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Gluon fragmentation into $^3P_J^{[1,8]}$ quark pair and test of NRQCD factorization at two-loop level

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ABSTRACT: The next-to-leading order (NLO) ($\mathcal{O}(\alpha_s^3)$) corrections for gluon fragmentation functions to a heavy quark-antiquark pair in $^3P_J^{[1,8]}$ states are calculated within the NRQCD factorization. We use the integration-by-parts reduction and differential equations to semi-analytically calculate the fragmentation functions in full-QCD, and find that infrared divergences can be absorbed by the NRQCD long distance matrix elements. Thus, the NRQCD factorization conjecture is verified at two-loop level via a physical process, which is free of artificial ultraviolet divergences. Through the matching procedure, infrared-safe short distance coefficients and $\mathcal{O}(\alpha_s^2)$ perturbative NRQCD matrix elements $\langle \mathcal{O}^{^3P_J^{[1,8]}}(^3S_1^{[8]}) \rangle$ are obtained simultaneously. The NLO short distance coefficients are found to have significant corrections comparing with the LO ones.

KEYWORDS: NLO Computations, QCD Phenomenology

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Contents

1	Introduction	1
2	Full-QCD calculation	3
2.1	Definition	3
2.2	LO FFs	5
2.3	NLO FFs	6
2.4	Verification of the NRQCD factorization at two-loop level	8
3	Matching procedure and the SDCs	9
4	Numerical results and discussion	11
A	Operator renormalization integrals	17

1 Introduction

Heavy quarkonium provides an ideal physical system to explore the strong interaction, as the heavy quarkonium production contains both perturbative and non-perturbative effects in QCD. Non-relativistic QCD (NRQCD) factorization [1] is the most widely used theory to explain quarkonium production so far. When transverse momentum p_T of the produced quarkonium is large, fragmentation mechanism dominates and factorization is easier to hold, because long-distance interactions between quarkonium and initial-state particles are suppressed then.

Inclusive production differential cross section of a specific hadron H at high p_T can be calculated in collinear factorization [2],

$$d\sigma_{A+B \rightarrow H(p_T)+X} = \sum_i d\hat{\sigma}_{A+B \rightarrow i(p_T/z)+X'} \otimes D_{i \rightarrow H}(z, \mu) + \mathcal{O}(1/p_T^2), \quad (1.1)$$

where i sums over all quarks and gluons, z is the light-cone momentum fraction carried by H with respect to the parent parton i , and A and B are colliding particles whose effect should be further factorized into partons if they are hadrons. $d\hat{\sigma}_{A+B \rightarrow i(p_T/z)+X'}$ are perturbatively calculable hard parts, while $D_{i \rightarrow H}(z, \mu)$ are non-perturbative but universal fragmentation functions (FFs) describing the probability for the parton to hadronize to H with a momentum fraction z . For heavy quarkonium production, other important $\mathcal{O}(1/p_T^2)$ contributions are double parton FFs which can also be factorized [3–7]. In FFs, there is a collinear factorization scale μ dependence, which cancels with the similar dependence in hard parts perturbatively order by order, leaving physical differential cross section independent of the scale in principle. The evolution of single parton FFs with respect to μ

are controlled by the Dokshitzer-Gribov-Lipatov-Altarelli-Parisi (DGLAP) evolution equation [8–10], and similar evolution equations for double parton FFs are calculated in [4]. With the FFs at a given factorization scale $\mu = \mu_f$, they can be obtained at other scales through the evolution.

When μ_f is close to the quarkonium mass m_H , it is customary to calculate FFs via NRQCD factorization. For single parton FFs that will be considered in this paper, we have

$$D_{i \rightarrow H}(z, \mu_f) = \sum_n d_{i \rightarrow Q\bar{Q}(n)}(z, \mu_f) \langle \bar{\mathcal{O}}_n^H \rangle, \quad (1.2)$$

where $d_{i \rightarrow Q\bar{Q}(n)}$ represent the perturbatively calculable short-distance coefficients (SDCs) to produce a heavy quark-antiquark pair $Q\bar{Q}$ with quantum number n , and $\langle \bar{\mathcal{O}}_n^H \rangle$ are normalized long-distance matrix elements (LDMEs).¹ The quantum number is usually expressed in spectroscopic notation $n = {}^{2S+1}L_J^{[c]}$, with $c = 1, 8$ respectively for color-singlet state and color-octet state. According to the velocity scaling rule [1], $\langle \bar{\mathcal{O}}_n^H \rangle$ is usually suppressed if L is too large. Therefore, the most important states for phenomenological purpose are S -wave and P -wave states. Because LDMEs are supposed to be process independent, they can be determined by fitting experimental data, while the SDCs can be calculated perturbatively through the matching procedure.

All the SDCs for single parton FFs to both S -wave and P -wave states up to $\mathcal{O}(\alpha_s^2)$ are available [11–21] (see [22, 23] for a summary and comparison). At α_s^3 order, the leading order (LO) SDCs of $g \rightarrow Q\bar{Q}({}^3S_1^{[1]}) + X$ and $g \rightarrow Q\bar{Q}({}^1P_1^{[1]}) + X$ are calculated separately in refs. [12, 24–27] and ref. [28], and the next-to-leading order (NLO) SDCs of $g \rightarrow Q\bar{Q}({}^1S_0^{[1,8]}) + X$ have also been calculated in refs. [29–31] recently. To perform phenomenological analysis at a consistent precision, such as that for J/ψ or χ_{cJ} production, at this order, one also needs the NLO SDCs of $g \rightarrow Q\bar{Q}({}^3P_J^{[1,8]}) + X$ and the next-to-next-to-leading order (NNLO) SDCs of $g \rightarrow Q\bar{Q}({}^3S_1^{[8]}) + X$. In this paper, we will focus on the former.

Another motivation to calculate the NLO FFs for processes $g \rightarrow Q\bar{Q}({}^3P_J^{[1,8]}) + X$ is to test the NRQCD factorization conjecture at two-loop level with a physical process. More explicitly, for the processes $g \rightarrow Q\bar{Q}({}^3P_J^{[1]}) + X$, the infrared (IR) divergences in the LO full-QCD FFs are absolutely absorbed in the $\mathcal{O}(\alpha_s)$ perturbative NRQCD matrix element (PME) $\langle \mathcal{O}^{3P_J^{[1]}}({}^3S_1^{[8]}) \rangle_{\text{LO}}$ [18, 22], which verified the factorization conjecture at one-loop level. At two-loop level, the IR divergences in the NLO full-QCD FFs for processes $g \rightarrow Q\bar{Q}({}^3P_J^{[1,8]}) + X$ should be absorbed in the $\mathcal{O}(\alpha_s^2)$ PME $\langle \mathcal{O}^{3P_J^{[1,8]}}({}^3S_1^{[8]}) \rangle_{\text{NLO}}$, which can serve as a test of the NRQCD factorization conjecture at this level. The similar test at two-loop level exists in literature [32–35] but within the framework of the eikonal approximation for infrared (IR) divergences. The eikonal approximation introduces artificial ultraviolet (UV) divergences which makes the extraction of IR divergences beyond one-loop level highly nontrivial. Because we do not use the eikonal approximation, the extraction of IR divergences in our case is straightforward.

¹ $\langle \bar{\mathcal{O}}_n^H \rangle$ can be related to the original definition of NRQCD LDME $\langle \mathcal{O}_n^H \rangle$ [1] by the following rules. They are the same if n is color-octet, and $\langle \bar{\mathcal{O}}_n^H \rangle = \langle \mathcal{O}_n^H \rangle / (2N_c)$ if n is color-singlet.

In this paper, we aim at calculating NLO SDCs of $g \rightarrow Q\bar{Q}({}^3P_J^{[1,8]}) + X$ to sufficiently high precision using similar methods in our previous paper [29]. The rest of the paper is organized as follows. In section 2, we calculate the process to LO and NLO in full-QCD. The calculation method is very similar to that in ref. [29]. A small improvement is the computation of operator renormalization shown in section 2.3 and appendix. A. We argue that the NRQCD factorization at two-loop level without the eikonal approximation is verified in section 2.4. The $\mathcal{O}(\alpha_s^2)$ perturbative NRQCD matrix elements (PMEs) $\langle \mathcal{O}^{3P_J^{[1]}}({}^3S_1^{[8]}) \rangle_{\text{NLO}}$ and $\langle \mathcal{O}^{3P_J^{[8]}}({}^3S_1^{[8]}) \rangle_{\text{NLO}}$ are matched, and the corresponding IR-safe SDCs are obtained simultaneously in section 3. Our results will be discussed in section 4.

