Heavy quarkonium production at collider energies: Partonic cross section and polarization

Zhong-Bo Kang,[1,*] Yan-Qing Ma,[2,3,†] Jian-Wei Qiu,[4,5,‡] and George Sterman[5,§]

[1]*Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*
[2]*Maryland Center for Fundamental Physics, University of Maryland, College Park, Maryland 20742, USA*
[3]*Center for High-Energy Physics, Peking University, Beijing 100871, China*
[4]*Physics Department, Brookhaven National Laboratory, Upton, New York 11973-5000, USA*
[5]*C. N. Yang Institute for Theoretical Physics and Department of Physics and Astronomy, Stony Brook University, Stony Brook, New York 11794-3840, USA*

(Received 17 November 2014; published 27 January 2015)

We calculate the $\mathcal{O}(\alpha_s^3)$ short-distance, QCD collinear-factorized coefficient functions for all partonic channels that include the production of a heavy quark pair at short distances. This provides the first power correction to the collinear-factorized inclusive hadronic production of heavy quarkonia at large transverse momentum, p_T, including the full leading-order perturbative contributions to the production of heavy quark pairs in all color and spin states employed in NRQCD treatments of this process. We discuss the role of the first power correction in the production rates and the polarizations of heavy quarkonia in high-energy hadronic collisions. The consistency of QCD collinear factorization and nonrelativistic QCD factorization applied to heavy quarkonium production is also discussed.

DOI: 10.1103/PhysRevD.91.014030 PACS numbers: 12.38.Bx, 12.39.-x, 12.39.St, 13.88.+e

I. INTRODUCTION

Both the cross section and polarization of heavy quarkonium production in high-energy collisions have posed significant challenges to our understanding of the production mechanism [1]. Although the nonrelativistic QCD (NRQCD) treatment of heavy quarkonium production is by far the most theoretically sound [2–5], and generally consistent with experimental data on inclusive production of J/ψ and Υ of large transverse momentum, p_T, at the Tevatron and the LHC [6–9], it has not been able to explain fully the polarization of these heavy quarkonia produced at high p_T [10–13]. With a larger heavy quark mass, m_Q, it was expected that the NRQCD factorization formalism should do a better job in describing the production of Υ and its polarization. However, recent data on polarization of $\Upsilon(1S, 2S, 3S)$ measured by the CMS Collaboration at the LHC [14] also show inconsistency with full next-to-leading-order (NLO) NRQCD calculations [9,15]. In addition, global fits of data on J/ψ production from various high-energy collisions, including e^+e^-, lepton-hadron, and hadron-hadron collisions [7,16] show some discrepancies in the shape of momentum spectra between theory predictions and data [17]. For some production channels of the NRQCD calculations, the NLO corrections are orders larger than their corresponding leading-order (LO) results, which raises questions as to whether yet higher-order contributions can be neglected. Motivated in part by these challenges to existing theory, new approaches based on QCD factorization [18–22] and soft-collinear effective theory [23,24] have been proposed for the systematic study of heavy quarkonium production at collider energies.

In Ref. [22], we developed an extended QCD factorization formalism for heavy quarkonium production at large transverse momentum $p_T \gg m_H \gg \Lambda_{\rm QCD}$ in hadronic collisions (or at a large energy $E \gg m_H$ in e^+e^- collisions) with heavy quarkonium mass m_H. The new QCD factorization formalism includes both collinear-factorized leading-power (LP) and collinear-factorized next-to-leading-power (NLP) terms in the $1/p_T$ expansion of the production cross section,

$$
\begin{aligned}
E_P\frac{d\sigma_{A+B\to H+X}}{d^3P}(P) \approx{}& \sum_f\int\frac{dz}{z^2}D_{f\to H}(z;m_Q)E_c\frac{d\hat{\sigma}_{A+B\to f(p_c)+X}}{d^3p_c}\left(p_c=\frac{1}{z}p\right)\\
&+\sum_{[Q\bar{Q}(\kappa)]}\int\frac{dz}{z^2}dudv\mathcal{D}_{[Q\bar{Q}(\kappa)]\to H}(z,u,v;m_Q)\\
&\times E_c\frac{d\hat{\sigma}_{A+B\to[Q\bar{Q}(\kappa)](p_c)+X}}{d^3p_c}\left(P_Q=\frac{u}{z}p,P_{\bar{Q}}=\frac{\bar{u}}{z}p,P'_Q=\frac{v}{z}p,P'_{\bar{Q}}=\frac{\bar{v}}{z}p\right),
\end{aligned}
\tag{1}
$$

