

# Three-loop matching of heavy flavor-changing (axial-)tensor currents

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**ABSTRACT:** We present the three-loop calculations of the nonrelativistic QCD (NRQCD) current renormalization constants and corresponding anomalous dimensions, and the matching coefficients for the spatial-temporal tensor and spatial-spatial axial-tensor currents with two different heavy quark masses. We obtain the convergent decay constant ratio up to the next-to-next-to-next-to-leading order (N<sup>3</sup>LO) for the *S*-wave vector meson  $B_c^*$  involving the tensor and axial-tensor currents. We obtain the three-loop finite ( $\epsilon^0$ ) term in the ratio of the QCD heavy flavor-changing tensor current renormalization constant in the on-shell (OS) scheme to that in the modified-minimal-subtraction ( $\overline{\text{MS}}$ ) scheme, which is helpful to obtain the three-loop matching coefficients for all heavy flavor-changing (axial-)tensor currents.

**KEYWORDS:** Higher-Order Perturbative Calculations, Automation, Effective Field Theories of QCD, Quarkonium

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## 1 Introduction

In the Standard Model (SM), the  $c\bar{b}$  meson family is the only meson system whose states are formed from two heavy quarks of different flavors. As a result, the  $c\bar{b}$  mesons can not annihilate into gluons and consequently they are more stable than the double heavy charmonium  $c\bar{c}$  and bottomonium  $b\bar{b}$ . Therefore, the  $c\bar{b}$  meson family provides a good platform for a systematic study of the QCD dynamics in the heavy quark interactions.

The excited  $c\bar{b}$  states can pass through electromagnetic radiative decays and hadronic transitions to the low-lying states, which then decay via the charged weak currents. Since the  $c\bar{b}$  meson family shares dynamical properties with the quarkonium, i.e.,  $c$  and  $\bar{b}$  move nonrelativistically, it is appropriate to study the low-lying  $c\bar{b}$  meson states by the NRQCD effective field theory [1]. The meson decay constant is a fundamental physical quantity describing the leptonic decay of a meson state. With the framework of the NRQCD factorization, at the lowest order in quark relative velocity expansion, the decay constant can be factorized into the short-distance coefficient (matching coefficient) and the long-distance matrix element (wave function at the origin).

Using the NRQCD theory, the matching coefficients for heavy flavor-changing currents have been calculated in various perturbative orders of the strong coupling constant  $\alpha_s$ . The one-loop matching coefficient for the heavy flavor-changing temporal axial-vector current was first calculated in ref. [2]. The one-loop calculation of the heavy flavor-changing spatial vector and temporal axial-vector currents allowing for higher order relativistic corrections can be found in refs. [3, 4]. Two-loop corrections to the heavy flavor-changing pseudo-scalar, spatial vector and temporal axial-vector currents are available in the literature [5–7]. At the N<sup>3</sup>LO of  $\alpha_s$ , the matching coefficients for the heavy flavor-changing pseudo-scalar, spatial vector, scalar, temporal axial-vector and spatial axial-vector currents have been numerically

evaluated in refs. [8–11], and our calculations in refs. [10, 11] confirm the earlier results presented in refs. [8, 12] with agreement in almost all of their significant digits.

The aim of this work is to calculate the N<sup>3</sup>LO QCD corrections to the matching coefficients and decay constants for the  $S$ -wave vector meson  $B_c^*$  coupled with the heavy flavor-changing tensor and axial-tensor currents. Apart from testing the perturbative convergence of the NRQCD theory, the three-loop matching of heavy flavor-changing (axial-)tensor currents will reveal the nonrelativistic dynamics in  $B_c^*$  decays via different currents and shed light on the internal structure when the heavy bottom and charm quarks are combined into the  $c\bar{b}$  meson.

The (axial-)tensor decay constants can appear in the calculations of meson distribution amplitudes, form factors and branching ratios for the leptonic, semileptonic, nonleptonic and rare decays [13–18], which along with experimental measurement are helpful to determine the fundamental parameters in particle physics. As well as being significant inputs to factorization formulae, the (axial-)tensor decay constants play an important role in QCD sum rule analysis [19–22]. Furthermore, the (axial-)tensor currents can be included in effective field theory extensions of the SM and may be related to anomalous interactions and new physics beyond the SM [23–25].

By using lattice QCD and QCD sum rules, the (axial-)tensor decay constants of heavy quarkonia (such as  $\Upsilon$ ,  $J/\psi$ ) and light mesons (such as  $\rho$ ,  $\phi$  mesons) have been calculated in various literature [26–41]. Additionally, the accurate calculations of the higher-order perturbative corrections to the decay constants involving heavy-light (axial-)tensor currents have been performed within various QCD effective field theories [19, 42, 43]. In this paper, with the help of the NRQCD theory we will fill the gap in the higher-order perturbative QCD calculations for the (axial-)tensor decay constants of beauty-charmed mesons. Our predictions for  $B_c^*$  decay constants involving vector, tensor and axial-tensor currents will provide valuable information for experimental searches for the ground vector  $B_c^*$  meson. Additionally, our calculations will serve as a probe to test the SM and explore potential new physics.

The rest of the paper is organized as following. In section 2, we introduce the matching formulas between QCD and NRQCD. In section 3, we describe the details of our calculation for the QCD vertex function. In section 4, we study the current renormalization constants in QCD. In section 5, we study the current renormalization constants in NRQCD. In section 6, we present the three-loop numeric results of the matching coefficients and decay constants. Section 7 contains a summary.

## 2 Matching formulas

We first introduce the definitions of the decay constants for the  $S$ -wave vector  $c\bar{b}$  meson  $B_c^*(1^-)(^3S_1)$  coupled with the vector  $v$ , tensor  $t$ , axial-tensor  $t5$  currents [30, 42, 44–58]

$$\begin{aligned}
 \langle 0 | j_v^\mu | B_c^*(q, \varepsilon) \rangle &\doteq f_{B_c^*}^{v,i} m_{B_c^*} \varepsilon^\mu, \\
 \langle 0 | j_t^{\mu\nu} | B_c^*(q, \varepsilon) \rangle &\doteq f_{B_c^*}^{t,i0} (q^\mu \varepsilon^\nu - q^\nu \varepsilon^\mu), \\
 \langle 0 | j_{t5}^{\mu\nu} | B_c^*(q, \varepsilon) \rangle &\doteq f_{B_c^*}^{t5,ij} \epsilon^{\mu\nu\alpha\beta} q_\alpha \varepsilon_\beta,
 \end{aligned} \tag{2.1}$$

where  $q$  and  $\varepsilon$  represent the momentum and polarization vector of  $B_c^*$ , respectively. The superscript  $(v, i)/(t, i0)/(t5, ij)$  denotes the contributing (see below) spatial/spatial-temporal/spatial-spatial component of the vector/tensor/axial-tensor current, respectively. The heavy flavor-changing currents in the full QCD are defined by

$$\begin{aligned} j_v^\mu &= \bar{\psi}_b \gamma^\mu \psi_c, \\ j_t^{\mu\nu} &= \bar{\psi}_b \sigma^{\mu\nu} \psi_c, \\ j_{t5}^{\mu\nu} &= \bar{\psi}_b \sigma^{\mu\nu} \gamma_5 \psi_c, \end{aligned} \tag{2.2}$$

where  $\sigma_{\mu\nu} = \frac{i}{2}(\gamma_\mu \gamma_\nu - \gamma_\nu \gamma_\mu)$ . The QCD current components contributing to the decay constants of  $B_c^*$  can be expanded in terms of NRQCD currents as follows,

$$\begin{aligned} j_v^i &= \mathcal{C}_{v,i} \tilde{j}_v^i + \mathcal{O}(|\vec{k}|^2), \\ j_t^{i0} &= \mathcal{C}_{t,i0} \tilde{j}_t^{i0} + \mathcal{O}(|\vec{k}|^2), \\ j_{t5}^{ij} &= \mathcal{C}_{t5,ij} \tilde{j}_{t5}^{ij} + \mathcal{O}(|\vec{k}|^2), \end{aligned} \tag{2.3}$$

where  $|\vec{k}|$  is the small half relative spatial momentum between the bottom and charm quarks.  $\mathcal{C}_{v,i}, \mathcal{C}_{t,i0}, \mathcal{C}_{t5,ij}$  are the matching coefficients for the heavy flavor-changing spatial vector, spatial-temporal tensor, spatial-spatial axial-tensor currents, respectively. And the NRQCD currents read [3, 4, 59]

$$\begin{aligned} \tilde{j}_v^i &= \varphi_b^\dagger \sigma^i \chi_c, \\ \tilde{j}_t^{i0} &= i \tilde{j}_v^i, \\ \tilde{j}_{t5}^{ij} &= -\epsilon^{ijk} \tilde{j}_v^k, \end{aligned} \tag{2.4}$$

where  $\varphi_b^\dagger$  and  $\chi_c$  denote 2-component Pauli spinor fields annihilating the  $\bar{b}$  and  $c$  quarks, respectively.

After inserting the currents in eq. (2.3) between the vacuum state and the free  $c\bar{b}$  pair of on-shell heavy charm and bottom quarks with small relative velocity [5, 60], we can write the matching formulas as

$$\sqrt{Z_{2,b}^{\text{OS}} Z_{2,c}^{\text{OS}}} Z_J^{\text{OS}} \Gamma_J = \mathcal{C}_J(\mu_f, \mu, m_b, m_c) \sqrt{\tilde{Z}_{2,b}^{\text{OS}} \tilde{Z}_{2,c}^{\text{OS}}} \tilde{Z}_J^{-1} \tilde{\Gamma}_J + \mathcal{O}(|\vec{k}|^2), \tag{2.5}$$

$$\sqrt{Z_{2,b}^{\text{OS}} Z_{2,c}^{\text{OS}}} Z_J^{\text{MS}} \Gamma_J = \bar{\mathcal{C}}_J(\mu_f, \mu, m_b, m_c) \sqrt{\tilde{Z}_{2,b}^{\text{OS}} \tilde{Z}_{2,c}^{\text{OS}}} \tilde{Z}_J^{-1} \tilde{\Gamma}_J + \mathcal{O}(|\vec{k}|^2). \tag{2.6}$$

Since NRQCD is obtained from QCD by factorizing (‘integrating out’) the hard contributions, which go into the matching coefficient [59, 61, 62],  $\tilde{\Gamma}_J$  does not contain contributions from the hard region of loop momenta on the NRQCD side. Due to expansion (prior to integration) in momenta that are not hard within dimensional regularization [63], contributions from the soft, potential and ultrasoft regions of loop momenta agree in QCD and NRQCD, and thus drop out of both  $\Gamma_J$  and  $\tilde{\Gamma}_J$  before performing integration [5, 59, 60]. As a consequence, in eqs. (2.5) and (2.6),  $\Gamma_J$  becomes the on-shell unrenormalized vertex function in the pure hard integration region of QCD, whereas  $\tilde{\Gamma}_J$  becomes the on-shell tree level vertex function independent of  $\alpha_s$  in NRQCD. The left and right parts in eqs. (2.5) and (2.6) represent the renormalization of  $\Gamma_J$  and  $\tilde{\Gamma}_J$ , respectively.

