Penguin contribution to the 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 Γ_{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 Γ_{12}^q with full dependence on the charm quark mass. This is the first step toward the prediction of the *CP* asymmetry $a_{\rm fs}^q$ 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 nonzero charm mass and our partial NNLO result decreases the NLO penguin corrections to $a_{\rm fs}^q$ by 37% and those to $\Delta\Gamma_q$ by 16%. We further update the Standard-Model NLO predictions for $a_{\rm fs}^q$ 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 $a_{\rm fs}^s=(2.07\pm0.10)\times10^{-5}$, $a_{\rm fs}^d=(-4.71\pm0.24)\times10^{-4}$, $\Delta\Gamma_s/\Delta M_s=(4.33\pm1.26)\times10^{-3}$, and $\Delta\Gamma_d/\Delta M_d=(4.48\pm1.19)\times10^{-3}$. In the $\overline{\rm MS}$ scheme these numbers read $a_{\rm fs}^s=(2.04\pm0.11)\times10^{-5}$, $a_{\rm fs}^d=(-4.64\pm0.25)\times10^{-4}$, $\Delta\Gamma_s/\Delta M_s=(4.97\pm1.02)\times10^{-3}$, and $\Delta\Gamma_d/\Delta M_d=(5.07\pm0.96)\times10^{-3}$.

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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 2×2 matrices, the mass matrix M and the decay matrix Γ. 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]

$$a_{\rm fs}^q={\rm Im}\frac{\Gamma_{12}^q}{M_{12}^q}. \tag{1}$$

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

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

In the absence of direct *CP* violation in the semileptonic decay amplitude one has $a_{\rm fs}^q=a_{\rm sl}^q$. Direct *CP* violation in $B\to X\ell^+\nu_\ell$ 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

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$B \to D\ell^+\nu_\ell$, because the needed CP-conserving phase comes from QED corrections only.) The ratio $\Delta\Gamma_q/\Delta M_q$ is given by

$$\frac{\Delta\Gamma_q}{\Delta M_q} = -\mathrm{Re}\,\frac{\Gamma_{12}^q}{M_{12}^q}. \tag{3}$$

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

The mass differences $\Delta M_s = (17.757 \pm 0.021)\ \mathrm{ps}^{-1}$ and $\Delta M_d = (0.5064 \pm 0.0019)\ \mathrm{ps}^{-1}$ [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],

$$\Delta\Gamma_s^{\mathrm{exp}} = (8.9 \pm 0.6) \times 10^{-2}\ \mathrm{ps}^{-1}, \tag{4}$$

$$\Delta\Gamma_d^{\mathrm{exp}} = (-1.32 \pm 6.58) \times 10^{-3}\ \mathrm{ps}^{-1} \tag{5}$$

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]

$$a_{\mathrm{sl}}^{s,\mathrm{exp}} = (60 \pm 280) \times 10^{-5}, \tag{6}$$

$$a_{\mathrm{sl}}^{d,\mathrm{exp}} = (-21 \pm 17) \times 10^{-4}. \tag{7}$$

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_{fs}^d and $\Delta\Gamma_d$ it is worthwhile to study the clean sample of $B \to J/\psi K_s$ decays [13]. While new physics will primarily enter M_{12}^q, scenarios in which Γ_{12}^q is affected have been studied as well [14,15], especially the doubly Cabibbo-suppressed Γ_{12}^d could play a role in new-physics studies.

The state of the art of the theory predictions of a_{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 $\mathcal{O}(\Lambda_{\mathrm{QCD}}/m_b)$ power-suppressed corrections [19,20]. The accuracy of $\Delta\Gamma_s^{\mathrm{exp}}$ 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 Γ_{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_{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 Γ_{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 toward the prediction of a_{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 Γ_{12}^q is desirable.

This paper is organized as follows: In the following section we summarize the theoretical framework of the calculation. In Sec. III we present our analytical results and subsequently perform a phenomenological analysis in Sec. 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 $b \to s$ transition, reads [23]

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

where

$$\lambda_t^s = V_{ts}^* V_{tb}, \qquad \lambda_u^s = V_{us}^* V_{ub} \tag{9}$$

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

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

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 $(1 \pm \gamma_5)$. $C_1, \ldots, C_6$ 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 formulas for $b \to d$ transitions can be obtained from Eqs. (8)–(10) by replacing s with d.

