = (4 - D)/2$  appears in the ultraviolet poles in dimensional regularization. We decompose the matrix element as

$$M = M_{\text{cc}} + M_{\text{peng}}, \quad (\text{A1})$$

where the first term denotes the contribution with two insertions of the current-current operators  $O_{1,2}$  and the second term comprises the diagrams with at least one penguin operator. Recall that we count  $C_{3-6}$  as order  $\alpha_s$ , so that one loop less is needed for  $M_{\text{peng}}$  compared to  $M_{\text{cc}}$ . We expand  $M_{\text{peng}}^{ab} = M_{\text{peng}}^{ab,(0)} + \frac{\alpha_s}{4\pi} M_{\text{peng}}^{ab,(1)} + \dots$

## 1. Penguin operators

Here and in the following  $\langle \dots \rangle^{(0)}$  denotes tree-level matrix element and  $C_k^b = \sum_j C_j Z_{jk}$  are bare Wilson coefficients (see eq. (3.10) of [21]).

We decompose the NLO penguin diagrams according to the diagrams in figure 1 as

$$M_{\text{peng}}^{(1)} = -\frac{G_F^2 m_b^2}{12\pi} \left[ \lambda_c^2 \left( M_{D_{11}}^{cc,(1)} + M_{D_{12}}^{c,(1)} \right) + \lambda_c \lambda_u \left( 2M_{D_{11}}^{cu,(1)} + M_{D_{12}}^{c,(1)} + M_{D_{12}}^{u,(1)} \right) + \lambda_u^2 \left( M_{D_{11}}^{uu,(1)} + M_{D_{12}}^{u,(1)} \right) \right],$$

where

$$\begin{aligned} M_{D_{11}}^{q_1 q_2, (1)} = & -\frac{5\langle Q \rangle^{(0)} + 8\langle \tilde{Q}_S \rangle^{(0)}}{9} C_2^{b2} \left( \frac{\sqrt{1-4z_1}(1+2z_1) + \sqrt{1-4z_2}(1+2z_2)}{2\epsilon} \right. \\ & + \sqrt{1-4z_2} \left( \frac{1}{2}(2z_2+1) \left( 4\log\left(\frac{\mu_1}{m_b}\right) - \log(z_1) - \log(1-4z_2) \right) + 2z_1(2z_2+1) + \frac{1}{3}(7z_2+2) \right) \\ & + \sqrt{1-4z_1} \left( \frac{1}{2}(2z_1+1) \left( 4\log\left(\frac{\mu_1}{m_b}\right) - \log(1-4z_1) - \log(z_2) \right) + 2(2z_1+1)z_2 + \frac{1}{3}(7z_1+2) \right) \\ & + \frac{1}{2}\sqrt{1-4z_1}(2z_1+1)\sqrt{1-4z_2}(2z_2+1)(\log(\sigma_1) + \log(\sigma_2)) + \epsilon \left( \sqrt{1-4z_1} \left( \left( \frac{2+7z_1}{3} + 2(1+2z_1)z_2 \right) \right. \right. \\ & \times \left. \left( 4\log\left(\frac{\mu_1}{m_b}\right) - \log(1-4z_1) - \log(z_2) \right) + \frac{1}{4}(1+2z_1) \left( \left( 4\log\left(\frac{\mu_1}{m_b}\right) - \log(1-4z_1) - \log(z_2) \right)^2 - \frac{\pi^2}{3} \right) \right. \\ & + \left. \frac{1}{3}(40z_1z_2 + 17z_1 + 14z_2 + 5) \right) + \sqrt{1-4z_2} \left( \left( \frac{2+7z_2}{3} + 2(1+2z_2)z_1 \right) \left( 4\log\left(\frac{\mu_1}{m_b}\right) - \log(1-4z_2) - \log(z_1) \right) \right. \\ & + \left. \frac{1}{4}(1+2z_2) \left( \left( 4\log\left(\frac{\mu_1}{m_b}\right) - \log(1-4z_2) - \log(z_1) \right)^2 - \frac{\pi^2}{3} \right) + \frac{1}{3}(40z_1z_2 + 17z_2 + 14z_1 + 5) \right) \\ & + \sqrt{1-4z_1}\sqrt{1-4z_2} \left( \frac{1}{3}(20z_1z_2 + 7(z_1+z_2) + 2)(\log(\sigma_1) + \log(\sigma_2)) - (2z_1+1)(2z_2+1) \left( -\frac{1}{2}(\log(\sigma_1) + \log(\sigma_2)) \right. \right. \\ & \times \left. \left. \left( 4\log\left(\frac{\mu_1}{m_b}\right) - \log(1-4z_1) - \log(1-4z_2) \right) + \text{Li}_2(\sigma_1) + \text{Li}_2(\sigma_2) + \frac{1}{4}(\log^2(\sigma_1) + \log^2(\sigma_2)) + \frac{2\pi^2}{3} \right) \right) \left. \right), \quad (\text{A2}) \end{aligned}$$