$Z_{2,b(c)}^{\text{OS}}$  is the  $b(c)$  quark field OS renormalization constant in QCD, which can be obtained from refs. [64, 65].  $\tilde{Z}_{2,b(c)}^{\text{OS}}$  is the  $b(c)$  quark field OS renormalization constant in NRQCD and  $\tilde{Z}_{2,b}^{\text{OS}} = \tilde{Z}_{2,c}^{\text{OS}} = 1$  because heavy bottom and charm quarks are decoupled in the NRQCD effective theory.  $\tilde{Z}_J$  is the NRQCD heavy flavor-changing current renormalization constant in the  $\overline{\text{MS}}$  scheme.  $Z_J^{\text{OS}(\overline{\text{MS}})}$  is the QCD heavy flavor-changing current renormalization constant in OS( $\overline{\text{MS}}$ ) scheme.

At the leading-order (LO) of  $\alpha_s$ , the matching coefficient  $\mathcal{C}_J^{\text{LO}} = \bar{\mathcal{C}}_J^{\text{LO}} = 1$ , while in a fixed high order perturbative calculation, both  $\mathcal{C}_J$  and  $\bar{\mathcal{C}}_J$  are finite and depend on the NRQCD factorization scale  $\mu_f$  and the QCD renormalization scale  $\mu$ . For  $J \in \{(t, i0), (t5, ij)\}$ , we can not directly calculate  $\mathcal{C}_J$  by eq. (2.5) because both  $Z_J^{\text{OS}}$  and  $\tilde{Z}_J$  are not known at present, however we can obtain  $\mathcal{C}_J$  by first introducing eq. (2.6) and calculating  $\bar{\mathcal{C}}_J$ , which will be elucidated in section 4.

### 3 QCD vertex function

Let  $q_1(q_2)$  denote the charm (bottom) external momentum,  $q = q_1 + q_2$  represent the total external momentum, and the small momentum  $k$  [66] refer to the relative movement between the bottom and charm quarks. From eq. (2.3) and eq. (2.4), terms at  $\mathcal{O}(k)$  are not needed in QCD and NRQCD so that we can safely set  $k = 0$  throughout the calculation to obtain the vertex function  $\Gamma_J$  in the hard region of the full QCD [60]. Based on the on-shell condition  $q_1^2 = m_c^2, q_2^2 = m_b^2$ , the external momentum configuration can be written as

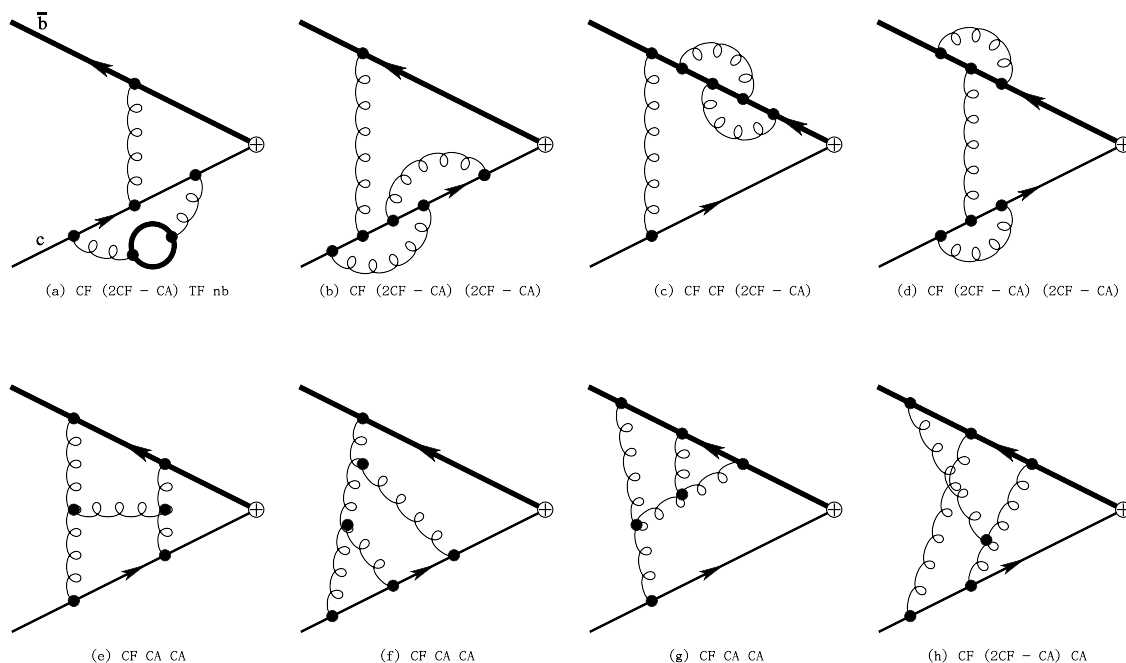
$$\begin{aligned} q_1 &= \frac{m_c}{m_b + m_c} q, \\ q_2 &= \frac{m_b}{m_b + m_c} q, \\ q^2 &= (m_b + m_c)^2. \end{aligned} \tag{3.1}$$

Following the literature [67], we employ the appropriate projector to obtain the hard QCD vertex function  $\Gamma_J$

$$\begin{aligned} \Gamma_{t,i0} &= \text{Tr} \left[ P_{(t,i0),\mu\nu} \Gamma_{(t)}^{\mu\nu} \right], \\ \Gamma_{t5,ij} &= \text{Tr} \left[ P_{(t5,ij),\mu\nu} \Gamma_{(t5)}^{\mu\nu} \right], \end{aligned} \tag{3.2}$$

where  $\Gamma_{(t)}^{\mu\nu} = \dots \sigma^{\mu\nu} \dots$ ,  $\Gamma_{(t5)}^{\mu\nu} = \dots \sigma^{\mu\nu} \gamma_5 \dots$  denote on-shell amputated QCD amplitudes with tensor structures for the tensor and axial-tensor currents, respectively. And the projectors for the heavy flavor-changing spatial-temporal tensor and spatial-spatial axial-tensor currents are constructed as

$$\begin{aligned} P_{(t,i0),\mu\nu} &= \frac{1}{4(D-1)(m_b + m_c)^2} \left( \frac{m_c}{m_b + m_c} \not{q} + m_c \right) \sigma_{\mu\nu} \left( -\frac{m_b}{m_b + m_c} \not{q} + m_b \right), \\ P_{(t5,ij),\mu\nu} &= \frac{1}{2(D-1)(D-2)(m_b + m_c)^2} \left( \frac{m_c}{m_b + m_c} \not{q} + m_c \right) \sigma_{\mu\nu} \gamma_5 \left( -\frac{m_b}{m_b + m_c} \not{q} + m_b \right). \end{aligned} \tag{3.3}$$



**Figure 1.** Representative three-loop Feynman diagrams labelled with corresponding color factors for the QCD vertex function with the heavy flavor-changing current. The cross “ $\oplus$ ” implies the insertion of a certain heavy flavor-changing current. The solid closed circle represents the bottom quark loop with mass  $m_b$  and flavors  $n_b$  (physically,  $n_b = 1$ ).

It is worth mentioning that due to no singlet diagram [59] and no trace with an odd number of  $\gamma_5$  [11] for heavy flavor-changing currents, throughout our calculation we adopt the naively anticommuting  $\gamma_5$  dimensional regularization scheme, i.e.,  $\gamma_5\gamma_\mu + \gamma_\mu\gamma_5 = 0$ ,  $\gamma_5^2 = 1$ .

As following, we will outline our workflow to perform the higher-order calculation for the QCD vertex function. Firstly, we use `FeynCalc` [68] to obtain Feynman diagrams and corresponding Feynman amplitudes. In the Feynman diagrams, we have allowed for  $n_b$  bottom quarks with mass  $m_b$ ,  $n_c$  charm quarks with mass  $m_c$  and  $n_l$  massless quarks appearing in the quark loop. Some representative three-loop Feynman diagrams contributing to the QCD vertex function are displayed in figure 1. By `$Apart` [69], each Feynman amplitude is decomposed into several Feynman integral families. Based on the symmetry among different families, we use our `Mathematica` code+`LiteRed` [70]+`FIRE6` [71] to minimize [72–74] the number of all Feynman integral families. For each heavy flavor-changing current, the total number of three-loop Feynman integral families is minimized from 841 to 110. Then, we use `FIRE6/Kira` [75]/`FiniteFlow` [76] based on Integration by Parts (IBP) [77] to reduce each Feynman integral family to master integral family. Next, we use our `Mathematica` code+`Kira`+`FIRE6` to minimize the number of all master integral families. For each heavy flavor-changing current, the total number of three-loop master integral families is minimized from 110 to 26 meanwhile the total number of three-loop master integrals is minimized into 300. Last, we use `AMFlow` [78], which is a proof-of-concept implementation of the auxiliary mass flow method [79–81], equipped with `FiniteFlow/Kira` to calculate each master integral family.