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

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

where "abs" denotes the absorptive part of the matrix element and T is the time ordering operator. Following [17] we write Γ_{12} as

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

where the coefficients Γ_{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 $\Lambda_{\mathrm{QCD}}/m_b$) 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

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

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

The hadronic matrix elements, which are calculated with nonperturbative methods like lattice QCD, are usually expressed in term of the "bag" parameters B_{B_q}, B'_{S,B_q} as

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

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 μ_2 is the scale of lattice-continuum matching. In the expression for Γ_{12} the matrix elements of Eq. (16) are multiplied by perturbative Wilson coefficients depending on μ_2 as well, resulting in a cancellation of the unphysical scale μ_2 from Γ_{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

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

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")

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

The HQE expresses these bilocal matrix elements in terms of the local matrix elements $\langle Q\rangle$, $\langle Q_S\rangle$ ("effective theory"), and 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 α_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

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

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

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

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 nonzero, 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 Fig. 1 of [21]). The diagrams P_{1-2} are not only needed for the contributions involving $C_{3-6,8}$, but also appear in counterterm 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 $z_i = 0$

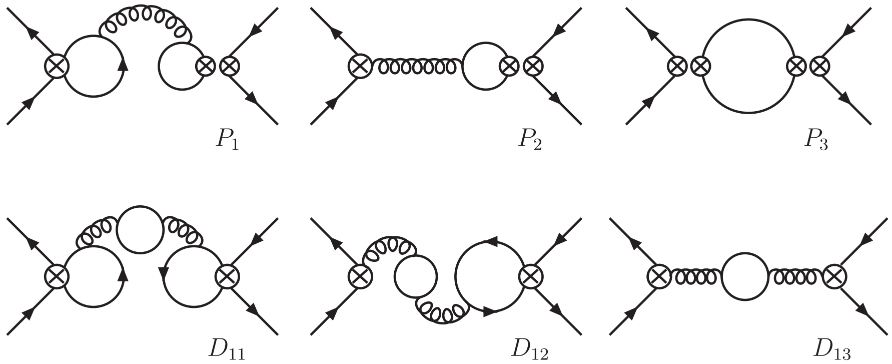

FIG. 1. Diagrams for the penguin contribution at $\mathcal{O}(\alpha_s^2 N_f)$. The small Wilson coefficients C_{3-6} are counted as $\mathcal{O}(\alpha_s)$. P_1, P_2 are diagrams with one insertion of a penguin operator $O_3, \ldots, O_6$, depicted as two circles with crosses, and one insertion of $O_2^{u,c}$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

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

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

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

$$\begin{aligned} P^{cc,(2),N_V}(z_i,z) = {}& \sqrt{1-4z_i}\bigg((1-z_i)M_1'(\mu_1) \\ & + \frac{1}{2}(1-4z_i)M_2'(\mu_1) + 3z_i M_3'(\mu_1)\bigg) \\ & + \frac{\alpha_s(\mu_1)}{4\pi} G_p^{cc,(1),N_V}(z_i,z) M_4'(\mu_1) \\ & + \frac{\alpha_s^2(\mu_1)}{(4\pi)^2} G_p^{cc,(2),N_V}(z_i,z) C_2^2(\mu_1), \end{aligned} \tag{23}$$

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

with

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

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

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

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

where we have defined

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

and

$$\sigma = \frac{1-\sqrt{1-4z}}{1+\sqrt{1-4z}}, \tag{30}$$

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

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

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

where

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

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

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

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

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

In this section we first show the impact of a nonzero charm quark mass in the $\alpha_s^2 N_f$ corrections to $\Delta\Gamma_s$ and a_{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_{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_{fs}^q in terms of m_b and $z = m_c^2/m_b^2$. As shown in Ref. [24], 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_{fs}^q, namely the $\overline{\mathrm{MS}}$ mass $\bar{m}_b(\bar{m}_b)$ and the pole mass m_b^{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 $m_b^{\mathrm{pole}} = (4.58 \pm 0.03)$ GeV at NLO and $m_b^{\mathrm{pole}} = (4.84 \pm 0.03)$ GeV at NNLO.