2 Full-QCD calculation

2.1 Definition

The FF of a gluon to a hadron (quarkonium) was defined by Collins and Soper [36],

$$D_{g \rightarrow H}(z, \mu_0) = \frac{-g_{\mu\nu} z^{D-3}}{2\pi P_g^+ (N_c^2 - 1)(D-2)} \int_{-\infty}^{+\infty} dx^- e^{-iP_g^+ x^-} \times \langle 0 | G_c^{+\mu}(0) \mathcal{E}^\dagger(0, 0, \mathbf{0}_\perp)_{cb} \mathcal{P}_{H(P)} \mathcal{E}(0, x^-, \mathbf{0}_\perp)_{ba} G_a^{+\nu}(0, x^-, \mathbf{0}_\perp) | 0 \rangle, \quad (2.1)$$

where $G_c^{\mu\nu}$ is the gluon field-strength operator, P and P_g are respectively the momenta of the produced hadron H and the initial-state fragmenting gluon g , and $z = P^+/P_g^+$ is the ratio of momenta along the “+” direction. It is convenient to choose the frame in which the hadron has zero transverse momentum, $P = (zP_g^+, M^2/(2zP_g^+), \mathbf{0}_\perp)$, with $P^2 = 2P^+P^- = M^2$. The projection operator $\mathcal{P}_{H(P)}$ is defined by

$$\mathcal{P}_{H(P)} = \sum_X |H(P) + X\rangle \langle H(P) + X|, \quad (2.2)$$

where X sums over all unobserved particles. The gauge link $\mathcal{E}(x^-)$ is an eikonal operator that involves a path-ordered exponential of gluon field operators along a light-like path,

$$\mathcal{E}(0, x^-, \mathbf{0}_\perp)_{ba} = \text{P exp} \left[+ig_s \int_{x^-}^{\infty} dz^- A^+(0, z^-, \mathbf{0}_\perp) \right]_{ba}, \quad (2.3)$$

where $g_s = \sqrt{4\pi\alpha_s}$ is the QCD coupling constant and $A^\mu(x)$ is the matrix-valued gluon field in the adjoint representation: $[A^\mu(x)]_{ac} = if^{abc} A_b^\mu(x)$.

Since the SDCs d ’s in the NRQCD factorization formula (1.2) are independent of the final state H , we can replace H by on-shell $Q\bar{Q}$ states to extract $d_{i \rightarrow Q\bar{Q}[n]}$ through the matching procedure [See below (3.1) and (3.6)].

Choosing the factorization scale $\mu_0 \sim 2m_Q$ with m_Q as the heavy quark mass, we can calculate FF for $g \rightarrow Q\bar{Q}[n]$ in the full-QCD in the Feynman gauge. All the Feynman rules are the same as those of QCD except for the addition of rules for the eikonal lines which can be found in ref. [29]. Amplitudes of all the Feynman diagrams are denoted as $\mathcal{M}_{\lambda_Q \lambda_{\bar{Q}} \lambda_i}(q)$, where λ_Q and $\lambda_{\bar{Q}}$ are respectively the spins of the produced on-shell heavy quark and heavy antiquark, λ_i ($i = 1, 2, \dots$) are the spins of the initial-state virtual gluon

or final-state unobserved light particles, and q is the heavy quark momentum in the rest frame of heavy quark pair. To project the free $Q\bar{Q}$ pair to the state of spin-triplet and specific color, one can multiply amplitudes by projection operators and obtain

$$\mathcal{M}_{\lambda_i}^\alpha(q) = \text{Tr} \left[\Gamma_c \Gamma_\lambda^\alpha \overline{\mathcal{M}}_{\lambda_Q \lambda_{\bar{Q}} \lambda_i}(q) \right], \quad (2.4)$$

where $\overline{\mathcal{M}}_{\lambda_Q \lambda_{\bar{Q}} \lambda_i}$ denotes amplitudes with external heavy-(anti)quark spinors removed for $\mathcal{M}_{\lambda_Q \lambda_{\bar{Q}} \lambda_i}$ and the projection operators are defined as

$$\begin{aligned} \Gamma_{c=1} &= \frac{1}{\sqrt{N_c}}, \\ \Gamma_{c=8} &= \frac{\sqrt{2}T^a}{\sqrt{N_c^2 - 1}}, \\ \Gamma_\lambda^\alpha &= \frac{1}{\sqrt{2E(E + m_Q)}} (\not{p} - m_Q) \frac{2E - \not{P}}{4E} \gamma^\alpha \frac{2E + \not{P}}{4E} (\not{p} - m_Q), \end{aligned} \quad (2.5)$$

where $p = P/2 + q$ and $\bar{p} = P/2 - q$ are the momenta respectively of the Q and $\bar{Q}$, m_Q is the mass of the heavy quark, and E is the energy of the quark Q or $\bar{Q}$ in the rest frame of the $Q\bar{Q}$ pair. With the on-shell conditions of the quark Q and $\bar{Q}$, we have

$$P \cdot q = 0, \quad P^2 = 4E^2 = 4(m_Q^2 - q^2). \quad (2.6)$$

To project the amplitude on a P-wave state, we also need to take the derivation over q^β ,

$$\mathcal{M}_{\lambda_i}^{\alpha\beta} = \frac{\partial}{\partial q^\beta} \mathcal{M}_{\lambda_i}^\alpha(q)|_{q \rightarrow 0}. \quad (2.7)$$

By summing over the spins and the colors of the initial-state and the final-state particles, we get the squared amplitude

$$A_J = \frac{N_{\text{CS}}}{N_J} \sum P_J^{\alpha\alpha'\beta\beta'} \text{Re} \left[\mathcal{M}_{\lambda_i}^{\alpha\beta} \mathcal{M}_{\lambda_i}^{*\alpha'\beta'} \right], \quad (2.8)$$

where $N_{\text{CS}} = \frac{z^{D-2}}{(N_c^2 - 1)(D - 2)}$ with $D = 4 - 2\epsilon$ being the space-time dimension. For different J , N_J and $P_J^{\alpha\alpha'\beta\beta'}$ are respectively

$$N_J = \begin{cases} 1, & \text{for } J = 0 \\ \frac{1}{2}(D - 1)(D - 2), & \text{for } J = 1 \\ \frac{1}{2}(D + 1)(D - 2), & \text{for } J = 2 \\ (D - 1)^2, & \text{for } \sum_J \end{cases}, \quad (2.9)$$

and

$$P_J^{\alpha\alpha'\beta\beta'} = \begin{cases} \frac{1}{D - 1} I^{\alpha\beta} I^{\alpha'\beta'}, & \text{for } J = 0 \\ \frac{1}{2} (I^{\alpha\alpha'} I^{\beta\beta'} - I^{\alpha\beta'} I^{\alpha'\beta}), & \text{for } J = 1 \\ \frac{1}{2} (I^{\alpha\alpha'} I^{\beta\beta'} - I^{\alpha\beta'} I^{\alpha'\beta}) - \frac{1}{D - 1} I^{\alpha\beta} I^{\alpha'\beta'}, & \text{for } J = 2 \\ I^{\alpha\alpha'} I^{\beta\beta'}, & \text{for } \sum_J \end{cases}, \quad (2.10)$$

Figure 1. One of the two Feynman diagrams representing a gluon fragmenting into $Q\bar{Q}[{}^3P_0^{[1]}]$ at the LO in α_s . Another diagram can be obtained by permuting the heavy quark and anti-quark.

where

$$I^{\alpha\beta} = -g^{\alpha\beta} + \frac{P^\alpha P^\beta}{P^2}. \quad (2.11)$$

Then, the fragmentation functions in the full-QCD can be denoted as

$$D \left[g \rightarrow Q\bar{Q}({}^3P_J^{[1,8]}) \right] = \int d\Phi A_J. \quad (2.12)$$

Here, $d\Phi$ is the final-state phase space,

$$d\Phi = \frac{P^+}{z^2 S} \delta \left(\frac{1-z}{z} P^+ - \sum_i k_i^+ \right) \prod_i \frac{d^D k_i}{(2\pi)^{D-1}} \delta_+(k_i^2), \quad (2.13)$$

where S is the symmetry factor for the final-state particles and k_i 's are momenta of the final-state light particles. In the rest of the paper, we will take the case of $g \rightarrow Q\bar{Q}({}^3P_0^{[1]}) + X$ as an explicit example to explain our calculations.