#### 4 QCD current renormalization constants

Based on the matching formulas in eq. (2.5) and eq. (2.6), we have the following relations for the QCD heavy flavor-changing spatial-temporal tensor  $(t, i0)$  and spatial-spatial axial-tensor  $(t5, ij)$  current OS( $\overline{\text{MS}}$ ) renormalization constants:

$$\begin{aligned} Z_{t,i0}^{\overline{\text{MS}}} &= Z_{t5,ij}^{\overline{\text{MS}}} = Z_t^{\overline{\text{MS}}}, \\ Z_{t,i0}^{\text{OS}} &= Z_{t5,ij}^{\text{OS}} = Z_t^{\text{OS}}, \\ \frac{C_{t,i0}}{\overline{C}_{t,i0}} &= \frac{C_{t5,ij}}{\overline{C}_{t5,ij}} = \frac{Z_t^{\text{OS}}}{Z_t^{\overline{\text{MS}}}} = z_t^g z_t^\mu + \mathcal{O}(\epsilon), \end{aligned} \tag{4.1}$$

where  $Z_t^{\text{OS}(\overline{\text{MS}})}$  is the QCD heavy flavor-changing tensor current OS( $\overline{\text{MS}}$ ) renormalization constant and  $z_t^g z_t^\mu$  is the finite ( $\epsilon^0$ ) term of the ratio  $Z_t^{\text{OS}}/Z_t^{\overline{\text{MS}}}$ .  $Z_t^{\text{OS}}$  is not available in the literature while  $Z_t^{\overline{\text{MS}}}$  can be obtained from refs. [19, 23, 42, 82, 83]:

$$\begin{aligned} Z_t^{\overline{\text{MS}}} &= 1 + \frac{\alpha_s^{(n_f)}(\mu) C_F}{\pi} \frac{C_F}{4\epsilon} + \left( \frac{\alpha_s^{(n_f)}(\mu)}{\pi} \right)^2 C_F \left[ C_F \left( \frac{1}{32\epsilon^2} - \frac{19}{64\epsilon} \right) \right. \\ &\quad \left. + C_A \left( -\frac{11}{96\epsilon^2} + \frac{257}{576\epsilon} \right) + T_F n_f \left( \frac{1}{24\epsilon^2} - \frac{13}{144\epsilon} \right) \right] \\ &\quad + \left( \frac{\alpha_s^{(n_f)}(\mu)}{\pi} \right)^3 C_F \left\{ C_F^2 \left[ \frac{1}{384\epsilon^3} - \frac{19}{256\epsilon^2} + \frac{1}{\epsilon} \left( \frac{365}{1152} - \frac{1}{3}\zeta_3 \right) \right] \right. \\ &\quad \left. + C_F C_A \left[ -\frac{11}{384\epsilon^3} + \frac{75}{256\epsilon^2} + \frac{1}{\epsilon} \left( -\frac{6823}{6912} + \frac{7}{12}\zeta_3 \right) \right] \right. \\ &\quad \left. + C_A^2 \left[ \frac{121}{1728\epsilon^3} - \frac{3439}{10368\epsilon^2} + \frac{1}{\epsilon} \left( \frac{13639}{20736} - \frac{5}{24}\zeta_3 \right) \right] \right. \\ &\quad \left. + C_F T_F n_f \left[ \frac{1}{96\epsilon^3} - \frac{13}{192\epsilon^2} + \frac{1}{\epsilon} \left( \frac{49}{864} + \frac{1}{12}\zeta_3 \right) \right] \right. \\ &\quad \left. - C_A T_F n_f \left[ \frac{11}{216\epsilon^3} - \frac{245}{1296\epsilon^2} + \frac{1}{\epsilon} \left( \frac{251}{1296} + \frac{1}{12}\zeta_3 \right) \right] \right. \\ &\quad \left. + T_F^2 n_f^2 \left[ \frac{1}{108\epsilon^3} - \frac{13}{648\epsilon^2} - \frac{1}{144\epsilon} \right] \right\} + \mathcal{O}(\alpha_s^4). \end{aligned} \tag{4.2}$$

On the one hand, we can use eq. (2.6) and eq. (4.2) to fit  $\tilde{Z}_J$  and calculate  $\overline{C}_J$  for  $J \in \{(t, i0), (t5, ij)\}$ . On the other hand, from eq. (2.3) and eq. (2.4), we obtain following relations between the spatial vector and spatial-temporal tensor currents:

$$\begin{aligned} \tilde{Z}_{t,i0} &= \tilde{Z}_{v,i}, \\ C_{t,i0} &= C_{v,i}, \\ f_{B_c^*}^{t,i0} &= f_{B_c^*}^{v,i}, \end{aligned} \tag{4.3}$$

where  $\tilde{Z}_{v,i}$ ,  $\mathcal{C}_{v,i}$  and  $f_{B_c^*}^{v,i}$  have been calculated and denoted as  $\tilde{Z}_v$ ,  $\mathcal{C}_v$  and  $f_{B_c^*}$  respectively in our previous publication [11]. Substituting eq. (4.3) into eq. (4.1), we obtain

$$z_t^g z_t^\mu = \frac{\mathcal{C}_{v,i}}{\bar{\mathcal{C}}_{t,i0}}. \quad (4.4)$$

For  $J \in \{(t, i0), (t5, ij)\}$ , with  $z_t^g z_t^\mu$  and  $\bar{\mathcal{C}}_J$  known, we can calculate  $\mathcal{C}_J$  by eq. (4.1), i.e.  $\mathcal{C}_J = z_t^g z_t^\mu \bar{\mathcal{C}}_J$ .

As following, we will present our result of  $z_t^g z_t^\mu$ . For brevity, we introduce several notations throughout the paper:

$$\begin{aligned} x &\equiv \frac{m_c}{m_b}, \\ L_\mu &\equiv \ln \frac{\mu^2}{m_b m_c}, \\ L_{\mu_f} &\equiv \ln \frac{\mu_f^2}{m_b m_c}. \end{aligned} \quad (4.5)$$

Let  $z_t^\mu(L_\mu = 0) = 1$ , and let  $z_t^g$  satisfy the renormalization group invariance (see eq. (5.14) in ref. [11]).<sup>1</sup> With the aid of numerical fitting techniques such as the PSLQ algorithm [65], we can obtain the following expressions for  $z_t^\mu$  and  $z_t^g$ :

$$\begin{aligned} z_t^\mu &= 1 + \frac{\alpha_s^{(n_f)}(\mu)}{\pi} \frac{C_F}{4} L_\mu + \left( \frac{\alpha_s^{(n_f)}(\mu)}{\pi} \right)^2 C_F \left[ C_F \left( \frac{1}{32} L_\mu^2 - \frac{19}{32} L_\mu \right) \right. \\ &\quad \left. + C_A \left( \frac{11}{96} L_\mu^2 + \frac{257}{288} L_\mu \right) - T_F n_f \left( \frac{1}{24} L_\mu^2 + \frac{13}{72} L_\mu \right) \right] \\ &\quad + \left( \frac{\alpha_s^{(n_f)}(\mu)}{\pi} \right)^3 C_F \left\{ C_F^2 \left[ \frac{1}{384} L_\mu^3 - \frac{19}{128} L_\mu^2 + \left( \frac{365}{384} - \zeta_3 \right) L_\mu \right] \right. \\ &\quad \left. + C_F C_A \left[ \frac{11}{384} L_\mu^3 - \frac{185}{576} L_\mu^2 + \left( \frac{7}{4} \zeta_3 - \frac{6823}{2304} \right) L_\mu \right] \right. \\ &\quad \left. + C_A^2 \left[ \frac{121}{1728} L_\mu^3 + \frac{3133}{3456} L_\mu^2 + \left( \frac{13639}{6912} - \frac{5}{8} \zeta_3 \right) L_\mu \right] \right. \\ &\quad \left. + C_F T_F n_f \left[ -\frac{1}{96} L_\mu^3 + \frac{35}{288} L_\mu^2 + \left( \frac{\zeta_3}{4} + \frac{49}{288} \right) L_\mu \right] \right. \\ &\quad \left. - C_A T_F n_f \left[ \frac{11}{216} L_\mu^3 + \frac{445}{864} L_\mu^2 + \left( \frac{\zeta_3}{4} + \frac{251}{432} \right) L_\mu \right] \right. \\ &\quad \left. + T_F^2 n_f^2 \left[ \frac{L_\mu^3}{108} + \frac{13 L_\mu^2}{216} - \frac{L_\mu}{48} \right] \right\} + \mathcal{O}(\alpha_s^4), \end{aligned} \quad (4.6)$$

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<sup>1</sup>We find that  $\mathcal{C}_J/z_t^g = z_t^\mu \bar{\mathcal{C}}_J$  ( $J \in \{(t, i0), (t5, ij)\}$ ) is renormalization group invariant and  $z_t^g z_t^\mu$  can be written as  $z_t^g z_t^\mu = \sum_{0 \leq j \leq i} \left( \alpha_s^{(n_f)}(\mu)/\pi \right)^i L_\mu^j c_{ij}(x)$ , which can always be factorized into the product of  $z_t^\mu = 1 + \sum_{1 \leq j \leq i} \left( \alpha_s^{(n_f)}(\mu)/\pi \right)^i L_\mu^j f_{ij}(x)$  and the renormalization group invariant  $z_t^g$  in eq. (4.7). In a word,  $z_t^\mu$  and  $z_t^g$  can be uniquely determined by  $\bar{\mathcal{C}}_{t,i0}$  and  $\mathcal{C}_{t,i0} = \mathcal{C}_{v,i}$ .



$$\begin{aligned}
 z_t^g &= 1 + \frac{\alpha_s^{(n_f)}(\mu)}{\pi} z_t^{(1)}(x) + \left( \frac{\alpha_s^{(n_f)}(\mu)}{\pi} \right)^2 \left( z_t^{(2)}(x) + \frac{z_t^{(1)}(x)}{4} \beta_0^{(n_f)} L_\mu \right) \\
 &+ \left( \frac{\alpha_s^{(n_f)}(\mu)}{\pi} \right)^3 \left\{ z_t^{(3)}(x) + \left( \frac{z_t^{(1)}(x)}{16} \beta_1^{(n_f)} + \frac{z_t^{(2)}(x)}{2} \beta_0^{(n_f)} \right) L_\mu \right. \\
 &\left. + \frac{z_t^{(1)}(x)}{16} \beta_0^{(n_f)2} L_\mu^2 \right\} + \mathcal{O}(\alpha_s^4), \tag{4.7}
 \end{aligned}$$

$$\begin{aligned}
 z_t^{(1)}(x) &= -\frac{C_F}{4} \frac{x-1}{x+1} \ln x, \\
 z_t^{(2)}(x) &= C_F \left[ C_F z_t^{FF}(x) + C_A z_t^{FA}(x) + T_F n_l z_t^{FL}(x) + T_F n_b z_t^{FB}(x) + T_F n_c z_t^{FC}(x) \right], \\
 z_t^{(3)}(x) &= C_F \left[ C_F^2 z_t^{FFF}(x) + C_F C_A z_t^{FFA}(x) + C_A^2 z_t^{FAA}(x) \right. \\
 &+ C_F T_F n_l z_t^{FFL}(x) + C_F T_F n_b z_t^{FFB}(x) + C_F T_F n_c z_t^{FFC}(x) \\
 &+ C_A T_F n_l z_t^{FAL}(x) + C_A T_F n_b z_t^{FAB}(x) + C_A T_F n_c z_t^{FAC}(x) \\
 &+ T_F^2 n_l^2 z_t^{FLL}(x) + T_F^2 n_l n_b z_t^{FLB}(x) + T_F^2 n_l n_c z_t^{FLC}(x) \\
 &\left. + T_F^2 n_b^2 z_t^{FBB}(x) + T_F^2 n_b n_c z_t^{FBC}(x) + T_F^2 n_c^2 z_t^{FCC}(x) \right], \tag{4.8}
 \end{aligned}$$