[*]zkang@lanl.gov
[†]yqma@bnl.gov
[‡]jqiu@bnl.gov
[§]sterman@insti.physics.sunysb.edu

where $p^\mu = P^\mu(m_H = 0)$ is the massless part of the heavy quarkonium momentum in a frame in which the quarkonium moves along the z-axis, and the renormalization scale μ and the factorization scale μ_F are suppressed. We will often refer to this result below as "QCD factorization" to distinguish it from NRQCD factorization. In this factorized expression, $\sum_f$ runs over all parton flavors $f = q, \bar{q}, g$, including heavy flavors when $m_Q \ll p_T$, while $\sum_{[Q\bar{Q}(\kappa)]}$ indicates a sum over both spin and color states of heavy quark pairs $[Q\bar{Q}(\kappa)]$, where $\kappa = sI$ with $s = v, a, t$ for vector, axial vector and tensor spin states, and $I = 1, 8$ for singlet and octet color states, respectively. In Eq. (1), the variables z, u, and v, with $\bar{u} = 1 - u$ and $\bar{v} = 1 - v$ are light-cone momentum fractions; and $D_{f\to H}(z; m_Q)$ and $\mathcal{D}_{[Q\bar{Q}(\kappa)]\to H}(z, u, v; m_Q)$ are single-parton and heavy quark-pair fragmentation functions (FFs), respectively [22]. In the factorization formula in Eq. (1), we neglect all contributions involving twist-4 multiparton correlation functions of colliding hadrons, as well as all terms at NLP involving FFs not from a heavy quark pair, because these contributions must create the heavy quark pair nonperturbatively. We thus expect them to be suppressed by powers of heavy quark mass [22], and they could be suppressed further by reasons similar to those that lead to the OZI rule in evaluating decay rates.

The QCD factorization formalism in Eq. (1) effectively organizes the contributions to heavy quarkonium production at large p_T in terms of the characteristic time when an active heavy quark pair, which is necessary for a final-state heavy quarkonuim, is produced. The LP contribution to the production cross section is given by the hard partonic scattering to produce an active parton (quark, antiquark, or gluon) at a distance scale of $\mathcal{O}(1/p_T)$, convolved with a fragmentation function for this parton to evolve into a heavy quark pair that transmutes into a heavy quarkonium. At LP accuracy, the heavy quark pair is effectively produced at the distance scale of $\mathcal{O}(1/2m_Q)$, a much longer distance compared to scales over which the active parton was initially produced. At NLP accuracy, the QCD factorization requires not only the factorized NLP term in Eq. (1), but also a new power-suppressed contribution to the DGLAP evolution of heavy quarkonium FFs from a single active parton [22]. The factorized NLP term in Eq. (1) describes the production of the heavy quark pair directly at $\mathcal{O}(1/p_T)$ where the initial hard collision took place. The power-suppressed contribution to the evolution of single-parton FFs sums up all leading logarithmic contributions to the production of the heavy quark pairs at distance scales from $\mathcal{O}(1/\mu_F)$ to $\mathcal{O}(1/\mu_0)$ where $\mu_F \sim p_T$ is the factorization scale and $\mu_0 \sim 2m_Q$ is the input scale at which the evolution of the FFs starts. Having both LP and NLP contribution, the QCD factorization formalism in Eq. (1) effectively covers all leading contributions to the production of the heavy quark pair, which transmutes into an observed heavy quarkonium, no matter where and when the heavy quark pair was produced [22]. If we keep only the factorized LP contribution to the cross section in Eq. (1), we include only the contribution to the heavy quarkonium production when the heavy quark pair is produced at the distance scale $\gtrsim\mathcal{O}(1/\mu_0)$.

The predictive power of the QCD factorization formalism in Eq. (1) relies on the universality of the FFs, and our ability to calculate the evolution kernels of these FFs, as well as the short-distance coefficient functions, perturbatively, to all orders in powers of α_s. In Ref. [22], we evaluated the mixing evolution kernels for one parton to evolve into a heavy quark pair at $\mathcal{O}(\alpha_s^2)$, as well as evolution kernels for a heavy quark pair to evolve into another heavy quark pair at $\mathcal{O}(\alpha_s)$. In this paper, we concentrate on the calculation of the short-distance coefficient functions of the QCD factorization formalism in Eq. (1). When A and B in Eq. (1) are hadrons, the cross section is found using the following expressions, reflecting collinear factorization for the incoming hadrons:

$$E_c \frac{d\hat{\sigma}_{A+B\to f(p_c)+X}}{d^3 p_c} = \sum_{a,b} \int dx_a \phi_{A\to a}(x_a) \int dx_b \phi_{B\to b}(x_b) E_c \frac{d\hat{\sigma}_{a+b\to f(p_c)+X}}{d^3 p_c},$$
$$E_c \frac{d\hat{\sigma}_{A+B\to [Q\bar{Q}(\kappa)](p_c)+X}}{d^3 p_c} = \sum_{a,b} \int dx_a \phi_{A\to a}(x_a) \int dx_b \phi_{B\to b}(x_b) E_c \frac{d\hat{\sigma}_{a+b\to [Q\bar{Q}(\kappa)](p_c)+X}}{d^3 p_c}, \tag{2}$$

where a, b represent active parton flavors, running over quarks, antiquarks and gluons, and $\phi_{A\to a}(x)$ and $\phi_{B\to b}(x)$ are the parton distribution functions (PDFs) of hadrons A and B, respectively, with factorization scale dependence suppressed. The short-distance coefficient functions for producing a single parton at the LP, $\hat{\sigma}_{a+b\to f(p_c)+X}$ in Eq. (2), are the same as the perturbative coefficient functions for producing a light hadron, such as a pion, and are available for both the LO and NLO in powers of α_s in the literature [25]. This is because the factorized short-distance coefficient functions are not sensitive to the details of the hadron produced in the final state, but only the properties of the fragmenting parton. In the next section, we introduce the method to calculate the short-distance hard parts at NLP, $\hat{\sigma}_{a+b\to [Q\bar{Q}(\kappa)](p_c)+X}$ in Eq. (2), and present the detailed calculations of the $\mathcal{O}(\alpha_s^3)$ coefficient functions for all relevant spin-color states of a heavy quark pair produced from the scattering of a light quark and antiquark.