2.2 LO FFs

The Feynman diagrams representing a gluon fragmenting into $Q\bar{Q}[{}^3P_0^{[1]}]$ at the LO in α_s are shown in figure 1. These diagrams can be easily calculated, and the obtained FF can be expressed as

$$D_{\text{LO}} \left[g \rightarrow Q\bar{Q}({}^3P_0^{[1]}) \right] = \frac{N_{\text{LO}}}{1-\epsilon} \left[(1-z)^{-\epsilon} f_1(z) + (1-z)^{-1-2\epsilon} f_2(z) \right], \quad (2.14)$$

where

$$N_{\text{LO}} = \frac{\alpha_s^2}{(D-1)N_c m_Q^5} \left(\frac{\pi \mu_r^2}{m_Q^2} \right)^\epsilon \Gamma(1+\epsilon) \quad (2.15)$$

and

$$\begin{aligned} f_1(z) &= \frac{3(5-3z)}{\epsilon} + \frac{3}{2}(3z-4) - \frac{9z}{2}\epsilon, \\ f_2(z) &= \frac{3(1-z)(3z-5)}{\epsilon} + \frac{13z^3-42z^2+15z+18}{3} + 2(2z^2-2z-1)z\epsilon + \frac{2z^3\epsilon^2}{3}. \end{aligned} \quad (2.16)$$

With the following decomposition

$$(1-z)^{-1-2\epsilon} = -\frac{\delta(1-z)}{2\epsilon} + \frac{1}{[1-z]_+} - 2\epsilon \left[\frac{\ln(1-z)}{1-z} \right]_+ + \mathcal{O}(\epsilon^2), \quad (2.17)$$

Figure 2. Typical Feynman diagrams without gluon eikonal vertex for $g \rightarrow Q\bar{Q}(^3P_0^{[1]}) + X$. The gray circles in the last four diagrams represent the loop of the light particles such as the gluon, the light quarks and the ghost. The other diagrams can be obtained by permuting the heavy quark and anti-quark. The real and virtual diagrams can be obtained by cutting at different positions.

the FF can be expressed in the limit of $\epsilon \rightarrow 0$ as

$$D_{\text{LO}} \left[g \rightarrow Q\bar{Q}(^3P_0^{[1]}) \right] = N_{\text{LO}} \left(-\frac{2}{3\epsilon} \delta(1-z) + \frac{1}{3} \delta(1-z) + \frac{4}{3} \frac{z}{[1-z]_+} + \frac{1}{6} (85 - 26z)z + 3(5 - 3z) \ln(1-z) \right). \quad (2.18)$$

It is clear that there is an IR divergence in the full-QCD result. This divergence can be absorbed by the color-octet PME, which will be explained in section 3.

2.3 NLO FFs

The NLO full-QCD calculations of this process resemble closely to the NLO calculations of $g \rightarrow Q\bar{Q}(^1S_0^{[1,8]}) + X$ in ref. [29]. The relevant Feynman diagrams are shown in figure 2 and figure 3. In our calculation, we need to cut these diagrams at some specific positions. In figure 4, we give an example to show how to obtain cut diagrams for the real and the virtual corrections.

The calculation is almost the same as that in ref. [29]. Firstly we generate the amplitude from the Feynman diagrams for real or virtual corrections. Then we reduce them into linear combinations of master integrals (MIs). There are 95 MIs for real corrections and 66 MIs for virtual corrections. Fortunately, these MIs are the same as those in ref. [29], which can be calculated by using the differential equations (DEs) method [37–49]. We can estimate values of these MIs in regions $0 \sim 1/4$, $1/4 \sim 3/4$ and $3/4 \sim 1$ respectively by the

Figure 3. Typical Feynman diagrams with gluon eikonal vertex for $g \rightarrow Q\bar{Q}(^3P_0^{[1]}) + X$. The other diagrams can be obtained by permuting the heavy quark and anti-quark. The real and virtual diagrams can be obtained by cutting at different positions.

Figure 4. Real and virtual cut diagrams by cutting at different positions for the last diagrams in figure 3.

asymptotic expansions of them at $z = 0, 1/2$ and 1 . Finally, the real and virtual corrections can be expressed by asymptotic expansions in different regions as (see e.g. ref. [50])

$$\sum_s \sum_{i=0}^{n_s} (z - z_0)^s \ln^i(z - z_0) \sum_{j=0}^{\infty} I^{sij}(\epsilon) (z - z_0)^j, \quad (2.19)$$

where s are linear functions of ϵ which represent different regions, n_s are integers determined by s , and coefficients $I^{sij}(\epsilon)$ are functions of ϵ , which can be computed to sufficient high order with high precision. The sum over s implies the sum between different regions.

There are some differences between our renormalization procedure and that in ref. [29], because a $1/\epsilon$ pole is already presented at LO FF. Firstly, the on-shell renormalization constants of heavy quark field and mass (δ_2 and δ_m) should be expanded at least to $\mathcal{O}(\epsilon)$. To simplify the procedure, we use expressions with their exact ϵ dependence,

$$\delta_i = \frac{\alpha_s}{\pi} \Gamma(1 + \epsilon) \left(\frac{\pi \mu_r^2}{m_Q^2} \right)^\epsilon \hat{\delta}_i, \quad (2.20)$$

where $i = 2, m$ and

$$\begin{aligned} \hat{\delta}_2 &= -\frac{C_F}{4^{1-\epsilon}} \left(\frac{1}{\epsilon_{UV}} \frac{1+2\epsilon}{1-2\epsilon} + \frac{2}{\epsilon_{IR}} \right), \\ \hat{\delta}_m &= -\frac{C_F}{4^{1-\epsilon}} \frac{1}{\epsilon_{UV}} \frac{3-2\epsilon}{1-2\epsilon}, \end{aligned} \quad (2.21)$$

where $C_F = (N_c^2 - 1)/(2N_c)$.

Apart from the calculations of the QCD counter terms, some tricks are needed in the calculation of the operator renormalization. In the $\overline{\text{MS}}$ scheme, the operator counter term is given by

$$D_{\text{NLO}}^{\text{Operator}}(z) = -\frac{\alpha_s}{2\pi} \frac{\Gamma(1+\epsilon)}{\epsilon} \left(\frac{4\pi\mu_r^2}{\mu_0^2} \right)^\epsilon \int_z^1 \frac{dy}{y} P_{gg}(y) D_{\text{LO}}\left(\frac{z}{y}\right), \quad (2.22)$$

where μ_0 is the collinear factorization scale, and the Altarelli-Parisi splitting function $P_{gg}(z)$ is

$$P_{gg}(z) = b_0 \delta(1-z) + 2N_c \left(\frac{z}{(1-z)_+} + \frac{1-z}{z} + z(1-z) \right), \quad (2.23)$$

where $b_0 = (11N_c - 2n_f)/6$. If we take the eq. (2.18) as LO FF $D_{\text{LO}}(z)$, there will be two plus functions convolved in the integral in eq. (2.22) which is difficult to be defined and calculated. However, we can take eq. (2.14) as the input form of the $D_{\text{LO}}(z)$ to overcome this difficulty, with corresponding integrated results given in appendix A. In this way, operator renormalization results can be easily obtained in each region. As the real and the virtual corrections are also computed in each region, they can be summed more conveniently.

2.4 Verification of the NRQCD factorization at two-loop level

In the full-QCD calculations, the FF can be expressed by the phase space integral of the amplitude squared as shown in eq. (2.12). Before taking the derivative over q , the amplitude squared at $\mathcal{O}(q^2)$ can be expressed as

$$A(q, q') = (q \cdot q') A_1 + \frac{(q \cdot n)(q' \cdot n)}{(P \cdot n)^2} A_2, \quad (2.24)$$

where n is the light-like vector that defines the direction of the eikonal line of the fragmentation function. Because NRQCD LDMEs should be independent of the direction of the eikonal line of the fragmentation function, and all the remaining IR divergences in full-QCD calculation must be absorbed into the LDMEs if NRQCD factorization is valid, there should be no IR divergences in A_2 . On the other hand, if one can show that there is no IR divergence in A_2 , then all the IR divergences in the full-QCD FF can be absorbed into the NRQCD LDMEs in principle, and the NRQCD factorization can be verified at two-loop level.

The two-loop verification of NRQCD factorization was also done in refs. [32–35], in which the eikonal approximation was used to simplify the calculation. The eikonal approximation however introduced artificial UV divergences that make the extraction of IR divergences highly nontrivial.