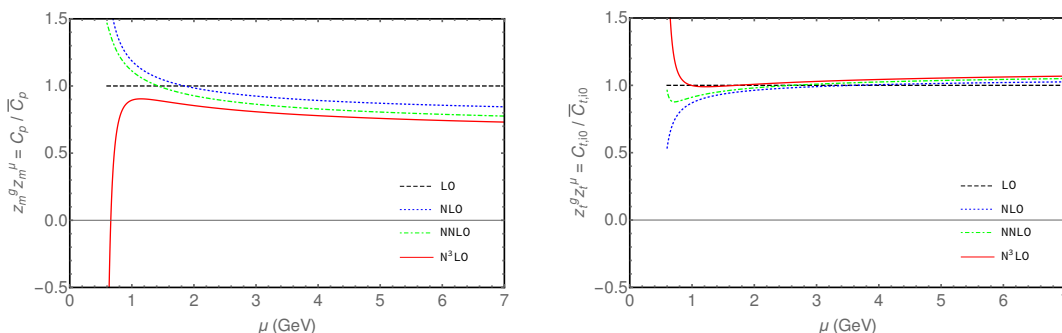
where  $\beta_0^{(n_f)} = \frac{11}{3}C_A - \frac{4}{3}T_F n_f$  and  $\beta_1^{(n_f)} = \frac{34}{3}C_A^2 - 4C_F T_F n_f - \frac{20}{3}C_A T_F n_f$  are respectively the one-loop and two-loop coefficients of the QCD  $\beta$  function [84] and  $n_f = n_l + n_b + n_c$  is the total number of flavors. The color-structure components of  $z_t^{(2)}(x)$  and  $z_t^{(3)}(x)$  read:

$$\begin{aligned}
 z_t^{FF}(x) &= -\frac{563}{384} - \frac{1}{6}\pi^2 \ln 2 + \frac{\zeta_3}{4} + \frac{3(x-1)}{32(x+1)} \ln x \\
 &- \frac{8x^4 - 20x^3 - 99x^2 - 46x - 35}{144(x+1)^2} \pi^2 \\
 &- \frac{32x^4 + 40x^3 - 19x^2 + 42x - 3}{96(x+1)^2} \ln^2 x \\
 &+ \frac{(x+1)(x-1)^3}{3x^2} [\ln(1-x) \ln x + \text{Li}_2(x)] \\
 &+ \frac{2x^4 + x^3 - x - 2}{6x^2} [\ln(1+x) \ln x + \text{Li}_2(-x)], \\
 z_t^{FA}(x) &= \frac{5141}{3456} + \frac{1}{12}\pi^2 \ln 2 - \frac{\zeta_3}{8} - \frac{209(x-1)}{288(x+1)} \ln x \\
 &+ \frac{x^4 - 2x^3 - 10x^2 - 4x - 3}{36(x+1)^2} \pi^2 \\
 &+ \frac{16x^4 + 16x^3 - 5x^2 + 22x + 11}{96(x+1)^2} \ln^2 x \\
 &- \frac{(x+1)(x-1)^3}{6x^2} [\ln(1-x) \ln x + \text{Li}_2(x)] \\
 &- \frac{x^4 - 1}{6x^2} [\ln(1+x) \ln x + \text{Li}_2(-x)], \\
 z_t^{FL}(x) &= -\frac{205}{864} - \frac{\pi^2}{36} + \frac{13(x-1)}{72(x+1)} \ln x - \frac{1}{24} \ln^2 x,
 \end{aligned}$$

$$\begin{aligned}
z_t^{FB}(x) &= -\frac{205}{864} - \frac{1}{4x} + \frac{\pi^2}{18(x+1)} \\
&\quad + \frac{13x^2 - 13x + 12}{72x(x+1)} \ln x + \frac{(3x-1)}{24(x+1)} \ln^2 x \\
&\quad - \frac{(x^2+x+1)(x-1)^2}{6x^3(x+1)} [\ln(1-x) \ln x + \text{Li}_2(x)] \\
&\quad - \frac{x^3+1}{6x^3} [\ln(x+1) \ln x + \text{Li}_2(-x)], \\
z_t^{FC}(x) &= -\frac{205}{864} - \frac{x}{4} - \frac{x^4 - 3x^3 - 5x + 1}{36(x+1)} \pi^2 \\
&\quad - \frac{12x^2 - 13x + 13}{72(x+1)} \ln x - \frac{4x^4 + x + 1}{24(x+1)} \ln^2 x \\
&\quad + \frac{(x^2+x+1)(x-1)^2}{6(x+1)} [\ln(1-x) \ln x + \text{Li}_2(x)] \\
&\quad + \frac{x^3+1}{6} [\ln(x+1) \ln x + \text{Li}_2(-x)], \tag{4.9} \\
z_t^{FFF}(x_0) &= -2.322282618854114578537016108614, \\
z_t^{FFA}(x_0) &= 0.63952094914985889385999778652907, \\
z_t^{FAA}(x_0) &= 4.91543462857763455194218954249917, \\
z_t^{FFL}(x_0) &= 0.48535345668429975701679412257185, \\
z_t^{FBB}(x_0) &= -0.96788752784853089190831478824595, \\
z_t^{FBC}(x_0) &= -0.030004714341714672058240640021062, \\
z_t^{FAL}(x_0) &= -3.7810411909098785095485086146338, \\
z_t^{FAB}(x_0) &= 2.00151369570156466157964680499125, \\
z_t^{FAC}(x_0) &= -0.64029413850834349156677913068544, \\
z_t^{FLL}(x) &= \frac{2665}{23328} + \frac{13\pi^2}{324} + \frac{7\zeta_3}{54} - \frac{89(x-1)}{648(x+1)} \ln x \\
&\quad - \frac{x-1}{54(x+1)} \pi^2 \ln x + \frac{13}{216} \ln^2 x - \frac{x-1}{108(x+1)} \ln^3 x, \\
z_t^{FLB}(x_0) &= -0.18426684902451221497413586356109, \\
z_t^{FLC}(x_0) &= 0.24724217746243652013783508427839, \\
z_t^{FBB}(x_0) &= 0.24641742011807953984404155385694, \\
z_t^{FBC}(x_0) &= 0.069455208354306644824678292877365, \\
z_t^{FCC}(x_0) &= 0.043546270000908910321578999401716, \tag{4.10}
\end{aligned}$$

where the numerical results with about 30-digit precision for various color-structure components of  $z_t^{(3)}(x)$  at the physical point  $x = x_0 = 150/475$  are presented because it is difficult to obtain the analytic expressions of them involving Goncharov polylogarithms (see ref. [64]). In the supplementary material attached to the paper, we provide the numerical results with about 30-digit precision for them at the following ten points:

$$x \in \left\{ \frac{1}{20}, \frac{1}{5}, \frac{100}{475}, \frac{150}{525}, \frac{150}{475}, \frac{150}{425}, \frac{204}{498}, \frac{200}{475}, \frac{1}{2}, 1 \right\}. \tag{4.11}$$



**Figure 2.** The renormalization scale  $\mu$  dependence of  $z_m^g z_m^\mu = \frac{C_p}{\bar{C}_p}$  and  $z_t^g z_t^\mu = \frac{C_{t,i0}}{\bar{C}_{t,i0}}$  at LO, NLO, NNLO and N<sup>3</sup>LO accuracy. The central values are calculated inputting the physical values with  $\mu_f = 1.2$  GeV,  $m_b = 4.75$  GeV and  $m_c = 1.5$  GeV. There are no visible error bands from the variation of the NRQCD factorization scale  $\mu_f$  between 7 and 0.4 GeV.

The values of them for  $x > 1$  can be obtained by employing the invariance of  $z_t^g$  under the exchange  $m_b \leftrightarrow m_c$  meanwhile  $n_b \leftrightarrow n_c$ .

To verify our calculation of  $z_t^g z_t^\mu$  and investigate the deviation between  $\mathcal{C}_J$  and  $\bar{\mathcal{C}}_J$ , following eq. (4.1), we also study the relations [43] for the QCD heavy flavor-changing scalar ( $s$ ) and pseudo-scalar ( $p$ ) current OS( $\overline{\text{MS}}$ ) renormalization constants:

$$\begin{aligned}
 Z_s^{\overline{\text{MS}}} &= Z_p^{\overline{\text{MS}}} = Z_m^{\overline{\text{MS}}}, \\
 Z_s^{\text{OS}} &= Z_p^{\text{OS}} = \frac{m_b Z_{m,b}^{\text{OS}} + m_c Z_{m,c}^{\text{OS}}}{m_b + m_c}, \\
 \frac{\mathcal{C}_s}{\bar{\mathcal{C}}_s} &= \frac{\mathcal{C}_p}{\bar{\mathcal{C}}_p} = \frac{m_b Z_{m,b}^{\text{OS}} + m_c Z_{m,c}^{\text{OS}}}{(m_b + m_c) Z_m^{\overline{\text{MS}}}} = z_m^g z_m^\mu + \mathcal{O}(\epsilon),
 \end{aligned}
 \tag{4.12}$$

where  $Z_m^{\overline{\text{MS}}}$  is the quark mass  $\overline{\text{MS}}$  renormalization constant in QCD, which can be found in refs. [19, 42, 82, 85].  $Z_{m,b(c)}^{\text{OS}}$  is the  $b(c)$  quark mass OS renormalization constant in QCD, which can be obtained from ref. [64].  $z_m^g$  and  $z_m^\mu$  can be defined by analogizing to the definitions of  $z_t^g$  and  $z_t^\mu$  respectively in the above context.