In our partial NNLO results we further use the complete NNLO $\Delta B = 1$ Wilson coefficients C_1, C_2 [25,26] 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 Table I we obtain

$$\frac{\lambda_u^d}{\lambda_t^d} = (0.0122 \pm 0.0097) - (0.4203 \pm 0.0090)i, \tag{35}$$

$$\frac{\lambda_u^s}{\lambda_t^s} = -(0.00865 \pm 0.00042) + (0.01832 \pm 0.00039)i. \tag{36}$$

For all central values quoted in the following we took $\mu_1 = m_b^{\mathrm{pole}}$ and $\mu_1 = \bar{m}_b$ for the pole and $\overline{\mathrm{MS}}$ schemes, respectively. For the contribution to the width differences

TABLE I. Input parameters used in Sec. IV. $\bar{m}_s(\bar{m}_b)$ is calculated from $\bar{m}_s(2\ \mathrm{GeV}) = 0.09344 \pm 0.00068$ 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. [28] by 8/3 and 3, respectively [see Eq. (16)]. m_B^{pow} is a redundant parameter calibrating the overall size of the hadronic parameters B_{R_i} which quantify the matrix elements at order $\Lambda_{\mathrm{QCD}}/m_b$. $B_{R_0}^q$ is calculated from $\langle B_s|R_0|\bar{B}_s\rangle = -(0.66 \pm 0.27)\ \mathrm{GeV}^4$ and $\langle B_d|R_0|\bar{B}_d\rangle = -(0.36 \pm 0.20)\ \mathrm{GeV}^4$ [28] (with $\langle R_0\rangle$ defined as in Refs. [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 $\langle B_s|\tilde{R}_2|\bar{B}_s\rangle = (0.28 \pm 0.11)\ \mathrm{GeV}^4$ and $\langle B_s|\tilde{R}_3|\bar{B}_s\rangle = (0.44 \pm 0.15)\ \mathrm{GeV}^4$ [29]. The expressions for $B_{R_2}^q$ and $B_{R_3}^q$ hold up to $\Lambda_{\mathrm{QCD}}/m_b$ corrections. $B_{R_1}^q = 1.5$ and $B_{\tilde{R}_1}^q = 1.2$ [29] 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.

$\bar{m}_b(\bar{m}_b) = (4.18 \pm 0.03)$ GeV	[30]	$\bar{m}_c(\bar{m}_c) = (1.2982 \pm 0.0013_{\mathrm{stat}} \pm 0.0120_{\mathrm{syst}})$ GeV	[31–33]
$\bar{m}_s(\bar{m}_b) = (0.0786 \pm 0.0006)$ GeV	[27]	$\bar{m}_t(m_t) = (165.26 \pm 0.11_{\mathrm{stat}} \pm 0.30_{\mathrm{syst}})$ GeV	[33]
$m_b^{\mathrm{pow}} = 4.7$ GeV	[19]	$\alpha_s(M_Z) = 0.1181(11)$	[34]
$M_{B_s} = 5366.88$ MeV	[34]	$M_{B_d} = 5279.64$ MeV	[34]
$B_{B_s} = 0.813 \pm 0.034$	[28]	$B_{B_d} = 0.806 \pm 0.041$	[28]
$\tilde{B}'_{S,B_s} = 1.31 \pm 0.09$	[28]	$\tilde{B}'_{S,B_d} = 1.20 \pm 0.09$	[28]
$B_{R_0}^s = 1.27 \pm 0.52$	[28]	$B_{R_0}^d = 1.02 \pm 0.55$	[28]
$B_{\tilde{R}_2}^s = 0.89 \pm 0.35$	[29]	$B_{\tilde{R}_2}^d = B_{\tilde{R}_2}^s$	
$B_{\tilde{R}_3}^s = 1.14 \pm 0.39$	[29]	$B_{\tilde{R}_3}^d = B_{\tilde{R}_3}^s$	
$B_{R_2}^q = -B_{\tilde{R}_2}^q$	[20]	$B_{R_3}^q = \frac{5}{7}B_{\tilde{R}_3}^q + \frac{2}{7}B_{\tilde{R}_2}^q$	[20]
$f_{B_s} = (0.2307 \pm 0.0013)$ GeV	[35]	$f_{B_d} = (0.1905 \pm 0.0013)$ GeV	[20]
$\sin(2\beta) = 0.7083^{+0.0127}_{-0.0098}$	[33]	$R_t = 0.9124^{+0.0064}_{-0.0100}$	[33]
$\lvert V_{us}\rvert = 0.22483^{+0.00025}_{-0.00006}$	[33]		