In this subsection, we verify the NRQCD factorization without applying the eikonal approximation. We take the process $g \rightarrow Q\bar{Q}({}^3P_J^{[1]}) + X$ with J summed as an example. To extract the part A_2 only, we use the following projection operator

$$P_{qn}^{\alpha\alpha'\beta\beta'} = I^{\alpha\alpha'} \left((D-2)I^{\beta\beta'} - (D-1)d^{\beta\beta'} \right), \quad (2.25)$$

where

$$d^{\beta\beta'} = -g^{\beta\beta'} + \frac{P^\beta n^{\beta'} + P^{\beta'} n^\beta}{P \cdot n} - \frac{P^2 n^\beta n^{\beta'}}{(P \cdot n)^2}, \quad (2.26)$$

and we get

$$P_{qn}^{\alpha\alpha'\beta\beta'} \frac{\partial}{\partial q^\beta \partial q'^{\beta'}} A(q, q') = I^{\alpha\alpha'} (D-2) \frac{1}{P^2} A_2. \quad (2.27)$$

Performing the calculations similar to those introduced in section 2, we find that all divergences are canceled out after adding the real corrections, the virtual corrections as well as the UV renormalization contributions. As a result, IR divergences in $A(q, q')$ are free of the gauge line vector n . Thus the NRQCD factorization is verified to hold at the two-loop level, which is consistent with the observation in refs. [32–35].

3 Matching procedure and the SDCs

As SDCs are independent of the specifics of the hadronic states, we can match the $\mathcal{O}(\alpha_s^2)$ PME from the divergences in full-QCD FFs and obtain the IR-safe SDCs simultaneously, thanks to the fact that NRQCD factorization holds at this order.

For $g \rightarrow Q\bar{Q}(^3P_J^{[1,8]})$ process, the LO FF can be expressed by

$$\begin{aligned} D_{\text{LO}} [g \rightarrow Q\bar{Q}(^3P_J^{[1,8]})] &= d_{\text{LO}} [g \rightarrow Q\bar{Q}(^3P_J^{[1,8]})] \langle \mathcal{O}^{^3P_J^{[1,8]}}(^3P_J^{[1,8]}) \rangle_{\text{LO}} \\ &\quad + d_{\text{LO}} [g \rightarrow Q\bar{Q}(^3S_1^{[8]})] \langle \mathcal{O}^{^3P_J^{[1,8]}}(^3S_1^{[8]}) \rangle_{\text{LO}}, \end{aligned} \quad (3.1)$$

where $\langle \mathcal{O}^{^3P_J^{[1]}}(^3P_J^{[1]}) \rangle_{\text{LO}} = \langle \mathcal{O}^{^3P_J^{[8]}}(^3P_J^{[8]}) \rangle_{\text{LO}} = 1$ is normalized. The LO SDC of gluon to $^3S_1^{[8]}$ in (3.1) has been calculated in refs. [17, 18], which is given in D -dimension by

$$d_{\text{LO}} [g \rightarrow Q\bar{Q}(^3S_1^{[8]})] = \frac{\pi\alpha_s\delta(1-z)}{(D-1)(N_c^2-1)m_Q^3}, \quad (3.2)$$

and the $\mathcal{O}(\alpha_s)$ PMEs in the $\overline{\text{MS}}$ subtraction scheme can be expressed as

$$\langle \mathcal{O}^{^3P_J^{[1]}}(^3S_1^{[8]}) \rangle_{\text{LO}} = -C_F \frac{4\alpha_s}{3\pi m_Q^2} \frac{\Gamma(1+\epsilon)}{\epsilon_{\text{IR}}} \left(\frac{4\pi\mu_r^2}{\mu_\Lambda^2} \right)^\epsilon, \quad (3.3)$$

$$\langle \mathcal{O}^{^3P_J^{[8]}}(^3S_1^{[8]}) \rangle_{\text{LO}} = -B_F \frac{4\alpha_s}{3\pi m_Q^2} \frac{\Gamma(1+\epsilon)}{\epsilon_{\text{IR}}} \left(\frac{4\pi\mu_r^2}{\mu_\Lambda^2} \right)^\epsilon, \quad (3.4)$$

where $B_F = (N_c^2 - 4)/(4N_c)$ and μ_Λ is the NRQCD factorization scale. With full-QCD FF in eq. (2.18), the D -dimension SDC $d_{\text{LO}}[g \rightarrow Q\bar{Q}(^3P_J^{[1]})]$ can be matched as

$$\begin{aligned} d_{\text{LO}} [g \rightarrow Q\bar{Q}(^3P_0^{[1]})] &= \frac{\alpha_s^2 \Gamma(1+\epsilon)}{(D-1)N_c m_Q^5} \left(\frac{\pi\mu_r^2}{m_Q^2} \right)^\epsilon \times \left(\left(\frac{1}{3} - \frac{2}{3} \ln \left(\frac{\mu_\Lambda^2}{4m_Q^2} \right) \right) \delta(1-z) \right. \\ &\quad \left. + \frac{4}{3} \frac{z}{[1-z]_+} + \frac{1}{6} (85 - 26z)z + 3(5 - 3z) \ln(1-z) \right), \end{aligned} \quad (3.5)$$

which equals the finite part of the full-QCD FF in eq. (2.18) if factorization scale is chosen as $\mu_\Lambda = 2m_Q$. We find that the IR divergence in full-QCD FF $D_{\text{LO}}[g \rightarrow Q\bar{Q}(^3P_0^{[1]})]$ is absorbed into the $\mathcal{O}(\alpha_s)$ PME $\langle \mathcal{O}^{^3P_J^{[1]}}(^3S_1^{[8]}) \rangle_{\text{LO}}$, and the SDCs are IR-safe up to LO. This result is consistent with that in ref. [22].

Similarly, $D_{\text{NLO}}[g \rightarrow Q\bar{Q}(^3P_J^{[1,8]})]$ can be expressed in the NRQCD factorization as

$$\begin{aligned} D_{\text{NLO}}[g \rightarrow Q\bar{Q}(^3P_J^{[1,8]})] &= d_{\text{NLO}}[g \rightarrow Q\bar{Q}(^3P_J^{[1,8]})] \langle \mathcal{O}^{^3P_J^{[1,8]}}(^3P_J^{[1,8]}) \rangle_{\text{LO}} \\ &\quad + d_{\text{LO}}[g \rightarrow Q\bar{Q}(^3P_J^{[1,8]})] \langle \mathcal{O}^{^3P_J^{[1,8]}}(^3P_J^{[1,8]}) \rangle_{\text{NLO}} \\ &\quad + d_{\text{NLO}}[g \rightarrow Q\bar{Q}(^3S_1^{[8]})] \langle \mathcal{O}^{^3P_J^{[1,8]}}(^3S_1^{[8]}) \rangle_{\text{LO}} \\ &\quad + d_{\text{LO}}[g \rightarrow Q\bar{Q}(^3S_1^{[8]})] \langle \mathcal{O}^{^3P_J^{[1,8]}}(^3S_1^{[8]}) \rangle_{\text{NLO}}, \end{aligned} \quad (3.6)$$

where all LO terms are known. For NLO terms, $D_{\text{NLO}}[g \rightarrow Q\bar{Q}(^3P_J^{[1,8]})]$ are calculated in this work, $\langle \mathcal{O}^{^3P_J^{[1,8]}}(^3P_J^{[1,8]}) \rangle_{\text{NLO}}$ are well-known, which have only Coulomb divergences and vanish in dimensional regularization with $\overline{\text{MS}}$ subtraction scheme, and $d_{\text{NLO}}[g \rightarrow Q\bar{Q}(^3S_1^{[8]})]$ has been calculated in refs. [18, 22], whose D -dimension form is given by

$$\begin{aligned} d_{\text{NLO}}[g \rightarrow Q\bar{Q}(^3S_1^{[8]})] &= \frac{\alpha_s^2 \Gamma(1+\epsilon)}{4(D-1)C_F m_Q^3} \left(\frac{\pi \mu_r^2}{m_Q^2} \right)^\epsilon \left[A(\mu_r) \delta(1-z) + \frac{1}{N_c} P_{gg}(z) \times \right. \\ &\quad \left. \left(\ln \left(\frac{\mu_0^2}{4m_Q^2} \right) - 1 \right) + \frac{2(1-z)}{z} - \frac{4(1-z+z^2)^2}{2} \left[\frac{\ln(1-z)}{1-z} \right]_+ \right], \end{aligned} \quad (3.7)$$

with

$$A(\mu_r) = \frac{b_0}{N_c} \left(\ln \left(\frac{\mu_r^2}{4m_Q^2} \right) + \frac{13}{3} \right) + \frac{4}{N_c^2} - \frac{\pi^2}{3} + \frac{16}{3} \ln 2. \quad (3.8)$$

Therefore, SDCs $d_{\text{NLO}}[g \rightarrow Q\bar{Q}(^3P_J^{[1,8]})]$ and PMEs $\langle \mathcal{O}^{^3P_J^{[1,8]}}(^3S_1^{[8]}) \rangle_{\text{NLO}}$ can be extracted from eq. (3.6) thanks to the fact that the former one is finite and the latter one is IR-divergent defined in $\overline{\text{MS}}$ subtraction scheme.