$$\begin{aligned} M_{D_{12}}^{q_1, (1)} = & -\frac{1}{3} \left( 5\langle Q \rangle^{(0)} + 8\langle \tilde{Q}_S \rangle^{(0)} \right) C_2^b C_8^b \\ & \cdot \sqrt{1-4z_1} \left( 1 + 2z_1 + \epsilon \left( \frac{2(1+5z_1)}{3} + (1+2z_1) \left( 2\log\frac{\mu_1}{m_b} - \log(1-4z_1) \right) \right) \right). \quad (\text{A3}) \end{aligned}$$

$q_1$  and  $q_2$  represent either  $c$  or  $u$  quark; and  $z_1$  and  $z_2$  are equal to  $m_c^2/m_b^2$  when originating from the operator  $O_2$  or equal to zero when related to a  $u$  quark associated with operator  $O_2^u$ .

For the matrix elements with one QCD penguin operator we write

$$M_{\text{peng}} = -\frac{G_F^2 m_b^2}{12\pi} \sum_{j=3}^6 \left[ \lambda_c^2 M_{j2}(z) + \lambda_c \lambda_u \left( M_{j2}(z) + M_{j2}(0) \right) + \lambda_u^2 M_{j2}(0) \right]. \quad (\text{A4})$$

As usual we expand  $M_{jk}$  as  $M_{jk} = M_{jk}^{(0)} + \frac{\alpha_s}{4\pi} M_{jk}^{(1)} + \dots$ . The unrenormalized LO and NLO matrix elements necessary for the renormalization of the penguin diagrams  $D_{11}$  and  $D_{12}$  are the following:

$$\begin{aligned} M_{32}^{(0)}(z) &= 2C_2^b C_3^b T_3, & M_{42}^{(0)}(z) &= 2C_2^b C_4^b T_4, \\ M_{52}^{(0)}(z) &= 2C_2^b C_5^b T_5, & M_{62}^{(0)}(z) &= 2C_2^b C_6^b T_5, \end{aligned} \quad (\text{A5})$$

$$M_{42}^{(1)}(z) = 2C_2^b C_4^b (N_H T_1 + N_V T_2 + N_L T_2'), \quad M_{62}^{(1)}(z) = 2C_2^b C_6^b (N_H T_1 + N_V T_2 + N_L T_2'), \quad (\text{A6})$$