Furthermore, we expand  $z_m^g z_m^\mu = \frac{C_p}{\bar{C}_p}$  and  $z_t^g z_t^\mu = \frac{C_{t,i0}}{\bar{C}_{t,i0}}$  in power series of  $\alpha_s^{(n_l=3)}(\mu)$  (where  $n_l$  is the number of massless quark flavors. See the following sections for the definition of  $\alpha_s$ .) and plot the renormalization scale  $\mu$  dependence of them in figure 2. We see both  $z_m^g z_m^\mu$  and  $z_t^g z_t^\mu$  are convergent and show good renormalization scale dependence. Note that both  $z_m^g z_m^\mu$  and  $z_t^g z_t^\mu$  are free from  $\mu_f$  due to the fact that the QCD current renormalization constant  $Z_J^{\text{OS}(\overline{\text{MS}})}$  is independent of the NRQCD factorization scale  $\mu_f$ . We also find although  $\mathcal{C}_J$  satisfies the renormalization group invariance (see eq. (5.14) in ref. [11]) while  $\bar{\mathcal{C}}_J$  does not, the deviation between  $\mathcal{C}_J$  and  $\bar{\mathcal{C}}_J$  is relatively small. In addition, our calculation verifies both  $\bar{\mathcal{C}}_J$  and  $\mathcal{C}_J$  are gauge invariant so that  $z_m^g z_m^\mu$ ,  $z_t^g z_t^\mu$ ,  $Z_J^{\overline{\text{MS}}}$  and  $Z_J^{\text{OS}}$  are also gauge invariant. We conclude that our calculation results for  $z_t^g z_t^\mu$  are reasonable and reliable.

## 5 NRQCD current renormalization constants

We employ the matching formula in eq. (2.6) to obtain  $\tilde{Z}_J$  for  $J \in \{(t, i0), (t5, ij)\}$ . To perform the conventional QCD renormalization procedure [86] for  $\Gamma_J$  on the l.h.s. of eq. (2.6), we need to implement the QCD heavy quark field and mass OS renormalization, the QCD coupling constant  $\overline{\text{MS}}$  renormalization [84, 87, 88], and the QCD heavy flavor-changing current  $\overline{\text{MS}}$  renormalization, after which the QCD vertex function gets rid of the ultra-violet(UV) divergences, yet still contains uncanceled infra-red(IR) poles starting from order  $\alpha_s^2$ . The remaining IR poles in QCD should be exactly cancelled by the UV poles of the NRQCD heavy flavor-changing current  $\overline{\text{MS}}$  renormalization constant  $\tilde{Z}_J$  on the r.h.s. of eq. (2.6), which renders the matching coefficient finite. Therefore, eq. (2.6) can completely determine  $\tilde{Z}_J$  and subsequently determine  $\bar{C}_J$ .

Based on the high-precision numerical results and the PSLQ algorithm [65], we have fitted and reconstructed the exact analytical expressions of  $\tilde{Z}_J$  for  $J \in \{(t, i0), (t5, ij)\}$ , which verify  $\tilde{Z}_{t,i0} \equiv \tilde{Z}_{v,i}$ . The results of  $\tilde{Z}_{t,i0}$  and  $\tilde{Z}_{t5,ij}$  are presented as following:

$$\begin{aligned}
 \tilde{Z}_J(L_{\mu_f}; x) &= 1 + \left(\frac{\alpha_s^{(n_l)}(\mu_f)}{\pi}\right)^2 \tilde{Z}_J^{(2)}(x) + \left(\frac{\alpha_s^{(n_l)}(\mu_f)}{\pi}\right)^3 \tilde{Z}_J^{(3)}(L_{\mu_f}; x) + \mathcal{O}(\alpha_s^4), \\
 \tilde{Z}_{t,i0}^{(2)}(x) &= \tilde{Z}_{t5,ij}^{(2)}(x) = \pi^2 C_F \frac{1}{\epsilon} \left( \frac{3x^2 + 2x + 3}{24(x+1)^2} C_F + \frac{1}{8} C_A \right), \\
 \tilde{Z}_J^{(3)}(L_{\mu_f}; x) &= \pi^2 C_F \left\{ C_F^2 \left[ \frac{3x^2 - x + 3}{36\epsilon^2(x+1)^2} + \frac{1}{\epsilon} \left( \frac{19x^2 + 5x + 19}{36(x+1)^2} - \frac{2}{3} \ln 2 \right. \right. \right. \\
 &\quad \left. \left. \left. + \frac{x^3 - 4x^2 - 2x - 3}{12(x+1)^3} \ln x + \frac{1}{6} \ln(x+1) + \frac{3x^2 - x + 3}{12(x+1)^2} L_{\mu_f} \right) \right] \right. \\
 &\quad \left. + C_F C_A \left[ \frac{x}{216\epsilon^2(x+1)^2} + \frac{1}{\epsilon} \left( \frac{78x^2 + c_1^J x + 78}{324(x+1)^2} \right. \right. \right. \\
 &\quad \left. \left. \left. - \frac{x+11}{48(x+1)} \ln x + \frac{1}{4} \ln(x+1) + \frac{11x^2 + 8x + 11}{48(x+1)^2} L_{\mu_f} \right) \right] \right. \\
 &\quad \left. + C_A^2 \left[ \frac{-1}{16\epsilon^2} + \frac{1}{\epsilon} \left( \frac{2}{27} + \frac{1}{6} \ln 2 - \frac{1}{24} \ln x + \frac{1}{12} \ln(x+1) + \frac{1}{24} L_{\mu_f} \right) \right] \right. \\
 &\quad \left. + C_F T_F n_l \left[ \frac{3x^2 + 2x + 3}{108\epsilon^2(x+1)^2} - \frac{21x^2 + c_2^J x + 21}{324\epsilon(x+1)^2} \right] + C_F T_F n_b \frac{x^2}{15\epsilon(x+1)^2} \right. \\
 &\quad \left. + C_F T_F n_c \frac{1}{15\epsilon(x+1)^2} + C_A T_F n_l \left[ \frac{1}{36\epsilon^2} - \frac{37}{432\epsilon} \right] \right\}, \tag{5.1}
 \end{aligned}$$

where  $c_1^{t,i0} = 296$ ,  $c_1^{t5,ij} = 227$ ,  $c_2^{t,i0} = 58$ ,  $c_2^{t5,ij} = 10$ . And the corresponding anomalous dimension  $\tilde{\gamma}_J$  [89–94] related to  $\tilde{Z}_J$  reads

$$\begin{aligned}
 \tilde{\gamma}_J(L_{\mu_f}; x) &= \left(\frac{\alpha_s^{(n_l)}(\mu_f)}{\pi}\right)^2 \tilde{\gamma}_J^{(2)}(x) + \left(\frac{\alpha_s^{(n_l)}(\mu_f)}{\pi}\right)^3 \tilde{\gamma}_J^{(3)}(L_{\mu_f}; x) + \mathcal{O}(\alpha_s^4), \\
 \tilde{\gamma}_J^{(2)}(x) &= -4 \tilde{Z}_J^{(2)[1]}(x), \quad \tilde{\gamma}_J^{(3)}(L_{\mu_f}; x) = -6 \tilde{Z}_J^{(3)[1]}(L_{\mu_f}; x), \tag{5.2}
 \end{aligned}$$

where  $\tilde{Z}_J^{(i)[1]}$  denotes the coefficient of  $\frac{1}{\epsilon}$  in  $\tilde{Z}_J^{(i)}$ . Note both  $\tilde{Z}_J$  and  $\tilde{\gamma}_J$  explicitly depend on  $\mu_f$  but not  $\mu$  [8, 9, 12, 61, 95]. One can check  $\tilde{Z}_J$  and  $\tilde{\gamma}_J$  are invariant under the exchange  $m_b \leftrightarrow m_c$  meanwhile  $n_b \leftrightarrow n_c$ .

In our calculation, we consider QCD where  $n_l$  massless flavors,  $n_b$  flavors with mass  $m_b$  and  $n_c$  flavors with mass  $m_c$  possibly appear in the quark loop. However the contributions from the loops of heavy charm and bottom quarks are decoupled in the NRQCD. To match QCD with NRQCD, we employ both the coupling running [10, 11, 96] and the decoupling relation [10, 11, 62, 94, 97–103] in  $D = 4 - 2\epsilon$  for the mutual conversion between  $\alpha_s^{(n_f)}(\mu)$ ,  $\alpha_s^{(n_l)}(\mu_f)$  and  $\alpha_s^{(n_l)}(\mu)$ , where  $n_f = n_l + n_b + n_c$  is the total number of flavors.

The numerical values of  $\alpha_s^{(n_l)}(\mu)$  with  $n_l = 3$ ,  $n_b = n_c = 1$  and  $\mu \in [0.4, 7]$  GeV can be calculated using the coupling running and the decoupling relation in  $D = 4$  [10, 11] or using the package RunDec [104–107] function AlphasLam with  $\Lambda_{\text{QCD}}^{(n_l=3)} = 0.3344\text{GeV}$  determined by inputting the initial value  $\alpha_s^{(n_f=5)}(m_Z = 91.1876\text{GeV}) = 0.1179$ .

## 6 Matching coefficients and decay constants

The final result of the matching coefficient  $\mathcal{C}_J$  for  $J \in \{(t, i0), (t5, ij)\}$  can be written as [8–11]:

$$\begin{aligned} \mathcal{C}_J(\mu_f, \mu, m_b, m_c) = & 1 + \frac{\alpha_s^{(n_l)}(\mu)}{\pi} \mathcal{C}_J^{(1)}(x) \\ & + \left( \frac{\alpha_s^{(n_l)}(\mu)}{\pi} \right)^2 \left[ \frac{\mathcal{C}_J^{(1)}(x)}{4} \beta_0^{(n_l)} L_\mu + \frac{\tilde{\gamma}_J^{(2)}(x)}{2} L_{\mu_f} + \mathcal{C}_J^{(2)}(x) \right] \\ & + \left( \frac{\alpha_s^{(n_l)}(\mu)}{\pi} \right)^3 \left\{ \frac{\mathcal{C}_J^{(1)}(x)}{16} \beta_0^{(n_l)2} L_\mu^2 + \left[ \frac{\mathcal{C}_J^{(1)}(x)}{16} \beta_1^{(n_l)} + \frac{\mathcal{C}_J^{(2)}(x)}{2} \beta_0^{(n_l)} \right] L_\mu \right. \\ & + \frac{\tilde{\gamma}_J^{(2)}(x)}{4} \beta_0^{(n_l)} L_\mu L_{\mu_f} + \left[ \frac{\partial \tilde{\gamma}_J^{(3)}(L_{\mu_f}; x)}{4 \partial L_{\mu_f}} - \frac{\tilde{\gamma}_J^{(2)}(x)}{8} \beta_0^{(n_l)} \right] L_{\mu_f}^2 \\ & \left. + \frac{1}{2} \left[ \mathcal{C}_J^{(1)}(x) \tilde{\gamma}_J^{(2)}(x) + \tilde{\gamma}_J^{(3)}(L_{\mu_f} = 0; x) \right] L_{\mu_f} + \mathcal{C}_J^{(3)}(x) \right\} + \mathcal{O}(\alpha_s^4), \end{aligned} \tag{6.1}$$