The $\mathcal{O}(\alpha_s^2)$ PMEs $\langle \mathcal{O}^{^3P_J^{[1,8]}}(^3S_1^{[8]}) \rangle_{\text{NLO}}$ are obtained numerically with high precision. Using PSLQ algorithm [51, 52] which is effective in recovering a relation when the input is known to only limited precision,² analytical expressions are obtained as

$$\langle \mathcal{O}^{^3P_J^{[1]}}(^3S_1^{[8]}) \rangle_{\text{NLO}} = -C_F \frac{\alpha_s^2}{27\pi^2 m_Q^2} \left(\frac{4\pi\mu_r^2}{\mu_\Lambda^2} \right)^{2\epsilon} \Gamma(1+\epsilon)^2 \left(\frac{9b_0}{\epsilon^2} + \frac{5n_f + (12\pi^2 - 47)N_c}{\epsilon} \right), \quad (3.9)$$

$$\langle \mathcal{O}^{^3P_J^{[8]}}(^3S_1^{[8]}) \rangle_{\text{NLO}} = -B_F \frac{\alpha_s^2}{27\pi^2 m_Q^2} \left(\frac{4\pi\mu_r^2}{\mu_\Lambda^2} \right)^{2\epsilon} \Gamma(1+\epsilon)^2 \left(\frac{9b_0}{\epsilon^2} + \frac{5n_f + (3\pi^2 - 47)N_c}{\epsilon} \right). \quad (3.10)$$

²The name ‘‘PSLQ’’ derives from its usage of a partial sum of squares vector and a LQ (lower-diagonal-orthogonal) matrix factorization.

Setting factorization scales $\mu_0 = \mu_\Lambda = 2m_Q$, the NLO SDC can be expressed as

$$d_{\text{NLO}} \left[g \rightarrow Q\bar{Q}({}^3P_0^{[1]}) \right] = \frac{\alpha_s^3}{3\pi N_c m_Q^5} \left(p_\delta \delta(1-z) + \sum_{i=0}^2 p_i \left[\frac{\ln^i(1-z)}{1-z} \right]_+ + p(z) \right. \\ \left. + \ln \left(\frac{\mu_r^2}{4m_Q^2} \right) b_0 d_{\text{LO}} \left[g \rightarrow Q\bar{Q}({}^3P_0^{[1]}) \right] \right), \quad (3.11)$$

where the coefficients p_δ, p_i can be fitted with the PSLQ algorithm from high-precision numerical values as follows

$$p_\delta = \frac{95 - 24\pi^2}{162} n_f + \frac{756\zeta(3) + 66\pi^2 - 1141 - 576\ln^2 2 - 1032\ln 2}{324} N_c - \frac{2(4\ln 2 - 1)}{3} \frac{1}{N_c}, \\ p_0 = -n_f + \frac{-12\pi^2 + 119 + 64\ln 2}{18} N_c + \frac{8}{3} \frac{1}{N_c}, \\ p_1 = \frac{4}{9} n_f - \frac{64}{9} N_c, \\ p_2 = -\frac{16}{3} N_c, \quad (3.12)$$

and $p(z)$ can be expressed as a piecewise function

$$p(z) = \begin{cases} \frac{63 - 8\pi^2}{36z} N_c + \sum_{i=0}^2 \sum_{j=0}^{\infty} \ln^i z (2z)^j \left(A_{ij}^f n_f + A_{ij} N_c + \frac{A_{ij}^N}{N_c} \right), & \text{for } 0 < z < \frac{1}{4} \\ \sum_{j=0}^{\infty} (2z - 1)^j \left(B_j^f n_f + B_j N_c + \frac{B_j^N}{N_c} \right), & \text{for } \frac{1}{4} \leq z \leq \frac{3}{4} \\ \sum_{i=0}^3 \sum_{j=0}^{\infty} \ln^i(1-z) (2-2z)^j \left(C_{ij}^f n_f + C_{ij} N_c + \frac{C_{ij}^N}{N_c} \right), & \text{for } \frac{3}{4} < z < 1 \end{cases}. \quad (3.13)$$

The coefficients $A_{ij}^k, B_j^k, C_{ij}^k$ can be evaluated numerically with high precision. In the Supplementary material, we give these coefficients calculated up to $j = 500$ to obtain the results with 140-digit precision at any value of z .

The SDCs of $g \rightarrow Q\bar{Q}({}^3P_J^{[1]}) + X$ with $J = 1, 2$ and $g \rightarrow Q\bar{Q}({}^3P_J^{[8]}) + X$ with sum J are calculated similarly, with results given as the Supplementary material.

4 Numerical results and discussion

In this section, we take the factorization scale $\mu_0 = \mu_\Lambda = 2m_Q$ and $N_c = 3$, and discuss the numerical results of the FFs for $c\bar{c}$ and $b\bar{b}$ respectively. We adopt the input parameters as

$$m_c = 1.67 \text{ GeV}, \quad \alpha_s(\mu_r = 2m_c) = 0.225, \quad n_f = 3 \quad (4.1)$$

for the charmonium and

$$m_b = 4.75 \text{ GeV}, \quad \alpha_s(\mu_r = 2m_b) = 0.181, \quad n_f = 4 \quad (4.2)$$

for the bottomonium, respectively. In figure 5 and figure 6, we plot the curves of LO SDCs and LO+NLO SDCs for the P -wave FFs of $c\bar{c}$ and $b\bar{b}$ respectively. The overall factors $9m_Q^5$ for color-singlet and $144m_Q^5/5$ for color-octet come from the normalization factors at NLO.

The sensitivities of LO and LO+NLO FFs with respect to the renormalization scale μ_r are illustrated in figure 5 and figure 6 with bands corresponding to μ_r varying from m_b to $4m_b$. We find that there are still large theoretical uncertainties after the NLO is revised and the uncertainties of $c\bar{c}$ are larger than those of $b\bar{b}$.

With $\mu_r = \mu_0 = \mu_\Lambda = 2m_Q$, we also provide K-factors (the ratio of LO+NLO over LO) for some special values of z in table 1 and table 2 respectively for $c\bar{c}$ and $b\bar{b}$, where we find that the K-factors are negative for most values of z .

As shown in figure 5 and figure 6, LO FFs are divergent at $z = 1$. These divergences come from the $\delta(1-z)$ and $1/[1-z]_+$ terms in eq. (3.5). Besides, the NLO FFs are negative and divergent at both $z = 0$ and $z = 1$. The leading behavior at $z \rightarrow 0$ is $1/z$, which means that the total fragmenting probability obtained by integrating the NLO FF over z from 0 to 1 is divergent. But fortunately, physical cross sections are not sensitive to the behavior at $z \rightarrow 0$ after convolving FFs with partonic hard parts, which behave as z^n in the small z region with n usually larger than 4. As shown in eq. (3.11), the divergences at $z \rightarrow 1$ behavior as $\delta(1-z)$ and plus functions with leading power $[\ln^2(1-z)/(1-z)]_+$, which comes from the expansion of $(1-z)^{-1-2\epsilon}\epsilon^{-2}$.