The complete results of short-distance hard parts for all parton-parton scattering channels at $\mathcal{O}(\alpha_s^3)$ are given in the Appendix.

With the perturbatively calculated short-distance hard parts in this paper, and the evolution kernels derived in Ref. [22], the predictive power of the QCD factorization formalism in Eq. (1) still requires our knowledge of the universal FFs at an input scale μ_0. Since both the short-distance hard parts and evolution kernels are perturbative, and the same for hadronic production of all heavy quarkonium states, it is these input FFs that carry the information on the characteristics of the individual heavy quarkonia. The universal input FFs are nonperturbative, and in principle, should be extracted from fitting experimental data, like the FFs for inclusive light hadron production. However, with the NLP contributions, we will need many more FFs (single-parton plus heavy quark pair FFs) for each heavy quarkonium state produced. Extracting all these FFs from inclusive cross sections of heavy quarkonium production would not be an easy task.

Unlike the FFs to a light hadron, heavy quarkonium FFs at the input scale μ_0 have essentially one intrinsic hard scale, the heavy quark mass $m_Q \sim \mathcal{O}(\mu_0)$, which is sufficiently separated from the momentum scale for the binding of heavy quarkonium, $m_Q v$, with the heavy quark relative velocity in the pair's rest frame, $v \ll 1$. The physics between the m_Q and μ_0 could be perturbatively calculable. It was proposed in Ref. [21], as a conjecture or a model, to use NRQCD factorization to calculate these input FFs by expressing all of them in terms of perturbatively calculated coefficients and a few local NRQCD matrix elements, organized in powers of v. Since the input momentum scale $\mu_0 \sim \mu_\Lambda$, the NRQCD factorization scale $\sim\mathcal{O}(m_Q)$, the perturbatively calculated coefficient functions should be free of the large logarithms and the power enhancement that were seen in the NLO NRQCD coefficient functions for heavy quarkonium production at large p_T at collider energies [6–9]. In Sec. III, we review the procedure to calculate the heavy quarkonium FFs at the input scale $\mu_0 \gtrsim 2m_Q$ in terms of NRQCD factorization.

Although there is no formal proof that ensures that NRQCD factorization works for evaluating these universal input FFs perturbatively to all orders in α_s and all powers in v-expansion, it has been demonstrated that such NRQCD factorization should work up to two-loop radiative corrections [18,19]. Explicit perturbative calculations in Refs. [26,27] show that such factorization is indeed possible for up to v^4 in the velocity expansion since all calculated perturbative coefficient functions are infrared safe for LP single-parton FFs at $\mathcal{O}(\alpha_s^2)$, as well as for NLP heavy quark-pair FFs at $\mathcal{O}(\alpha_s)$. Such perturbatively calculated input FFs in NRQCD factorization should provide a good starting point to estimate or determine these much needed universal but nonperturbative functions for heavy quarkonium production.

If the NRQCD factorization for calculating the input FFs is valid, the collinear factorization formalism in Eq. (1) may be thought of as a reorganization of the perturbatively calculated cross section by NRQCD factorization, with resummation of large fragmentation logarithms. It also provides a justification of NRQCD factorization applied to heavy quarkonium production at large transverse momentum, at least for the first and second power terms in the $1/p_T$ expansion. In Sec. III, we discuss the connection between the QCD factorization formalism in Eq. (1) and the NRQCD factorization approach to heavy quarkonium production [2]. With a proper matching, we introduce an expanded factorization formalism which could smoothly connect the QCD factorization in Eq. (1) for $p_T \gg \mu_0$ to the fixed-order calculation in NRQCD factorization for $p_T \gtrsim \mu_0 \gtrsim 2m_Q$, including heavy quark mass effects.

In Subsec. III C, we provide an explicit example to demonstrate that when $p_T \gg m_H$, the QCD factorization formalism in Eq. (1) catches all leading contributions to the heavy quarkonium production. We show that the extremely challenging calculation of the complete NLO contributions to the production of a color-singlet, spin-1 heavy quark pair in hadronic collisions can be effectively reproduced by the much simpler LO perturbative QCD calculation of the hard parts to produce a color-octet collinear and massless heavy quark pair, convolved with equally simple LO fragmentation functions for the perturbatively produced pair to fragment into the color-singlet, spin-1 heavy quark pair, calculated in NRQCD factorization. The combination of the two LO calculations reproduces more than 95% of the full NLO contribution when p_T is only a few times the heavy quark mass. The same conclusion is also true for other production channels in NRQCD calculations [28].