$\Delta\Gamma_s$ that originates from the penguin sector and is proportional to $\alpha_s^2 N_f$ (neglecting λ_u part) we find

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

Equation (37) shows that the effect of a nonzero 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 α_s [16] evaluates to

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

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

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

where $\delta\Delta\Gamma_s^{(1),p}(z)$ denotes the contribution to $\Delta\Gamma_s$ from the penguin sector at order α_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

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

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

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

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 α_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_{fs}^q is small [see Eqs. (39) and (41)], but in beyond-SM models [36,37] 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 $\Delta\Gamma_q/\Delta M_q$:

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

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

and a_{fs}^q:

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

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

The error indicated with "$\Lambda_{\mathrm{QCD}}/m_b$" comprises the uncertainty from the bag factors of Refs. [28,29]. The new lattice results for the bag parameters of the $\Lambda_{\mathrm{QCD}}/m_b$ corrections have errors comparable to those assumed in Ref. [21], but the central value of $B_{R_0}^s$ has shifted upward by more than a factor of 2. Furthermore, $\tilde{B}'_{S,B_s}/B_{B_s}$ decreased by 12%, which also lowered the μ_1 dependence. Adding the individual errors quoted in Eqs. (42)–(45) in quadrature yields the values quoted in the abstract.

With the input values of Table I we reproduce the measured ΔM_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 Table I by 16%, explaining why the $\Delta\Gamma_s$ values in Ref. [21] were larger by roughly the same amount compared to

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

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

In a_{fs}^q, however, the lattice results for the Λ_{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_{fs}^q is very sensitive to $B_{\tilde{R}_3}^s$, whose uncertainty of ± 0.39 is below the ± 0.5 assumed in older analyses done without the lattice input.

The scale dependence is calculated by varying μ_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 μ_1 dependence might well underestimate this error in the case of a_{fs}^q.

The central values of all our $\overline{\text{MS}}$ scheme results are in excellent agreement with Ref. [38]. Our error estimate of the Λ_{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. [38]. Our uncertainties for a_{fs}^q, though, are smaller compared to Ref. [38], as we find a smaller μ_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 Table I would contribute another 3% uncertainty to a_{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 asymmetry in flavor-specific decays of B_q mesons, a_{fs}^q. These and the mass difference ΔM_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. [24] 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_{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_{fs}^q, respectively, indicating a good convergence of the perturbative series.

In response to the recent progress in the lattice calculations of the nonperturbative matrix elements [28,29] we have further presented updated NLO values for $\Delta\Gamma_q$ and a_{fs}^q in Eqs. (42)–(46).

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APPENDIX: FULL-THEORY MATRIX ELEMENTS

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

$$M = M_{cc} + M_{\text{peng}}, \tag{A1}$$

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 α_s, so that one loop less is needed for M_{peng} compared to M_{cc}. We expand $M_{\text{peng}}^{ab} = M_{\text{peng}}^{ab,(0)} + \frac{\alpha_s}{4\pi} M_{\text{peng}}^{ab,(1)} + \cdots$.