Obviously, the distribution of FF will not give us direct information about physical cross sections. To see the impact of the NLO results to the physical cross sections, we evaluate the n -th moments of the SDCs,

$$\int_{z_0}^1 dz z^n (d_{\text{LO}}(z) + d_{\text{NLO}}(z)) \times c^{[1,8]}, \quad (4.3)$$

where $c^{[1]} = 9m_Q^5$ and $c^{[8]} = 144m_Q^5/5$. We plot the numerical results of the K-factors in the sense of the moments integration with different z_0 and n , which are shown in figure 7 and figure 8 respectively for $c\bar{c}$ and $b\bar{b}$. We find that for the same n , the K-factors are quite steady for different z_0 , meaning that cross sections are dominated by FFs at large z . Besides, the K-factors decrease with the increase of n . Especially, the color-singlet K-factors become negative for large n . And there may be a cancellation between the LO and the NLO FFs at about 5-th or 6-th moment respectively for color-singlet $c\bar{c}$ and $b\bar{b}$ quarkonium productions. Furthermore, it is clear that though the K-factors and values of FFs at each position $z = z_0$ are quite different for $j = 0, 1, 2$ as shown in table 1, table 2, figure 5 and figure 6, they are almost the same in the sense of integration as shown in figure 7 and figure 8.

For the special case $z_0 = 0$, we can estimate the impact of NLO calculations on physical cross sections. The numerical results are shown in table 3 and table 4 respectively for $c\bar{c}$ and $b\bar{b}$. For large n , the influence of the behavior at $z \rightarrow 1$ becomes more and more prominent and the NLO correction becomes more and more significant. In addition, the K-factors of color-octet process are much larger than those of color-singlet process.

The above discussion implies that resummation at large z region may be crucial. This can be done within the framework of soft gluon factorization [53], which we leave for future study.

Figure 5. SDCs of the fragmentation functions of $g \rightarrow c\bar{c}(^3P_J^{[1,8]}) + X$ at LO and NLO. The dashed line is for $d_{\text{LO}}(z) \times c^{[1,8]}$, and the solid line is for $(d_{\text{LO}}(z) + d_{\text{NLO}}(z)) \times c^{[1,8]}$, with scale choices $\mu_r = \mu_0 = \mu_\Lambda = 2m_c$, $c^{[1]} = 9m_c^5$ for color-singlet and $c^{[8]} = 144m_c^5/5$ for color-octet. The bands are obtained by varying the renormalization scale μ_r by a factor of 2.

Figure 6. SDCs of the fragmentation functions of $g \rightarrow b\bar{b}(^3P_J^{[1,8]}) + X$ at LO and NLO. The dashed line is for $d_{\text{LO}}(z) \times c^{[1,8]}$, and the solid line is for $(d_{\text{LO}}(z) + d_{\text{NLO}}(z)) \times c^{[1,8]}$, with scale choices $\mu_r = \mu_0 = \mu_\Lambda = 2m_b$, $c^{[1]} = 9m_b^5$ for color-singlet and $c^{[8]} = 144m_b^5/5$ for color-octet. The bands are obtained by varying the renormalization scale μ_r by a factor of 2.

z	$K_0^{[1]}$	$K_1^{[1]}$	$K_2^{[1]}$	$K_J^{[8]}$
0.10	-7.412858964	-30.86132449	-99.52466722	-48.15556379
0.20	-3.534687667	-6.817537936	-24.93756227	-12.02728887
0.30	-9.190767911	-2.206595589	-9.402148919	-4.311289749
0.40	-19.39892351	-0.4988135323	-3.777820293	-1.202945419
0.50	-21.10949630	0.3129612840	-1.377915789	0.3392035223
0.60	-11.72263315	0.6932778485	-0.3623956578	1.084994296
0.70	-5.898469652	0.7414714295	-0.1018449594	1.276662180
0.80	-3.774089668	0.3461515495	-0.4817748227	0.8858438033
0.90	-4.142548165	-1.162734740	-2.057490226	-0.7016062329

Table 1. K-factors at different values of z for $c\bar{c}$. $K_j^{[c]}$ denotes the K-factor of $g \rightarrow c\bar{c}(^3P_j^{[c]}) + X$ and the symbol J means the sum of $j = 0, 1, 2$.

z	$K_0^{[1]}$	$K_1^{[1]}$	$K_2^{[1]}$	$K_J^{[8]}$
0.10	-5.746823334	-24.60770220	-79.84997431	-38.52164437
0.20	-2.644346438	-5.288432534	-19.87280192	-9.481286949
0.30	-7.198593861	-1.593420613	-7.390964744	-3.288936921
0.40	-15.40618698	-0.2304903644	-2.878388543	-0.8000547312
0.50	-16.79362533	0.4131713893	-0.9577973668	0.4303450620
0.60	-9.270458907	0.7101131977	-0.1500652088	1.020569545
0.70	-4.605946556	0.7391584729	0.05021547782	1.164601499
0.80	-2.912955012	0.4091668085	-0.2661028908	0.8383434112
0.90	-3.226904801	-0.8227021717	-1.548987722	-0.4556362309

Table 2. K-factors at different values of z for $b\bar{b}$. $K_j^{[c]}$ denotes the K-factor of $g \rightarrow b\bar{b}(^3P_j^{[c]}) + X$ and the symbol J means the sum of $j = 0, 1, 2$.

Figure 7. The K-factors calculated by the integration results with eq. (4.3) for different z_0 and n .

Figure 8. The K-factors calculated by the integration results with eq. (4.3) for different z_0 and n .

state	SDCs*c ^[1,8]	z^2	z^4	z^6	z^8	z^{10}
$^3P_0^{[1]}$	LO	−0.198211	−0.209792	−0.219358	−0.227548	−0.234726
	LO+NLO	−0.128770	−0.0372559	0.0426356	0.115174	0.182351
	K-factor	0.649662	0.177585	−0.194365	−0.506153	−0.776869
$^3P_1^{[1]}$	LO	−0.133031	−0.158143	−0.176190	−0.190342	−0.202003
	LO+NLO	−0.0881088	−0.0209104	0.0442083	0.107158	0.167758
	K-factor	0.662316	0.132225	−0.250913	−0.562979	−0.830473
$^3P_2^{[1]}$	LO	−0.164250	−0.182375	−0.196234	−0.207512	−0.217045
	LO+NLO	−0.110276	−0.0319328	0.0398160	0.107090	0.170690
	K-factor	0.671393	0.175094	−0.202901	−0.516069	−0.786429
$^3P_J^{[8]}$	LO	−0.157617	−0.177344	−0.192122	−0.204015	−0.213995
	LO+NLO	−0.276873	−0.222739	−0.168856	−0.115754	−0.0639081
	K-factor	1.75662	1.25597	0.878899	0.567379	0.298643

Table 3. Moments and K-factors of $c\bar{c}$ SDCs.

state	SDCs*c ^[1,8]	z^2	z^4	z^6	z^8	z^{10}
$^3P_0^{[1]}$	LO	−0.128268	−0.135763	−0.141953	−0.147253	−0.151898
	LO+NLO	−0.0827831	−0.0358580	0.00517161	0.0424728	0.0770533
	K-factor	0.645389	0.264122	−0.0364318	−0.288434	−0.507269
$^3P_1^{[1]}$	LO	−0.0860886	−0.102339	−0.114018	−0.123176	−0.130722
	LO+NLO	−0.0569318	−0.0238177	0.00883562	0.0406816	0.0715000
	K-factor	0.661317	0.232733	−0.0774933	−0.330272	−0.546961
$^3P_2^{[1]}$	LO	−0.106291	−0.118021	−0.126989	−0.134287	−0.140456
	LO+NLO	−0.0710246	−0.0314452	0.00503849	0.0393863	0.0719469
	K-factor	0.668207	0.266438	−0.0396766	−0.293299	−0.512237
$^3P_J^{[8]}$	LO	−0.101999	−0.114765	−0.124328	−0.132024	−0.138483
	LO+NLO	−0.157138	−0.130328	−0.103237	−0.0763266	−0.0499276
	K-factor	1.54058	1.13561	0.830358	0.578126	0.360533

Table 4. Moments and K-factors of $b\bar{b}$ SDCs.