In Sec. IV, we discuss how to evaluate heavy quarkonium polarization in the QCD factorization approach. Since both short-distance partonic hard parts and evolution kernels of heavy quarkonium FFs are perturbative, and not sensitive to the long-distance details of the individual heavy quarkonium produced, the heavy quarkonium polarization should be completely determined by the heavy quarkonium FFs at the input factorization scale, μ_0. With $\mu_0 \gtrsim m_Q \gg m_Q v$, it is very reasonable to apply the same NRQCD factorization conjecture for calculating the unpolarized heavy quarkonium FFs at scale μ_0 to the calculation of polarized heavy quarkonium FFs at the same input scale. In this section, we present the projection operators, within the NRQCD factorization approach, for the calculation of polarized heavy quarkonium FFs with the produced heavy quarkonium in either a transverse or a longitudinal polarization state. As an example, we present our $\mathcal{O}(\alpha_s)$ calculation of polarized heavy quarkonium FFs via a color-singlet ${}^3S_1^{[1]}$ heavy quark pair in NRQCD. A complete calculation of polarized heavy quarkonium FFs in NRQCD for all partonic channels is now available [26,27,29]. With the perturbatively calculated polarized heavy quarkonium FFs, we demonstrate explicitly that the combination of QCD factorization for heavy quarkonium production in Eq. (1) and NRQCD factorization for the heavy quarkonium FFs can not only reproduce the NLO color-singlet model (CSM) calculation for the production rate, but also the polarization of the produced heavy quarkonia. Clearly, a full understanding of heavy quarkonium production and its polarization requires a new global analysis of all heavy quarkonium production data in terms of QCD factorization formalism and the new set of evolution equations for heavy quarkonium FFs [28]. Finally, our conclusions are summarized in Sec. V.

II. PRODUCTION CROSS SECTION AND PARTONIC HARD PARTS

In this section, we introduce a systematic method to calculate all partonic hard parts of the collinear-factorized NLP terms, $d\hat{\sigma}_{ab\to[Q\bar{Q}(\kappa)](p_c)}$, in Eq. (2) perturbatively. We provide a detailed derivation of the hard parts for producing a heavy quark pair in various spin-color states from the scattering of a quark and an antiquark at $\mathcal{O}(\alpha_s^3)$, and present our full results for all other partonic scattering channels, including quark-gluon and gluon-gluon scattering channels in the Appendix.

A. The formalism

As a consequence of QCD factorization, all factorized partonic hard parts for heavy quarkonium production in Eq. (2) are uniquely determined perturbatively by the factorization formalism and the definition of fragmentation functions (and parton distribution functions in the case of hadronic collisions). Like the LP hard parts, the NLP factorized partonic hard parts, $d\hat{\sigma}_{ab\to[Q\bar{Q}(\kappa)](p_c)}$ in Eq. (2), are insensitive to the long-distance details of the colliding hadrons and the produced heavy quarkonium. The factorization formalism in Eq. (1) is also valid when the colliding hadrons, A and B, are replaced by two asymptotic colliding parton states of flavor a and b, respectively, and the produced heavy quarkonium, H, is replaced by an asymptotic state of a heavy quark pair with momentum p and spin-color state $[Q\bar{Q}(\kappa)]$. Together, the partonic analogs of Eqs. (1) and (2) can be expressed symbolically as

$$d\sigma_{a+b\to[Q\bar{Q}(\kappa)](p)} \approx \sum_{i,j,f}\phi_{a\to i}\otimes\phi_{b\to j}\otimes d\hat{\sigma}_{i+j\to f(p_c)}\otimes D_{f\to[Q\bar{Q}(\kappa)]} + \sum_{i,j,[Q\bar{Q}(\kappa')]}\phi_{a\to i}\otimes\phi_{b\to j}\otimes d\hat{\sigma}_{i+j\to[Q\bar{Q}(\kappa')](p_c)}\otimes \mathcal{D}_{[Q\bar{Q}(\kappa')]\to[Q\bar{Q}(\kappa)]}, \tag{3}$$

where i, j, f represent the factorized active parton flavors, including q, $\bar{q}$, g, and Q; $[Q\bar{Q}(\kappa')]$ represents a heavy quark pair of spin-color state κ'; and $\otimes$ represents the convolution over partonic momentum fractions as shown in Eqs. (1) and (2). Unlike the cross section in Eq. (1), both the partonic cross section on the left-hand side (lhs), and the PDFs of a parton and FFs of a partonic state on the right-hand side (rhs) of Eq. (3) can be calculated perturbatively in terms of Feynman diagrams with proper regularizations. Most importantly, the short-distance partonic hard parts in Eq. (3) are the same as those in Eq. (2).

The fact that the cross section is factorizable ensures that the perturbatively calculated partonic cross sections on the lhs and PDFs and FFs on the rhs of Eq. (3) are all free of infrared (IR) divergence, while the ultraviolet (UV) divergences are taken care of by the renormalization, and all collinear (CO) divergences are process independent and canceled perturbatively order by order in powers of α_s between the lhs and the rhs to leave the partonic hard parts free of any divergences. To derive the partonic hard parts in Eq. (2), which are the same as those in Eq. (3), we expand both sides of Eq. (3) order by order in powers of α_s, and then extract all partonic hard parts perturbatively by calculating the corresponding partonic cross section in the lhs, and the PDFs and FFs of partons on the rhs.