where  $n_l$  is the number of the massless flavors.  $\mathcal{C}_J^{(n)}(x)$  ( $n = 1, 2, 3$ ) is a function only depending on  $x = m_c/m_b$ , which can be decomposed in terms of different color factor structures [8, 9, 12, 61, 95, 108]:

$$\begin{aligned} \mathcal{C}_{t,i0}^{(1)}(x) = \mathcal{C}_{t5,ij}^{(1)}(x) &= \frac{3}{4} C_F \left( \frac{x-1}{x+1} \ln x - \frac{8}{3} \right), \\ \mathcal{C}_J^{(2)}(x) &= C_F \left[ C_F \mathcal{C}_J^{FF}(x) + C_A \mathcal{C}_J^{FA}(x) + T_F n_l \mathcal{C}_J^{FL}(x) + T_F n_b \mathcal{C}_J^{FB}(x) + T_F n_c \mathcal{C}_J^{FC}(x) \right], \\ \mathcal{C}_J^{(3)}(x) &= C_F \left[ C_F^2 \mathcal{C}_J^{FFF}(x) + C_F C_A \mathcal{C}_J^{FFA}(x) + C_A^2 \mathcal{C}_J^{FAA}(x) \right. \\ &+ C_F T_F n_l \mathcal{C}_J^{FFL}(x) + C_F T_F n_b \mathcal{C}_J^{FFB}(x) + C_F T_F n_c \mathcal{C}_J^{FFC}(x) \\ &+ C_A T_F n_l \mathcal{C}_J^{FAL}(x) + C_A T_F n_b \mathcal{C}_J^{FAB}(x) + C_A T_F n_c \mathcal{C}_J^{FAC}(x) \\ &+ T_F^2 n_l^2 \mathcal{C}_J^{FLL}(x) + T_F^2 n_l n_b \mathcal{C}_J^{FLB}(x) + T_F^2 n_l n_c \mathcal{C}_J^{FLC}(x) \\ &\left. + T_F^2 n_b^2 \mathcal{C}_J^{FBB}(x) + T_F^2 n_b n_c \mathcal{C}_J^{FBC}(x) + T_F^2 n_c^2 \mathcal{C}_J^{FCC}(x) \right]. \end{aligned} \tag{6.2}$$

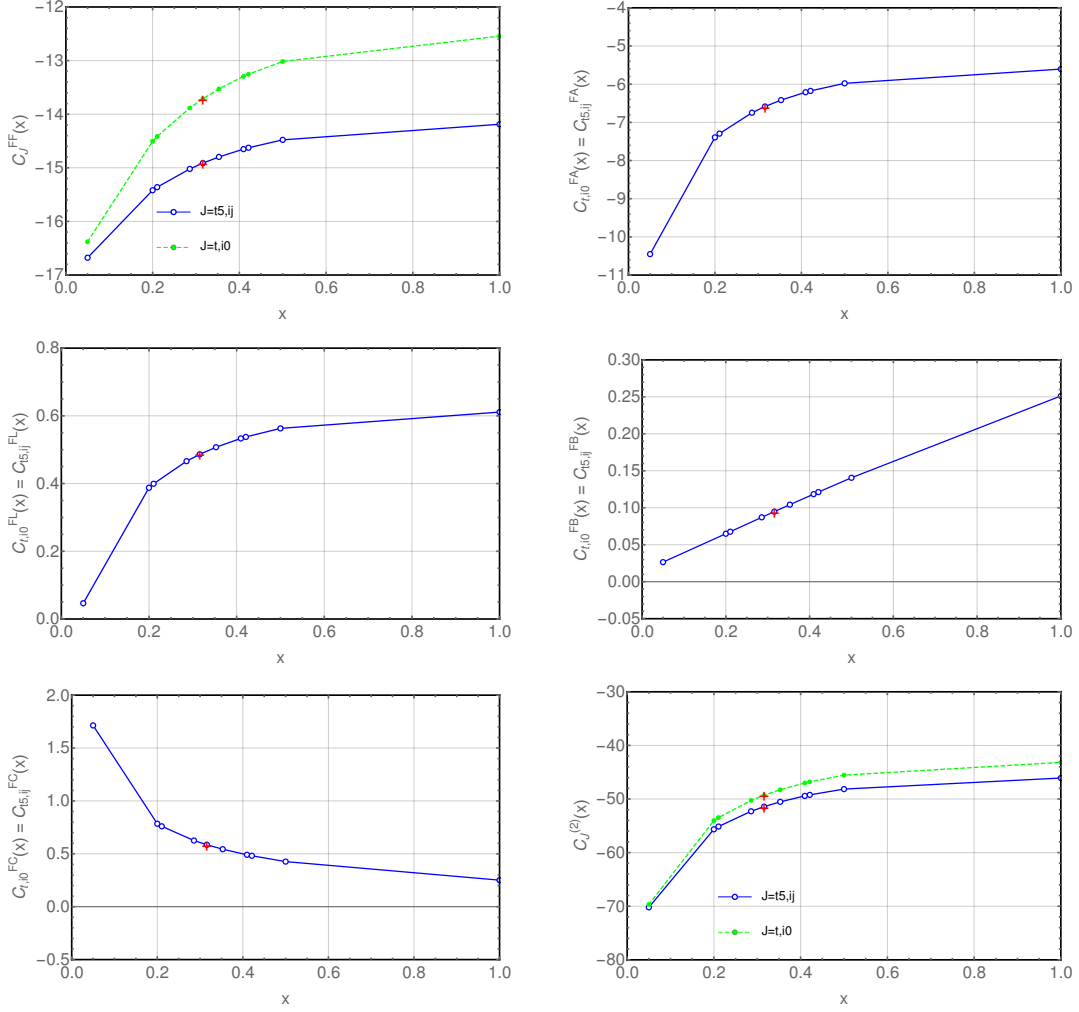
In the following, we will present the numerical results with about 30-digit precision for the color-structure components of  $\mathcal{C}_J^{(2)}(x)$  and  $\mathcal{C}_J^{(3)}(x)$  with  $J \in \{(t, i0), (t5, ij)\}$  at the physical heavy quark mass ratio  $x = x_0 = \frac{150}{475}$ :

$$\begin{aligned}
 \mathcal{C}_{t,i0}^{FF}(x_0) &= -13.7128908053312964335378688241536, \\
 \mathcal{C}_{t5,ij}^{FF}(x_0) &= -14.913034700503762441588142929738, \\
 \mathcal{C}_{t,i0}^{FA}(x_0) = \mathcal{C}_{t5,ij}^{FA}(x_0) &= -6.5854991351922034080659088041666, \\
 \mathcal{C}_{t,i0}^{FL}(x_0) = \mathcal{C}_{t5,ij}^{FL}(x_0) &= 0.48623749753445268636481818648117, \\
 \mathcal{C}_{t,i0}^{FB}(x_0) = \mathcal{C}_{t5,ij}^{FB}(x_0) &= 0.094767648112565260648796850397580, \\
 \mathcal{C}_{t,i0}^{FC}(x_0) = \mathcal{C}_{t5,ij}^{FC}(x_0) &= 0.58579656372904430515925102361910; \\
 \mathcal{C}_{t,i0}^{FFF}(x_0) &= 20.189694171293059999115718422862, \\
 \mathcal{C}_{t5,ij}^{FFF}(x_0) &= 22.306062127579275290403925140598, \\
 \mathcal{C}_{t,i0}^{FFA}(x_0) &= -203.43492648602951942325728768127, \\
 \mathcal{C}_{t5,ij}^{FFA}(x_0) &= -203.95472214521991932337123118763, \\
 \mathcal{C}_{t,i0}^{FAA}(x_0) = \mathcal{C}_{t5,ij}^{FAA}(x_0) &= -102.79687277377774222247635787879, \\
 \mathcal{C}_{t,i0}^{FFL}(x_0) &= 50.937750168903261462489070659559, \\
 \mathcal{C}_{t5,ij}^{FFL}(x_0) &= 50.848850621112708424855717022108, \\
 \mathcal{C}_{t,i0}^{FFB}(x_0) = \mathcal{C}_{t5,ij}^{FFB}(x_0) &= -0.12549350490181543572124489903965, \\
 \mathcal{C}_{t,i0}^{FFC}(x_0) = \mathcal{C}_{t5,ij}^{FFC}(x_0) &= -1.6854789447153670526748653363782, \\
 \mathcal{C}_{t,i0}^{FAL}(x_0) = \mathcal{C}_{t5,ij}^{FAL}(x_0) &= 40.225746623835199555381909178019, \\
 \mathcal{C}_{t,i0}^{FAB}(x_0) = \mathcal{C}_{t5,ij}^{FAB}(x_0) &= -0.20773504228300500317960484318926, \\
 \mathcal{C}_{t,i0}^{FAC}(x_0) = \mathcal{C}_{t5,ij}^{FAC}(x_0) &= 0.46466348732388629839619141994117, \\
 \mathcal{C}_{t,i0}^{FLL}(x_0) = \mathcal{C}_{t5,ij}^{FLL}(x_0) &= -2.0881487824796221669234777696960, \\
 \mathcal{C}_{t,i0}^{FLB}(x_0) = \mathcal{C}_{t5,ij}^{FLB}(x_0) &= -0.055625961762816926133354428478288, \\
 \mathcal{C}_{t,i0}^{FLC}(x_0) = \mathcal{C}_{t5,ij}^{FLC}(x_0) &= -0.77633957612352777786750825747681, \\
 \mathcal{C}_{t,i0}^{FBB}(x_0) = \mathcal{C}_{t5,ij}^{FBB}(x_0) &= 0.0155302263395316874159466507909598, \\
 \mathcal{C}_{t,i0}^{FBC}(x_0) = \mathcal{C}_{t5,ij}^{FBC}(x_0) &= 0.090304843884397461649988047441091, \\
 \mathcal{C}_{t,i0}^{FCC}(x_0) = \mathcal{C}_{t5,ij}^{FCC}(x_0) &= 0.166410566769625472334622650374377, \tag{6.3}
 \end{aligned}$$

where the color-structure components of  $\mathcal{C}_{t,i0}^{(n)}(x_0)$  are directly obtained from  $\mathcal{C}_{t,i0}^{(n)}(x) \equiv \mathcal{C}_{v,i}^{(n)}(x)$  while those of  $\mathcal{C}_{t5,ij}^{(n)}(x_0)$  are calculated by  $\mathcal{C}_{t5,ij} = z_t^g z_t^\mu \bar{\mathcal{C}}_{t5,ij}$ .