A Operator renormalization integrals

The operator convolution integration is shown in eq. (2.22) with the splitting functions shown in eq. (2.23). The splitting functions can be divided into three parts, while the LO FF have two regions. Thus there are 6 types of integrals,

$$\int_z^1 \frac{dy}{y} \delta(1-y) \left(1 - \frac{z}{y}\right)^{-\epsilon} f_1\left(\frac{z}{y}\right) = \lambda^{-\epsilon} f_1(1-\lambda), \quad (\text{A.1})$$

$$\int_z^1 \frac{dy}{y} \delta(1-y) \left(1 - \frac{z}{y}\right)^{-1-2\epsilon} f_2\left(\frac{z}{y}\right) = \lambda^{-1-2\epsilon} f_2(1-\lambda), \quad (\text{A.2})$$

$$\begin{aligned} & \int_z^1 \frac{dy}{y} g(y) \left(1 - \frac{z}{y}\right)^{-\epsilon} f_1\left(\frac{z}{y}\right) \\ &= \lambda^{-\epsilon} \int_0^1 dy h(y, \epsilon) \frac{\lambda}{1-\lambda y} g\left(\frac{1-\lambda}{1-\lambda y}\right) f_1(1-\lambda y), \end{aligned} \quad (\text{A.3})$$

$$\begin{aligned} & \int_z^1 \frac{dy}{y} g(y) \left(1 - \frac{z}{y}\right)^{-1-2\epsilon} f_2\left(\frac{z}{y}\right) \\ &= \lambda^{-1-2\epsilon} \left[-\frac{1}{2\epsilon} \lambda g(1-\lambda) f_2(1) \right. \\ & \quad \left. + \int_0^1 \frac{dy}{y} h(y, 2\epsilon) \left(\frac{\lambda}{1-\lambda y} g\left(\frac{1-\lambda}{1-\lambda y}\right) f_2(1-\lambda y) - \lambda g(1-\lambda) f_2(1) \right) \right], \end{aligned} \quad (\text{A.4})$$

$$\begin{aligned} & \int_z^1 \frac{dy}{y} \frac{1}{[1-y]_+} \left(1 - \frac{z}{y}\right)^{-\epsilon} f_1\left(\frac{z}{y}\right) \\ &= \lambda^{-\epsilon} \ln \lambda f_1(1-\lambda) + \lambda^{-\epsilon} \int_0^1 \frac{dy}{1-y} \left(h(y, \epsilon) f_1(1-\lambda y) - \frac{1-\lambda}{1-\lambda y} f_1(1-\lambda) \right), \end{aligned} \quad (\text{A.5})$$

$$\begin{aligned} & \int_z^1 \frac{dy}{y} \frac{1}{[1-y]_+} \left(1 - \frac{z}{y}\right)^{-1-2\epsilon} f_2\left(\frac{z}{y}\right) \\ &= \lambda^{-1-2\epsilon} \ln \lambda f_2(1-\lambda) \\ & \quad + \lambda^{-1-2\epsilon} \left[\left(-\frac{1}{2\epsilon} - H(-2\epsilon) - \ln(1-\lambda) \right) f_2(1) \right. \\ & \quad \left. + \int_0^1 \frac{dy}{1-y} \left(h(y, 2\epsilon) \frac{f_2(1-\lambda y) - f_2(1)}{y} - \frac{1-\lambda}{1-\lambda y} (f_2(1-\lambda) - f_2(1)) \right) \right], \end{aligned} \quad (\text{A.6})$$

where $\lambda = 1 - z$, $g(y) = (1 - 2y)/y + y(1 - y)$ comes from the splitting function, $H(-2\epsilon)$ is the Harmonic number which can be expanded in the limit of $\epsilon \rightarrow 0$ and

$$h(y, \epsilon) = y^{-\epsilon} = \sum_i \frac{(-\epsilon)^i}{i!} \ln^i(y) \quad (\text{A.7})$$

is the Taylor series at $\epsilon \rightarrow 0$. Based on these results, we find that two more behaviors $(1 - z)^{-\epsilon} \ln(1 - z)$ and $(1 - z)^{-1-2\epsilon} \ln(1 - z)$ are added to the region at $z \rightarrow 1$.

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References

- [1] G.T. Bodwin, E. Braaten and G.P. Lepage, *Rigorous QCD analysis of inclusive annihilation and production of heavy quarkonium*, *Phys. Rev. D* **51** (1995) 1125 [Erratum *ibid.* **55** (1997) 5853] [[hep-ph/9407339](#)] [[INSPIRE](#)].
- [2] J.C. Collins, D.E. Soper and G.F. Sterman, *Factorization of Hard Processes in QCD*, *Adv. Ser. Direct. High Energy Phys.* **5** (1989) 1 [[hep-ph/0409313](#)] [[INSPIRE](#)].
- [3] Z.-B. Kang, J.-W. Qiu and G. Sterman, *Heavy quarkonium production and polarization*, *Phys. Rev. Lett.* **108** (2012) 102002 [[arXiv:1109.1520](#)] [[INSPIRE](#)].
- [4] Z.-B. Kang, Y.-Q. Ma, J.-W. Qiu and G. Sterman, *Heavy Quarkonium Production at Collider Energies: Factorization and Evolution*, *Phys. Rev. D* **90** (2014) 034006 [[arXiv:1401.0923](#)] [[INSPIRE](#)].
- [5] Z.-B. Kang, Y.-Q. Ma, J.-W. Qiu and G. Sterman, *Heavy Quarkonium Production at Collider Energies: Partonic Cross Section and Polarization*, *Phys. Rev. D* **91** (2015) 014030 [[arXiv:1411.2456](#)] [[INSPIRE](#)].
- [6] S. Fleming, A.K. Leibovich, T. Mehen and I.Z. Rothstein, *The Systematics of Quarkonium Production at the LHC and Double Parton Fragmentation*, *Phys. Rev. D* **86** (2012) 094012 [[arXiv:1207.2578](#)] [[INSPIRE](#)].
- [7] S. Fleming, A.K. Leibovich, T. Mehen and I.Z. Rothstein, *Anomalous dimensions of the double parton fragmentation functions*, *Phys. Rev. D* **87** (2013) 074022 [[arXiv:1301.3822](#)] [[INSPIRE](#)].
- [8] V.N. Gribov and L.N. Lipatov, *Deep inelastic $e p$ scattering in perturbation theory*, *Sov. J. Nucl. Phys.* **15** (1972) 438 [[INSPIRE](#)].
- [9] G. Altarelli and G. Parisi, *Asymptotic Freedom in Parton Language*, *Nucl. Phys. B* **126** (1977) 298 [[INSPIRE](#)].
- [10] Y.L. Dokshitzer, *Calculation of the Structure Functions for Deep Inelastic Scattering and e^+e^- Annihilation by Perturbation Theory in Quantum Chromodynamics*, *Sov. Phys. JETP* **46** (1977) 641 [[INSPIRE](#)].
- [11] E. Braaten, K.-m. Cheung and T.C. Yuan, *Z^0 decay into charmonium via charm quark fragmentation*, *Phys. Rev. D* **48** (1993) 4230 [[hep-ph/9302307](#)] [[INSPIRE](#)].
- [12] E. Braaten and T.C. Yuan, *Gluon fragmentation into heavy quarkonium*, *Phys. Rev. Lett.* **71** (1993) 1673 [[hep-ph/9303205](#)] [[INSPIRE](#)].