To evaluate the hard parts at the first nontrivial order in hadronic collisions, we expand both sides of Eq. (3) to $\mathcal{O}(\alpha_s^3)$,

$$d\sigma^{(3)}_{a+b\to[Q\bar{Q}(\kappa)](p)} \approx \sum_{i,j,f}\phi^{(0)}_{a\to i}\otimes\phi^{(0)}_{b\to j}\otimes d\hat{\sigma}^{(2)}_{i+j\to f(p_c)}\otimes D^{(1)}_{f\to[Q\bar{Q}(\kappa)]} + \sum_{i,j,[Q\bar{Q}(\kappa')]}\phi^{(0)}_{a\to i}\otimes\phi^{(0)}_{b\to j}\otimes d\hat{\sigma}^{(3)}_{i+j\to[Q\bar{Q}(\kappa')](p_c)}\otimes \mathcal{D}^{(0)}_{[Q\bar{Q}(\kappa')]\to[Q\bar{Q}(\kappa)]}, \tag{4}$$

where the superscript (m) with $m = 0, 1, 2, 3$ indicates the power of α_s of the corresponding quantity. Since the zeroth-order parton PDFs and FFs are given by the δ-functions that fix the corresponding convolutions, the short-distance hard parts for all possible channels of partonic scattering between parton flavors a and b are given by

$$d\hat{\sigma}^{(3)}_{a+b\to[Q\bar{Q}(\kappa)](p)} = d\sigma^{(3)}_{a+b\to[Q\bar{Q}(\kappa)](p)} - d\hat{\sigma}^{(2)}_{a+b\to g(p_c)} \otimes D^{(1)}_{g\to[Q\bar{Q}(\kappa)](p)}, \quad (5)$$

where the first term on the rhs, $d\sigma^{(3)}_{a+b\to[Q\bar{Q}(\kappa)](p)}$, is the perturbative cross section for two partons of flavors a and b to produce a heavy quark pair of momentum p in a spin-color quantum state $[Q\bar{Q}(\kappa)]$ at the order of α_s^3, which covers all LO partonic processes to produce a heavy quark pair at a large transverse momentum. Since we neglect the heavy quark mass when $p_T \gg m_Q$, this partonic scattering amplitude, like the one in Fig. 1, can have a perturbative divergence caused by the mass singularity of the gluon propagator, when its invariant mass goes on shell, $p^2 \to 0$, which leads to a divergent partonic cross section, $d\sigma^{(3)}_{a+b\to[Q\bar{Q}(\kappa)](p)}$. This perturbatively divergent contribution is in fact a LP contribution, and is already included in the LP fragmentation contribution, the first term on the rhs of Eq. (1). Therefore, it should be systematically removed when we calculate the short-distance partonic hard parts of the NLP contribution to avoid double counting. In Eq. (5), the second term is a natural result of the QCD factorization formalism. Its role is to remove all possible LP contributions from the first term, and it can be referred to as a subtraction term for removing the mass singularity or the LP contribution.

Similarly, by expanding the factorized formalism for the partonic scattering cross section in Eq. (3) to order α_s^4, we derive the factorization formula for calculating the NLO short-distance partonic hard parts of the NLP contribution as

$$\begin{aligned} d\hat{\sigma}^{(4)}_{a+b\to[Q\bar{Q}(\kappa)](p)} = {} & d\sigma^{(4)}_{a+b\to[Q\bar{Q}(\kappa)](p)} - d\hat{\sigma}^{(3)}_{a+b\to g(p_c)} \otimes D^{(1)}_{g\to[Q\bar{Q}(\kappa)](p)} \\ & - \sum_f d\hat{\sigma}^{(2)}_{a+b\to f(p_c)} \otimes D^{(2)}_{f\to[Q\bar{Q}(\kappa)](p)} \\ & - \sum_i \phi^{(1)}_{a\to i} \otimes d\hat{\sigma}^{(2)}_{i+b\to g(p_c)} \otimes D^{(1)}_{g\to[Q\bar{Q}(\kappa)](p)} \\ & - \sum_j \phi^{(1)}_{b\to j} \otimes d\hat{\sigma}^{(2)}_{a+j\to g(p_c)} \otimes D^{(1)}_{g\to[Q\bar{Q}(\kappa)](p)} \\ & - \sum_i \phi^{(1)}_{a\to i} \otimes d\hat{\sigma}^{(3)}_{i+b\to[Q\bar{Q}(\kappa)](p)} - \sum_j \phi^{(1)}_{b\to j} \otimes d\hat{\sigma}^{(3)}_{a+j\to[Q\bar{Q}(\kappa)](p)}, \end{aligned} \quad (6)$$