where

$$\begin{aligned}
T_1 = & -\frac{1}{9}(8\langle\tilde{Q}_S\rangle^{(0)} + 5\langle Q\rangle^{(0)})\sqrt{1-4z} \left[ \frac{1+2z}{2\epsilon} + \frac{19+44z}{6} + \frac{1}{2} \left( 4\log\left(\frac{\mu_1}{m_b}\right) - \log(1-4z) - \sqrt{3}\pi \right) \right. \\
& + \epsilon \left( \frac{1}{4}(1+2z) \left( \left( 4\log\left(\frac{\mu_1}{m_b}\right) - \log(1-4z) \right)^2 - \frac{\pi^2}{3} + 2\sqrt{3}\pi \left( \frac{\log(3)}{2} - 4\log\left(\frac{\mu_1}{m_b}\right) + \log(1-4z) \right. \right. \right. \\
& \left. \left. \left. - \frac{3i(\text{Li}_2(\frac{1}{6}(3-i\sqrt{3})) - \text{Li}_2(\frac{1}{6}(3+i\sqrt{3})))}{\pi} \right) \right) \right) + \frac{19+44z}{6} \left( 4\log\left(\frac{\mu_1}{m_b}\right) - \log(1-4z) \right) - \frac{\sqrt{3}\pi}{2}(3+8z) \\
& \left. + \frac{57+158z}{6} \right], \tag{A7}
\end{aligned}$$

$$\begin{aligned}
T_2 = & -\frac{1}{9}(8\langle\tilde{Q}_S\rangle^{(0)} + 5\langle Q\rangle^{(0)}) \left[ \frac{\sqrt{1-4z}(1+2z) + \sqrt{1-4z_i}(1+2z_i)}{2\epsilon} + \frac{1}{2}\sqrt{1-4z}(1+2z)\sqrt{1-4z_i}(1+2z_i) \right. \\
& \times (\log(\sigma) + \log(\sigma_i)) + \frac{1}{6}\sqrt{1-4z_i} \left( 7 + 20z_i + 3(1+2z_i) \left( 4z + 4\log\left(\frac{\mu_1}{m_b}\right) - \log(z) - \log(1-4z_i) \right) \right) \\
& + \frac{1}{6}\sqrt{1-4z} \left( 7 + 20z + 3(1+2z) \left( 4z_i + 4\log\left(\frac{\mu_1}{m_b}\right) - \log(z_i) - \log(1-4z) \right) \right) \\
& + \epsilon \frac{1}{12} \left( \sqrt{1-4z_i} \left( 2(17+40z+54z_i+104zz_i) + 2(7+12z+20z_i+24zz_i) \cdot \left( 4\log\left(\frac{\mu_1}{m_b}\right) - \log(z) \right. \right. \right. \\
& \left. \left. \left. - \log(1-4z_i) \right) + 3(1+2z_i) \left( \left( 4\log\left(\frac{\mu_1}{m_b}\right) - \log(z) - \log(1-4z_i) \right)^2 - \pi^2(1+2z_i) \right) \right) \right) \\
& + \sqrt{1-4z} \left( 2(17+40z_i+54z+104zz_i) + 2(7+12z_i+20z+24zz_i) \cdot \left( 4\log\left(\frac{\mu_1}{m_b}\right) - \log(z_i) - \log(1-4z) \right) \right) \\
& + 3(1+2z) \left( \left( 4\log\left(\frac{\mu_1}{m_b}\right) - \log(z_i) - \log(1-4z) \right)^2 - \pi^2(1+2z) \right) \\
& + \sqrt{1-4z}\sqrt{1-4z_i} \left( (1+2z)(1+2z_i) \left( 6(\log(\sigma) + \log(\sigma_i)) \left( 4\log\left(\frac{\mu_1}{m_b}\right) - \log(1-4z) - \log(1-4z_i) \right) \right. \right. \\
& \left. \left. + 12\text{Li}_2(\sigma) + 12\text{Li}_2(\sigma_i) + 3\log^2(\sigma) + 3\log^2(\sigma_i) + 8\pi^2 \right) + 2(7+20z+20z_i+52zz_i)(\log(\sigma) + \log(\sigma_i)) \right) \right], \tag{A8}
\end{aligned}$$