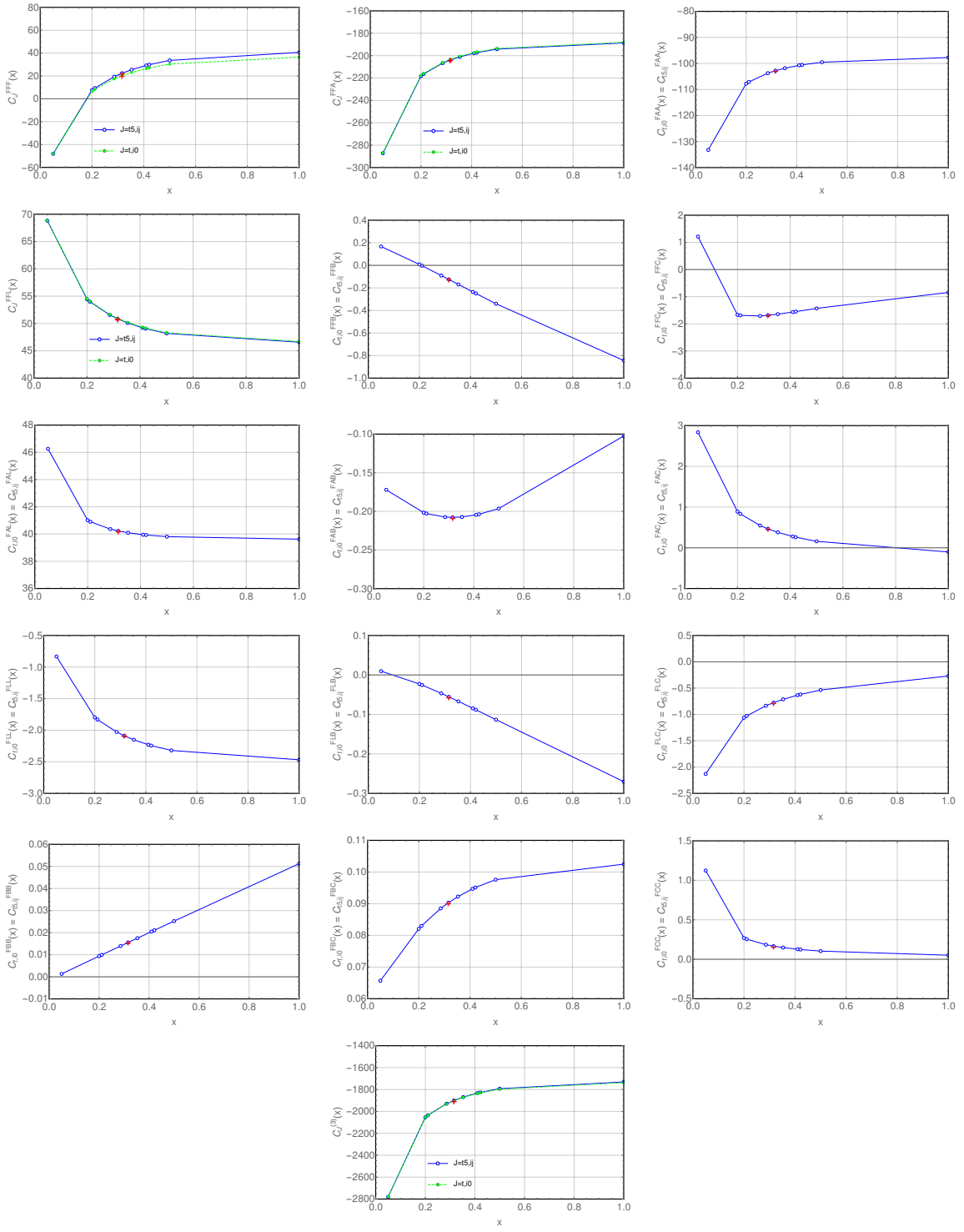
We want to mention that all contributions up to N<sup>3</sup>LO have been calculated for a general QCD gauge parameter  $\xi$  ( $\xi = 0$  corresponds to Feynman gauge) but only with the  $\xi^0, \xi^1$  terms, and the final N<sup>3</sup>LO results of the matching coefficients for the heavy flavor-changing spatial-temporal tensor and spatial-spatial axial-tensor currents are all independent of  $\xi$ , which constitutes an important check on our calculation. In the supplementary material attached to this paper, we provide the numerical results with about 30-digit precision for the color-structure components of  $\mathcal{C}_J^{(2)}(x)$  and  $\mathcal{C}_J^{(3)}(x)$  at the ten points<sup>2</sup> of  $x$  in eq. (4.11).

<sup>2</sup>It is worth mentioning that at the point  $x = 204/498$  the agreement between our three-loop numerical results of  $\mathcal{C}_{v,i}$  ( $\mathcal{C}_{v,i} \equiv \mathcal{C}_{t,i0}$ ) and the corresponding results of the  $\mathcal{C}$  in eqs. (20a)–(20c) in ref. [9] is limited to a precision of only about two significant digits.



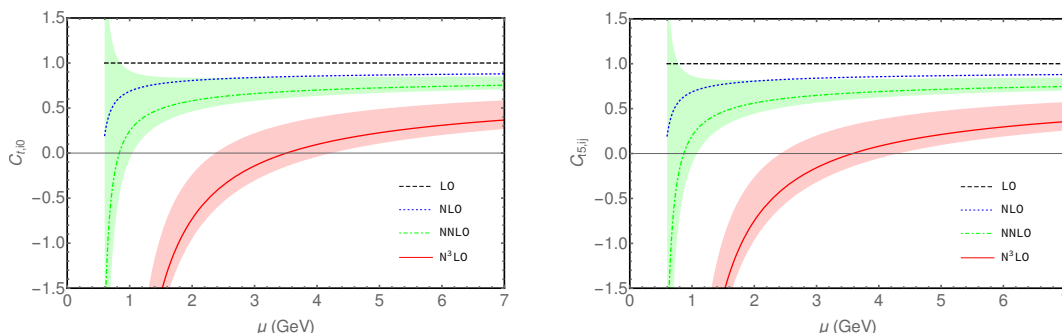
**Figure 3.** The two-loop coefficient  $\mathcal{C}_J^{(2)}(x)$  ( $J \in \{(t, i0), (t5, ij)\}$ ) with  $n_l = 3, n_b = n_c = 1$  and its five color-structure components as functions of the heavy quark mass ratio  $x$  within the range of  $x \in (0, 1]$ . The blue hollow dots and green solid dots on the curves represent sample points at ten different values of  $x$  in eq. (4.11). The red crosses on the curves correspond to the results at the physical heavy quark mass ratio with  $x = x_0 = 150/475$ .

Choosing our results at the ten points of  $x$  as sample data points, we plot the dependence of  $\mathcal{C}_J^{(n)}(x)$  ( $J \in \{(t, i0), (t5, ij)\}, n \in \{2, 3\}$ ) with  $n_l = 3, n_b = n_c = 1$  and its color-structure components on the heavy quark mass ratio  $x$  within the range of  $x \in (0, 1]$  in figure 3 and figure 4, from which one can see  $\mathcal{C}_J^{(n)}(x)$  and its color-structure components have a relatively weak  $x$ -dependence in the physical region, indicating that the  $B_c^*$  meson might be viewed both as a heavy-heavy meson and as a heavy-light meson [47, 109]. From eq. (6.3) and figures 3 and 4, we find the dominant contributions in  $\mathcal{C}_J^{(2)}(x)$  and  $\mathcal{C}_J^{(3)}(x)$  come from the components corresponding to the color structures  $C_F^2, C_F C_A, C_F^2 C_A$  and  $C_F C_A^2$ , while the contributions from the bottom and charm quark loops are negligible. We also find almost all color-structure components of  $\mathcal{C}_{t5,ij}^{(n)}(x)$  are exactly equal to the corresponding components of  $\mathcal{C}_{t,i0}^{(n)}(x)$ , except that  $|\mathcal{C}_{t5,ij}^{FFF}(x) - \mathcal{C}_{t,i0}^{FFF}(x)| \gtrsim |\mathcal{C}_{t5,ij}^{FF}(x) - \mathcal{C}_{t,i0}^{FF}(x)| > |\mathcal{C}_{t5,ij}^{FFA}(x) - \mathcal{C}_{t,i0}^{FFA}(x)| \gtrsim |\mathcal{C}_{t5,ij}^{FFL}(x) - \mathcal{C}_{t,i0}^{FFL}(x)| \gtrsim 0$ .



**Figure 4.** The same as figure 3, but for the three-loop coefficient  $C_J^{(3)}(x)$  ( $J \in \{(t, i0), (t5, ij)\}$ ) with  $n_t = 3, n_b = n_c = 1$  and its fifteen color-structure components.





**Figure 5.** The renormalization scale  $\mu$  dependence of the matching coefficients  $\mathcal{C}_{t,i0}$  and  $\mathcal{C}_{t5,ij}$  at LO, NLO, NNLO and N<sup>3</sup>LO accuracy. The central values of the matching coefficients are calculated inputting the physical values with  $\mu_f = 1.2$  GeV,  $m_b = 4.75$  GeV and  $m_c = 1.5$  GeV. The error bands come from the variation of  $\mu_f$  between 2 and 0.4 GeV.

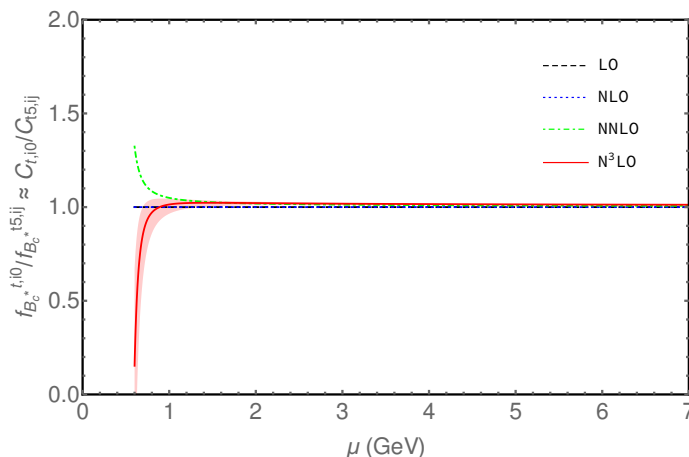
The values of  $\mathcal{C}_J^{(n)}(x)$  and its color-structure components for  $x > 1$  can be obtained by employing the invariance [2–6, 8, 9, 11] of  $\mathcal{C}_J$  under the exchange  $m_b \leftrightarrow m_c$  meanwhile  $n_b \leftrightarrow n_c$ . Furthermore, we have checked that both  $\mathcal{C}_J^{(2)}(x)$  and  $\mathcal{C}_J^{(3)}(x)$  for  $J \in \{(v, i), (t, i0), (t5, ij)\}$  are indeed approximately linear with respect to  $\frac{1}{x}$  in the range of  $\frac{1}{x} \in [2, 4]$  as the description for the  $\mathcal{C}^{(3)}(r)$  in figure 3 in ref. [9]. However, it's worth noting that the linear approximation may not be applicable to other values of  $x$  within the range of  $x \in (0, \infty)$ .