where the sum of i, j, f runs over all parton flavors, and all lower-order short-distance partonic hard parts are well-defined and calculable. For example, the $d\hat{\sigma}^{(3)}_{a+b\to[Q\bar{Q}(\kappa)](p_c)}$ are given by Eq. (5), and $d\hat{\sigma}^{(2)}_{a+b\to f(p_c)}$ are the lowest-order partonic cross sections given by lowest-order $2\to 2$ partonic scattering amplitudes, and are finite. In Eq. (6), the subtraction term in the first line plays the same role as that of the subtraction term in Eq. (5); the subtraction term in the second line is to remove the power collinear divergence of the partonic cross section, $d\sigma^{(4)}_{a+b\to[Q\bar{Q}(\kappa)](p)}$, which has been included in the evolution of the single-parton FFs via the mixing kernels from a single fragmenting parton to a heavy quark pair [22]. The four other subtraction terms in the last three lines of Eq. (6) are needed to remove the logarithmic collinear contributions that have been included in the evolution of initial-state PDFs. The factorization formula in Eq. (6) can be adapted for calculating the NLO contribution of the power corrections in other scattering processes—for example, we only need the first two lines for high-energy heavy quarkonium production in e^+e^- collisions.

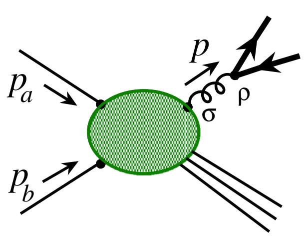

FIG. 1 (color online). Sample partonic scattering amplitude for $a(p_a) + b(p_b) \to [Q\bar{Q}(\kappa)](p) + X$ that includes a leading power contribution to the production rate of a heavy quark pair.

In the remainder of this section, we provide the detailed derivation of the first nontrivial short-distance hard parts for a quark and an antiquark to produce a heavy quark pair in all possible spin and color states. Because the heavy quark mass is set to zero in the hard parts, we only need to consider the production of a heavy quark pair in axial-vector and vector spin states at the order of α_s^3. That is, we calculate the partonic hard parts by using Eq. (5) with $a = q(p_1)$ and $b = \bar{q}(p_2)$ of momentum p_1 and p_2, respectively, and

$$\begin{aligned} & d\hat{\sigma}^{(3)}_{q(p_1)+\bar{q}(p_2)\to[Q\bar{Q}(\kappa)](p)} \\ & \quad = d\sigma^{(3)}_{q(p_1)+\bar{q}(p_2)\to[Q\bar{Q}(\kappa)](p)} \\ & \quad\quad - d\hat{\sigma}^{(2)}_{q(p_1)+\bar{q}(p_2)\to g(p_c)} \otimes D^{(1)}_{g(p_c)\to[Q\bar{Q}(\kappa)](p)}, \end{aligned} \quad (7)$$

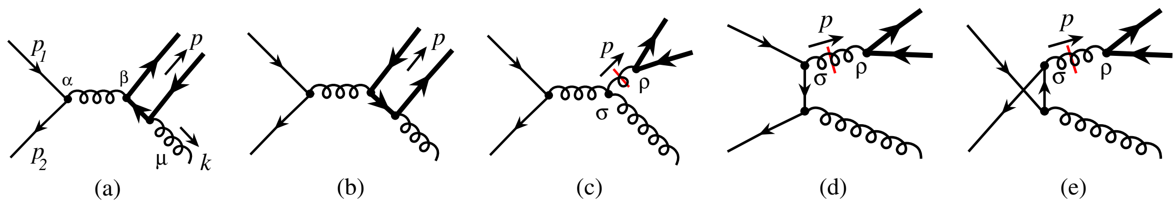

FIG. 2 (color online). Leading-order Feynman diagrams for the $q\bar{q} \to Q\bar{Q}g$ subprocess at $\mathcal{O}(\alpha_s^3)$.

where the produced pair $[Q\bar{Q}(\kappa)]$ can be in an axial-vector or a vector spin state while in either singlet or octet color state.

At the order of α_s^3, the scattering amplitude for $d\sigma^{(3)}_{q(p_1)+\bar{q}(p_2)\to[Q\bar{Q}(\kappa)](p)}$ is given by the Feynman diagrams in Fig. 2. The diagrams in Figs. 2(c), 2(d), and 2(e) all have divergent contributions caused by the same mass singularity when the momentum of the gluon with a short bar goes on shell, $p^2 \to 0$. As discussed above, any such perturbatively divergent LP contribution should be removed by a subtraction term, the second term on the rhs of Eq. (7). The $d\hat{\sigma}^{(2)}_{q(p_1)+\bar{q}(p_2)\to g(p_c)}$ of the subtraction term is the lowest-order cross section for the partonic process, $q(p_1) + \bar{q}(p_2) \to g(p) + g$, given by the Feynman diagrams in Fig. 3. At order α_s^2, the partonic cross section $d\hat{\sigma}^{(2)}_{q(p_1)+\bar{q}(p_2)\to g(p_c)}$ is perturbatively finite. The function $D^{(1)}_{g(p_c)\to[Q\bar{Q}(\kappa)](p)}$ of the subtraction term in Eq. (7) is the lowest-order fragmentation function for a gluon to a heavy quark pair. At order α_s, it is given by the Feynman diagram in Fig. 4, which is in cut diagram notation, where the amplitude and complex conjugate are combined into a forward scattering diagram and the final state is identified by a vertical line. From the definition of the gluon fragmentation function, two gluon lines in Fig. 4 are contracted by the cut vertex [22],

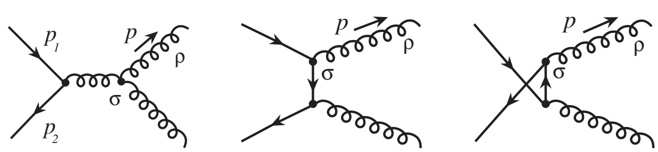

FIG. 3. Leading-order Feynman diagrams for $q\bar{q} \to gg$ subprocess at $\mathcal{O}(\alpha_s^2)$.