1. Penguin operators

Here and in the following $\langle\cdots\rangle^{(0)}$ 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 Fig. 1 as

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

where

$$
\begin{aligned}
M_{D_{11}}^{q_1q_2,(1)} = &-\frac{5\langle Q\rangle^{(0)}+8\langle\tilde{Q}_S\rangle^{(0)}}{9}C_2^{b2}\Bigg(\frac{\sqrt{1-4z_1}(1+2z_1)+\sqrt{1-4z_2}(1+2z_2)}{2\epsilon}\\
&+\sqrt{1-4z_2}\left(\frac{1}{2}(2z_2+1)\left(4\log\left(\frac{\mu_1}{m_b}\right)-\log(z_1)-\log(1-4z_2)\right)+2z_1(2z_2+1)+\frac{1}{3}(7z_2+2)\right)\\
&+\sqrt{1-4z_1}\left(\frac{1}{2}(2z_1+1)\left(4\log\left(\frac{\mu_1}{m_b}\right)-\log(1-4z_1)-\log(z_2)\right)+2(2z_1+1)z_2+\frac{1}{3}(7z_1+2)\right)\\
&+\frac{1}{2}\sqrt{1-4z_1}(2z_1+1)\sqrt{1-4z_2}(2z_2+1)(\log(\sigma_1)+\log(\sigma_2))+\epsilon\Bigg(\sqrt{1-4z_1}\Bigg(\left(\frac{2+7z_1}{3}+2(1+2z_1)z_2\right)\\
&\times\left(4\log\left(\frac{\mu_1}{m_b}\right)-\log(1-4z_1)-\log(z_2)\right)+\frac{1}{4}(1+2z_1)\left(\left(4\log\left(\frac{\mu_1}{m_b}\right)-\log(1-4z_1)-\log(z_2)\right)^2-\frac{\pi^2}{3}\right)\\
&+\frac{1}{3}(40z_1z_2+17z_1+14z_2+5)\Bigg)+\sqrt{1-4z_2}\Bigg(\left(\frac{2+7z_2}{3}+2(1+2z_2)z_1\right)\Bigg(4\log\left(\frac{\mu_1}{m_b}\right)\\
&-\log(1-4z_2)-\log(z_1)\Bigg)+\frac{1}{4}(1+2z_2)\left(\left(4\log\left(\frac{\mu_1}{m_b}\right)-\log(1-4z_2)-\log(z_1)\right)^2-\frac{\pi^2}{3}\right)\\
&+\frac{1}{3}(40z_1z_2+17z_2+14z_1+5)\Bigg)+\sqrt{1-4z_1}\sqrt{1-4z_2}\Bigg(\frac{1}{3}(20z_1z_2+7(z_1+z_2)+2)(\log(\sigma_1)+\log(\sigma_2))\\
&-(2z_1+1)(2z_2+1)\Bigg(-\frac{1}{2}(\log(\sigma_1)+\log(\sigma_2))\times\left(4\log\left(\frac{\mu_1}{m_b}\right)-\log(1-4z_1)-\log(1-4z_2)\right)\\
&+\mathrm{Li}_2(\sigma_1)+\mathrm{Li}_2(\sigma_2)+\frac{1}{4}(\log^2(\sigma_1)+\log^2(\sigma_2))+\frac{2\pi^2}{3}\Bigg)\Bigg)\Bigg)\Bigg),
\end{aligned}
\tag{A2}
$$

$$
\begin{aligned}
M_{D_{12}}^{q_1,(1)} = &-\frac{1}{3}(5\langle Q\rangle^{(0)}+8\langle\tilde{Q}_S\rangle^{(0)})C_2^bC_8^b\\
&\cdot\sqrt{1-4z_1}\left(1+2z_1+\epsilon\left(\frac{2(1+5z_1)}{3}+(1+2z_1)\left(2\log\frac{\mu_1}{m_b}-\log(1-4z_1)\right)\right)\right).
\end{aligned}
\tag{A3}
$$

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

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

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

$$
\begin{aligned}
M_{32}^{(0)}(z) &= 2C_2^bC_3^bT_3, \qquad M_{42}^{(0)}(z) = 2C_2^bC_4^bT_4,\\
M_{52}^{(0)}(z) &= 2C_2^bC_5^bT_5, \qquad M_{62}^{(0)}(z) = 2C_2^bC_6^bT_5,
\end{aligned}
\tag{A5}
$$

$$
M_{42}^{(1)}(z) = 2C_2^bC_4^b(N_HT_1+N_VT_2+N_LT_2'), \qquad M_{62}^{(1)}(z) = 2C_2^bC_6^b(N_HT_1+N_VT_2+N_LT_2'), \tag{A6}
$$

where

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

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

and

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

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

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

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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