We consider the ratio of the  $B_c^*$  decay constant involving the spatial-temporal tensor current to that involving the spatial-spatial axial-tensor current, from which the wave function at the origin is eliminated [5, 8, 9, 11, 60, 108, 110, 111] so that the ratio of the physical decay constants is approximately equal to the ratio of the nonphysical matching coefficients [42], i.e.

$$\frac{f_{B_c^*}^{t,i0}}{f_{B_c^*}^{t5,ij}} \approx \frac{\mathcal{C}_{t,i0} \times |\Psi_{B_c^*}(0)|}{\mathcal{C}_{t5,ij} \times |\Psi_{B_c^*}(0)|} \approx \frac{\mathcal{C}_{t,i0}}{\mathcal{C}_{t5,ij}}. \quad (6.4)$$

Throughout our calculation in the remaining part of this section, we will expand both the matching coefficients and the ratio of the matching coefficients (decay constants) in power series of  $\alpha_s^{(n)}(\mu)$  and study the numerical results up to  $\mathcal{O}(\alpha_s^3)$  for them. Setting  $\mu_f = 1.2$  GeV,  $\mu = \mu_0 = 3$  GeV,  $m_b = 4.75$  GeV,  $m_c = 1.5$  GeV, the  $\alpha_s$ -expansions of eq. (6.1) and eq. (6.4) reduce to

$$\begin{aligned} \mathcal{C}_{t,i0} &= 1 - 2.067273 \frac{\alpha_s^{(3)}(\mu_0)}{\pi} - 29.29166 \left( \frac{\alpha_s^{(3)}(\mu_0)}{\pi} \right)^2 - 1689.867 \left( \frac{\alpha_s^{(3)}(\mu_0)}{\pi} \right)^3 + \mathcal{O}(\alpha_s^4), \\ \mathcal{C}_{t5,ij} &= 1 - 2.067273 \frac{\alpha_s^{(3)}(\mu_0)}{\pi} - 31.42525 \left( \frac{\alpha_s^{(3)}(\mu_0)}{\pi} \right)^2 - 1696.499 \left( \frac{\alpha_s^{(3)}(\mu_0)}{\pi} \right)^3 + \mathcal{O}(\alpha_s^4), \\ \frac{f_{B_c^*}^{t,i0}}{f_{B_c^*}^{t5,ij}} &\approx \frac{\mathcal{C}_{t,i0}}{\mathcal{C}_{t5,ij}} = 1 + 2.133589 \left( \frac{\alpha_s^{(3)}(\mu_0)}{\pi} \right)^2 + 11.04305 \left( \frac{\alpha_s^{(3)}(\mu_0)}{\pi} \right)^3 + \mathcal{O}(\alpha_s^4). \end{aligned} \quad (6.5)$$



**Figure 6.** The renormalization scale  $\mu$  dependence of the matching coefficient (decay constant) ratio at LO, NLO, NNLO and  $N^3$ LO accuracy. The central values are calculated inputting the physical values with  $\mu_f = 1.2$  GeV,  $m_b = 4.75$  GeV and  $m_c = 1.5$  GeV. The error band comes from the variation of  $\mu_f$  between 7 and 0.4 GeV.

	LO	NLO	NNLO	$N^3$ LO
$C_{t,i0}$	1	$0.83875_{+0}^{-0.04086+0.00753-0.01927}_{-0.06738-0.00790+0.03251}$	$0.66053_{+0.17632-0.16857-0.01477-0.03155}^{-0.08198+0.09301+0.01324+0.02563}$	$-0.14143_{+0.36305-1.41702-0.02078-0.15050}^{-0.16360+0.50840+0.01790+0.08745}$
$C_{t5,ij}$	1	$0.83875_{+0}^{-0.04086+0.00753-0.01927}_{-0.06738-0.00790+0.03251}$	$0.64755_{+0.17632-0.18168-0.01552-0.02879}^{-0.08198+0.09875+0.01392+0.02378}$	$-0.15756_{+0.35888-1.41796-0.02179-0.14861}^{-0.16166+0.51277+0.01881+0.08660}$

**Table 1.** The values of the matching coefficients  $C_{t,i0}$  and  $C_{t5,ij}$  up to  $N^3$ LO. The central values of the matching coefficients are calculated inputting the physical values with  $\mu_f = 1.2$  GeV,  $\mu = \mu_0 = 3$  GeV,  $m_b = 4.75$  GeV and  $m_c = 1.5$  GeV. The uncertainties are estimated by varying  $\mu_f$  from 2 to 0.4 GeV,  $\mu$  from 7 to 1.5 GeV,  $m_b$  from 5.25 to 4.25 GeV,  $m_c$  from 2 to 1 GeV, respectively.

	LO	NLO	NNLO	$N^3$ LO
$\frac{f_{B_c^{t,i0}}^*}{f_{B_c^{t5,ij}}^*} \approx \frac{C_{t,i0}}{C_{t5,ij}}$	1	1	$1.01298_{+0.01312+0.00074-0.00276}^{-0.000575-0.00068+0.00186}$	$1.01822_{+0.00417+0.00481+0.00124-0.00267}^{-0.00670-0.00559-0.00111+0.00143}$

**Table 2.** The same as table 1, but for the ratio of the matching coefficients (decay constants), with the uncertainties in the first column estimated by varying  $\mu_f$  from 7 to 0.4 GeV.

With the values of  $\alpha_s^{(n_i=3)}(\mu)$  calculated (see section 5), we investigate the QCD renormalization scale  $\mu$  dependence of the matching coefficients and the matching coefficient (decay constant) ratio at LO, NLO, NNLO and  $N^3$ LO accuracy in figure 5 and figure 6, respectively. The middle lines correspond to the choice of  $\mu_f = 1.2$  GeV for the NRQCD factorization scale, and the upper and lower edges of the error bands correspond to  $\mu_f = 0.4$  GeV and  $\mu_f = 2(7)$  GeV, respectively. Furthermore, we present our precise numerical results of the matching coefficients and the matching coefficient (decay constant) ratio at LO, NLO, NNLO and  $N^3$ LO accuracy in table 1 and table 2, respectively, where the uncertainties from  $\mu_f$ ,  $\mu$ ,  $m_b$  and  $m_c$  are included.

From eq. (6.5), the figures 5 and 6, as well as the tables 1 and 2, we have the following points:

- (1) Both the matching coefficients  $\mathcal{C}_{t,i0}$  and  $\mathcal{C}_{t5,ij}$  are nonconvergent up to N<sup>3</sup>LO; especially, the third order corrections to them are very large. Besides, the N<sup>3</sup>LO corrections to the matching coefficients also exhibit very strong dependence on both the QCD renormalization scale  $\mu$  and the NRQCD factorization scale  $\mu_f$ .
- (2) Due to a large cancellation at  $\mathcal{O}(\alpha_s^3)$  between the two nonconvergent matching coefficients, the matching coefficient ratio is becoming convergent,<sup>3</sup> or well-behaved say conservatively, up to N<sup>3</sup>LO. Then by the approximation in eq. (6.4), we obtain the convergent decay constant ratio  $f_{B_c^*}^{t,i0}/f_{B_c^*}^{t5,ij}$  up to N<sup>3</sup>LO. Note that each physical decay constant is also convergent (see ref. [11]).
- (3) The N<sup>3</sup>LO QCD correction to the ratio of the matching coefficients (decay constants) is almost independent of both  $\mu_f$  and  $\mu$ , which verifies the correctness of our calculation for the decay constant ratio based on eq. (6.4) (also see related discussion in ref. [11]).
- (4) From the tables 1 and 2, we also see the uncertainties of the matching coefficients and the matching coefficient (decay constant) ratio arising from the errors in the heavy quark masses  $m_b$  and  $m_c$  are relatively small compared to those resulting from the errors in  $\mu_f$  and  $\mu$  (also see ref. [7]).
- (5) For the  $B_c^*$  decay constants involving different heavy flavor-changing currents, we predict  $f_{B_c^*}^{v,i} = f_{B_c^*}^{t,i0} > f_{B_c^*}^{t5,ij}$ .

## 7 Summary

In this paper, we elaborate on the three-loop calculations of the NRQCD current renormalization constants (and corresponding anomalous dimensions), matching coefficients, (the ratio of) decay constants for the heavy flavor-changing spatial-temporal tensor  $(t, i0)$  current and spatial-spatial axial-tensor  $(t5, ij)$  current coupled to the  $S$ -wave vector  $c\bar{b}$  meson  $B_c^*$  within the NRQCD framework. Although the matching coefficients for both  $(t, i0)$  and  $(t5, ij)$  currents are nonconvergent, we can obtain the convergent ratio of  $B_c^*$  decay constants between  $(t, i0)$  and  $(t5, ij)$  currents up to N<sup>3</sup>LO. Our prediction for (the ratio of)  $B_c^*$  decay constants involving (axial-)tensor currents, along with the experiment, is useful to determine the fundamental parameters in particle physics and is also of interest in beyond the Standard Model studies.

As a byproduct, we obtain the three-loop finite term for the ratio of the QCD heavy flavor-changing tensor current renormalization constant in the OS scheme to that in the  $\overline{\text{MS}}$  scheme, which is a key ingredient to obtain matching coefficients for various heavy flavor-changing (axial-)tensor currents coupled to the  $S$ -wave and  $P$ -wave  $c\bar{b}$  mesons. And the study for  $P$ -wave  $c\bar{b}$  mesons is underway.

<sup>3</sup>In this paper, we use ‘convergence’ and ‘convergent’ to mean that the higher-order terms in the perturbation series up to  $\mathcal{O}(\alpha_s^3)$  are smaller than or comparable to the lower-order terms in size within the physical values of  $\alpha_s$ . Therefore, the meanings of ‘convergence’ and ‘convergent’ in this paper are somewhat different from the mathematical definitions of ‘convergence’ and ‘convergent’, respectively.

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