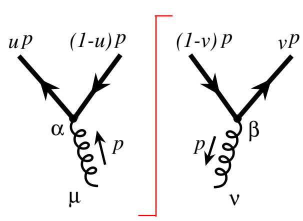

FIG. 4 (color online). Lowest-order Feynman diagram (α_s) for a gluon to fragment into a heavy quark pair.

$$\mathcal{V}_g(z) = \int \frac{d^4 p_c}{(2\pi)^4} z^2 \delta\left(z - \frac{p\cdot\hat{n}}{p_c\cdot\hat{n}}\right) \times \left[\frac{1}{N_c^2-1}\sum_{a=1}^{N_c^2-1} \delta_{a'a}\left(\frac{1}{2}\tilde{d}^{\mu\nu}_{\hat{n}}(p_c)\right)\right], \quad (8)$$

where the four-vector $\hat{n}^\mu$ with $\hat{n}^2 = 0$ is an auxiliary vector conjugate to the observed hadron momentum p^μ, introduced to help define the fragmenting gluon's light-cone momentum fraction, as well as its two transverse polarization states (or "physical" polarization states). In Eq. (8), the a and a' are color indices of the fragmenting gluon in the amplitude and its complex conjugate, respectively, and

$$\tilde{d}^{\mu\nu}_{\hat{n}}(p_c) = -g^{\mu\nu} + \frac{p_c^\mu \hat{n}^\nu + \hat{n}^\mu p_c^\nu}{p_c\cdot\hat{n}} - \frac{p_c^2}{(p_c\cdot\hat{n})^2}\hat{n}^\mu\hat{n}^\nu, \quad (9)$$

with $\tilde{d}^{\mu\nu}_{\hat{n}}(p_c)p_{c\mu} = \tilde{d}^{\mu\nu}_{\hat{n}}(p_c)\hat{n}_\mu = 0$. In a frame where the hadron is moving along the $+z$-axis, $p^\mu = (p^+, 0^-, 0_\perp)$ with hadron mass neglected, we can normalize the auxiliary vector $\hat{n}^\mu$ as $\hat{n}^\mu = (0^+, 1^-, 0_\perp)$, since the cut vertex, $\mathcal{V}_g(z)$, is invariant when we rescale the vector $\hat{n}^\mu$. At the lowest order, the fragmenting gluon momentum p_c above is effectively equal to the momentum of the heavy quark pair p in Fig. 4. Consequently, the LO perturbative gluon FF, $D^{(1)}_{g(p_c)\to[Q\bar{Q}(\kappa)](p)}$, is divergent as the gluon momentum goes on shell, $p_c^2 \to p^2 \to 0$. It is clear from above discussion that the second term in Eq. (7) matches precisely the structure of the divergent piece of the partonic cross section $d\sigma^{(3)}_{q(p_1)+\bar{q}(p_2)\to[Q\bar{Q}(\kappa)](p)}$ to remove its mass singularity when $p^2 \to 0$, and to leave the sum of these two terms in Eq. (7) infrared safe (IRS) and perturbative. This subtraction also avoids double counting of the LP contribution, as required by QCD factorization.

The cancellation of the divergence between the first and the second terms in Eq. (7) is exact at the phase space point where the gluons with a short bar in Figs. 2(c–e) is on the mass shell, with a physical polarization. It was shown in Ref. [22], as part of the calculation of the evolution kernels for a single parton to evolve into a heavy quark pair, that the net effect of the second term in Eq. (7) is to replace each gluon propagator with the short bar in Fig. 2 by a contact term, found by rewriting the propagator as

$$G^{\rho\sigma}(p) = \frac{i}{p^2 + i\varepsilon}\left[-g^{\rho\sigma} + \frac{p^\rho \hat{n}^\sigma + p^\sigma \hat{n}^\rho}{p\cdot\hat{n}} - \frac{p^2}{(p\cdot\hat{n})^2}\hat{n}^\rho\hat{n}^\sigma\right] + \frac{i}{p^2+i\varepsilon}\left[\frac{p^2}{(p\cdot\hat{n})^2}\hat{n}^\rho\hat{n}^\sigma\right], \tag{10}$$

and keeping only the final, unphysical term,

$$G^{\rho\sigma}(p) \to \frac{ip^2}{p^2+i\varepsilon}\left[\frac{\hat{n}^\rho\hat{n}^\sigma}{(p\cdot\hat{n})^2}\right] \equiv G_c^{\rho\sigma}(p). \tag{11}$$

Equation (11) shows the result of subtracting the contribution of these diagrams to gluon fragmentation, which is already included in the LP term.