- [13] P.L. Cho, M.B. Wise and S.P. Trivedi, *Gluon fragmentation into polarized charmonium*, *Phys. Rev. D* **51** (1995) R2039 [[hep-ph/9408352](#)] [[INSPIRE](#)].
- [14] E. Braaten and T.C. Yuan, *Gluon fragmentation into P wave heavy quarkonium*, *Phys. Rev. D* **50** (1994) 3176 [[hep-ph/9403401](#)] [[INSPIRE](#)].
- [15] M. Beneke and I.Z. Rothstein, *ψ' polarization as a test of color octet quarkonium production*, *Phys. Lett. B* **372** (1996) 157 [Erratum *ibid.* **389** (1996) 769] [[hep-ph/9509375](#)] [[INSPIRE](#)].
- [16] J.P. Ma, *Quark fragmentation into p wave triplet quarkonium*, *Phys. Rev. D* **53** (1996) 1185 [[hep-ph/9504263](#)] [[INSPIRE](#)].
- [17] E. Braaten and Y.-Q. Chen, *Dimensional regularization in quarkonium calculations*, *Phys. Rev. D* **55** (1997) 2693 [[hep-ph/9610401](#)] [[INSPIRE](#)].
- [18] E. Braaten and J. Lee, *Next-to-leading order calculation of the color octet $3S(1)$ gluon fragmentation function for heavy quarkonium*, *Nucl. Phys. B* **586** (2000) 427 [[hep-ph/0004228](#)] [[INSPIRE](#)].
- [19] G. Hao, Y. Zuo and C.-F. Qiao, *The Fragmentation Function of Gluon Splitting into P-wave Spin-singlet Heavy Quarkonium*, [arXiv:0911.5539](#) [[INSPIRE](#)].
- [20] Y. Jia, W.-L. Sang and J. Xu, *Inclusive h_c Production at B Factories*, *Phys. Rev. D* **86** (2012) 074023 [[arXiv:1206.5785](#)] [[INSPIRE](#)].
- [21] G.T. Bodwin, H.S. Chung, U.-R. Kim and J. Lee, *Quark fragmentation into spin-triplet S-wave quarkonium*, *Phys. Rev. D* **91** (2015) 074013 [[arXiv:1412.7106](#)] [[INSPIRE](#)].
- [22] Y.-Q. Ma, J.-W. Qiu and H. Zhang, *Heavy quarkonium fragmentation functions from a heavy quark pair. I. S wave*, *Phys. Rev. D* **89** (2014) 094029 [[arXiv:1311.7078](#)] [[INSPIRE](#)].
- [23] Y.-Q. Ma, J.-W. Qiu and H. Zhang, *Fragmentation functions of polarized heavy quarkonium*, *JHEP* **06** (2015) 021 [[arXiv:1501.04556](#)] [[INSPIRE](#)].
- [24] P. Zhang, Y.-Q. Ma, Q. Chen and K.-T. Chao, *Analytical calculation for the gluon fragmentation into spin-triplet S-wave quarkonium*, *Phys. Rev. D* **96** (2017) 094016 [[arXiv:1708.01129](#)] [[INSPIRE](#)].
- [25] E. Braaten and T.C. Yuan, *Gluon fragmentation into spin triplet S wave quarkonium*, *Phys. Rev. D* **52** (1995) 6627 [[hep-ph/9507398](#)] [[INSPIRE](#)].
- [26] G.T. Bodwin and J. Lee, *Relativistic corrections to gluon fragmentation into spin triplet S wave quarkonium*, *Phys. Rev. D* **69** (2004) 054003 [[hep-ph/0308016](#)] [[INSPIRE](#)].
- [27] G.T. Bodwin, U.-R. Kim and J. Lee, *Higher-order relativistic corrections to gluon fragmentation into spin-triplet S-wave quarkonium*, *JHEP* **11** (2012) 020 [[arXiv:1208.5301](#)] [[INSPIRE](#)].
- [28] Q.-F. Sun, Y. Jia, X. Liu and R. Zhu, *Inclusive h_c production and energy spectrum from e^+e^- annihilation at a super B factory*, *Phys. Rev. D* **98** (2018) 014039 [[arXiv:1801.10137](#)] [[INSPIRE](#)].
- [29] P. Zhang, C.-Y. Wang, X. Liu, Y.-Q. Ma, C. Meng and K.-T. Chao, *Semi-analytical calculation of gluon fragmentation into $^1S_0^{[1,8]}$ quarkonia at next-to-leading order*, *JHEP* **04** (2019) 116 [[arXiv:1810.07656](#)] [[INSPIRE](#)].
- [30] P. Artoisenet and E. Braaten, *Gluon fragmentation into quarkonium at next-to-leading order using FKS subtraction*, *JHEP* **01** (2019) 227 [[arXiv:1810.02448](#)] [[INSPIRE](#)].

- [31] F. Feng and Y. Jia, *Next-to-leading-order QCD corrections to gluon fragmentation into $^1S_0^{(1,8)}$ quarkonia*, [arXiv:1810.04138](#) [INSPIRE].
- [32] G.C. Nayak, J.-W. Qiu and G.F. Sterman, *Fragmentation, factorization and infrared poles in heavy quarkonium production*, *Phys. Lett. B* **613** (2005) 45 [[hep-ph/0501235](#)] [INSPIRE].
- [33] G.C. Nayak, J.-W. Qiu and G.F. Sterman, *Fragmentation, NRQCD and NNLO factorization analysis in heavy quarkonium production*, *Phys. Rev. D* **72** (2005) 114012 [[hep-ph/0509021](#)] [INSPIRE].
- [34] G.C. Nayak, J.-W. Qiu and G.F. Sterman, *NRQCD Factorization and Velocity-dependence of NNLO Poles in Heavy Quarkonium Production*, *Phys. Rev. D* **74** (2006) 074007 [[hep-ph/0608066](#)] [INSPIRE].
- [35] G.T. Bodwin, H.S. Chung, J.-H. Ee, U.-R. Kim and J. Lee, *Covariant calculation of a two-loop test of nonrelativistic QCD factorization*, *Phys. Rev. D* **101** (2020) 096011 [[arXiv:1910.05497](#)] [INSPIRE].
- [36] J.C. Collins and D.E. Soper, *Parton Distribution and Decay Functions*, *Nucl. Phys. B* **194** (1982) 445 [INSPIRE].
- [37] A.V. Kotikov, *Differential equations method: New technique for massive Feynman diagrams calculation*, *Phys. Lett. B* **254** (1991) 158 [INSPIRE].
- [38] Z. Bern, L.J. Dixon and D.A. Kosower, *Dimensionally regulated one loop integrals*, *Phys. Lett. B* **302** (1993) 299 [Erratum *ibid.* **318** (1993) 649] [[hep-ph/9212308](#)] [INSPIRE].
- [39] E. Remiddi, *Differential equations for Feynman graph amplitudes*, *Nuovo Cim. A* **110** (1997) 1435 [[hep-th/9711188](#)] [INSPIRE].
- [40] T. Gehrmann and E. Remiddi, *Differential equations for two loop four point functions*, *Nucl. Phys. B* **580** (2000) 485 [[hep-ph/9912329](#)] [INSPIRE].
- [41] J.M. Henn, *Multiloop integrals in dimensional regularization made simple*, *Phys. Rev. Lett.* **110** (2013) 251601 [[arXiv:1304.1806](#)] [INSPIRE].
- [42] R.N. Lee, *Reducing differential equations for multiloop master integrals*, *JHEP* **04** (2015) 108 [[arXiv:1411.0911](#)] [INSPIRE].
- [43] L. Adams, E. Chaubey and S. Weinzierl, *Simplifying Differential Equations for Multiscale Feynman Integrals beyond Multiple Polylogarithms*, *Phys. Rev. Lett.* **118** (2017) 141602 [[arXiv:1702.04279](#)] [INSPIRE].
- [44] M. Caffo, H. Czyz, M. Gunia and E. Remiddi, *BOKASUN: A Fast and precise numerical program to calculate the Master Integrals of the two-loop sunrise diagrams*, *Comput. Phys. Commun.* **180** (2009) 427 [[arXiv:0807.1959](#)] [INSPIRE].
- [45] M. Czakon, *Tops from Light Quarks: Full Mass Dependence at Two-Loops in QCD*, *Phys. Lett. B* **664** (2008) 307 [[arXiv:0803.1400](#)] [INSPIRE].
- [46] R. Mueller and D.G. Öztürk, *On the computation of finite bottom-quark mass effects in Higgs boson production*, *JHEP* **08** (2016) 055 [[arXiv:1512.08570](#)] [INSPIRE].
- [47] R.N. Lee, A.V. Smirnov and V.A. Smirnov, *Solving differential equations for Feynman integrals by expansions near singular points*, *JHEP* **03** (2018) 008 [[arXiv:1709.07525](#)] [INSPIRE].
- [48] X. Liu, Y.-Q. Ma and C.-Y. Wang, *A Systematic and Efficient Method to Compute Multi-loop Master Integrals*, *Phys. Lett. B* **779** (2018) 353 [[arXiv:1711.09572](#)] [INSPIRE].

- [49] X. Liu, Y.-Q. Ma, W. Tao and P. Zhang, *Calculation of Feynman loop integration and phase-space integration via auxiliary mass flow*, *Chin. Phys. C* **45** (2021) 013115 [[arXiv:2009.07987](#)] [[INSPIRE](#)].
- [50] J.M. Henn, *Lectures on differential equations for Feynman integrals*, *J. Phys. A* **48** (2015) 153001 [[arXiv:1412.2296](#)] [[INSPIRE](#)].
- [51] H.R.P. Ferguson, D.H. Bailey and S. Arno, *Analysis of pslq, an integer relation finding algorithm*, *Math. Comput.* **68** (1999) 351.
- [52] D.H. Bailey and D.J. Broadhurst, *Parallel integer relation detection: Techniques and applications*, *Math. Comput.* **70** (2001) 1719 [[math/9905048](#)] [[INSPIRE](#)].
- [53] Y.-Q. Ma and K.-T. Chao, *New factorization theory for heavy quarkonium production and decay*, *Phys. Rev. D* **100** (2019) 094007 [[arXiv:1703.08402](#)] [[INSPIRE](#)].