and

$$\begin{aligned}
T_3 = & \sqrt{1-4z} \left[ \langle Q\rangle^{(0)} \frac{1}{2}(1-4z) \left( 1 + \epsilon \left( \frac{2}{3} + 2\log\left(\frac{\mu_1}{m_b}\right) - \log(1-4z) \right) \right. \right. \\
& + \epsilon^2 \left( \left( 2\log\left(\frac{\mu_1}{m_b}\right) - \log(1-4z) \right) \left( \frac{2}{3} + \log\left(\frac{\mu_1}{m_b}\right) - \frac{1}{2}\log(1-4z) \right) - \frac{\pi^2}{4} + \frac{13}{9} \right) \\
& - \langle\tilde{Q}_S\rangle^{(0)} \left( 1 + 2z + \epsilon \left( \frac{2}{3}(1+5z) + (1+2z) \left( 2\log\left(\frac{\mu_1}{m_b}\right) - \log(1-4z) \right) \right) + \epsilon^2 \left( \frac{2}{3}(1+5z) \right. \right. \\
& \left. \left. \times \left( 2\log\left(\frac{\mu_1}{m_b}\right) - \log(1-4z) \right) + \frac{1+2z}{2} \left( \left( 2\log\left(\frac{\mu_1}{m_b}\right) - \log(1-4z) \right)^2 - \frac{\pi^2}{2} \right) + \frac{13+56z}{9} \right) \right) \right], \tag{A9}
\end{aligned}$$

$$\begin{aligned}
T_4 = & \sqrt{1-4z} \left[ \langle Q\rangle^{(0)} \left( 1 - z + \epsilon \left( \frac{2+z}{3} + (1-z) \left( 2\log\left(\frac{\mu_1}{m_b}\right) - \log(1-4z) \right) \right) \right. \right. \\
& + \epsilon^2 \left( \frac{2+z}{3} \left( 2\log\left(\frac{\mu_1}{m_b}\right) - \log(1-4z) \right) + \frac{1-z}{2} \left( \left( 2\log\left(\frac{\mu_1}{m_b}\right) - \log(1-4z) \right)^2 - \frac{\pi^2}{2} \right) + \frac{13+2z}{9} \right) \\
& + \langle\tilde{Q}_S\rangle^{(0)} \left( 1 + 2z + \epsilon \left( \frac{2(1+5z)}{3} + (1+2z) \left( 2\log\left(\frac{\mu_1}{m_b}\right) - \log(1-4z) \right) \right) + \epsilon^2 \left( \frac{2(1+5z)}{3} \right. \right. \\
& \left. \left. \times \left( 2\log\left(\frac{\mu_1}{m_b}\right) - \log(1-4z) \right) + \frac{1+2z}{2} \left( \left( 2\log\left(\frac{\mu_1}{m_b}\right) - \log(1-4z) \right)^2 - \frac{\pi^2}{2} \right) + \frac{13+56z}{9} \right) \right) \right], \tag{A10}
\end{aligned}$$

$$T_5 = \langle Q \rangle^{(0)} 3z\sqrt{1-4z} \left[ 1 + \epsilon \left( 2 \log \left( \frac{\mu_1}{m_b} \right) - \log(1-4z) + 1 \right) + \epsilon^2 \left( \frac{1}{2} \left( 2 \log \left( \frac{\mu_1}{m_b} \right) - \log(1-4z) \right) \left( 2 \log \left( \frac{\mu_1}{m_b} \right) - \log(1-4z) + 2 \right) - \frac{\pi^2}{4} + 2 \right) \right], \quad (\text{A11})$$

where  $z = m_c^2/m_b^2$  contains the charm mass on lines attached to  $O_{1,2}$  and  $z_i = m_c^2/m_b^2$  contains the charm mass from the closed fermion loop.  $T_2'$  is obtained from  $T_2$  by setting  $z_i$  to zero. For the matrix elements with two QCD penguin operators we refer to Eqs. (A.15)-(A.18) in Ref. [21].

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