As in Eq. (9), the first term in the right-hand side of Eq. (10) vanishes when it is contracted by either p_ρ or $\hat{n}_\rho$, defining the contribution from the gluon's two transverse polarization states. These are precisely the terms canceled by the subtraction, which takes the physical polarizations into account. In Eq. (10), the second term in the rhs is the contact term, which is finite when the gluon line goes on shell, $p^2 \to 0$. With this term included, the NLP contribution to the scattering amplitude in Fig. 2 is color gauge invariant [30]. Then, the effect of the subtraction is to specify a prescription for calculating the hard parts at this order following Eq. (7), which can be represented as [22]

$$d\hat{\sigma}^{(3)}_{q+\bar{q}\to[Q\bar{Q}(\kappa)](p)}(p_1,p_2,p) = d\sigma^{(3)}_{q+\bar{q}\to[Q\bar{Q}(\kappa)](p)}(p_1,p_2,p)_c, \tag{12}$$

where the subscript "c" indicates that the gluon propagators with a short bar in Fig. 2 are replaced by corresponding contact terms. These diagrams, in Figs. 2(c), 2(d) and 2(e), with their perturbatively divergent leading power contributions removed, are necessary for the gauge invariance of the NLP contribution. In addition to quark-antiquark scattering, the expression in Eq. (12) is also valid for scattering of two partons of any flavors a and b at this order.

In general, the removal of the LP contributions to the partonic scattering cross sections, or more specifically, the cancellation of divergences when $p^2 \to 0$ between the first and the second terms in Eq. (5), or the terms in Eq. (6), can be handled by introducing a regulator for the divergence of each term first, calculating all terms individually, and then removing the regulator after all terms are combined and divergent terms are canceled. Such a general approach for calculating partonic hard parts beyond the LO contribution derived here could be made algorithmic.

Having identified the contact-term prescription, Eq. (12), it is now straightforward to calculate NLP partonic hard parts for all partonic scattering channels at $\mathcal{O}(\alpha_s^3)$, once we specify the projection operators for the spin-color states of the produced heavy quark pair, $[Q\bar{Q}(\kappa)]$. The perturbatively produced collinear heavy quark pair should have four spin states, $s = v, a, t$ for vector, axial-vector, and two tensor states, respectively, and nine color states, $I = 1, 8$ for singlet and octet color states, respectively. The corresponding projection operators have been defined in Ref. [22],

$$\begin{aligned}
\tilde{\mathcal{P}}^{(v)}(p)_{ji,kl} &= (\gamma\cdot p)_{ji}(\gamma\cdot p)_{kl},\\
\tilde{\mathcal{P}}^{(a)}(p)_{ji,kl} &= (\gamma\cdot p\gamma_5)_{ji}(\gamma\cdot p\gamma_5)_{kl},\\
\tilde{\mathcal{P}}^{(t)}(p)_{ji,kl} &= \sum_{\alpha=1,2}(\gamma\cdot p\gamma_\perp^\alpha)_{ji}(\gamma\cdot p\gamma_\perp^\alpha)_{kl},
\end{aligned} \tag{13}$$

for spin states of the produced heavy quark pair, and

$$\begin{aligned}
\tilde{\mathcal{C}}^{[1]}_{ba,dc} &= \left[\frac{\delta_{ba}}{\sqrt{N_c}}\right]\left[\frac{\delta_{dc}}{\sqrt{N_c}}\right],\\
\tilde{\mathcal{C}}^{[8]}_{ba,dc} &= \sum_A [\sqrt{2}(t^A)_{ba}][\sqrt{2}(t^A)_{dc}],
\end{aligned} \tag{14}$$

for the color states of the same pair. In Eq. (13), the spin projection operators are independent of the momentum fractions of the produced heavy quark and antiquark, and the subscripts ji and kl represent the spinor indices of the heavy quark pair in the scattering amplitude and its complex conjugate, respectively. In Eq. (14), the t_A, with $A = 1, 2, \ldots, N_c^2 - 1$ are the generators in the fundamental representation of the group $\mathrm{SU}(N_c)$ color, and the subscripts ba and dc, represent the color indices of the heavy quark pair in the amplitude and those of its complex conjugate, respectively, but with $a, b, c, d = 1, 2, \ldots, N_c$.

From Eq. (12), calculating the short-distance hard part, $d\hat{\sigma}^{(3)}_{q+\bar{q}\to[Q\bar{Q}(\kappa)](p)}$, is the same as calculating the partonic cross section, $d\sigma^{(3)}_{q+\bar{q}\to[Q\bar{Q}(\kappa)](p)}$, with the divergent gluon propagator of momentum p replaced by its contact contribution. From the normalization defined by the factorization formalism in Eqs. (1) and (2), we obtain the expression for the NLP short-distance hard part as

$$E_p\frac{d\hat{\sigma}^{(3)}_{q+\bar{q}\to[Q\bar{Q}(\kappa)](p)}}{d^3p} = \frac{1}{2\hat{s}}|\overline{\mathcal{M}}_{q\bar{q}\to[Q\bar{Q}(\kappa)]}|_c^2\frac{1}{8\pi^2}\delta(\hat{s}+\hat{t}+\hat{u}), \tag{15}$$

where $1/2\hat{s}$ is the partonic flux factor, $|\overline{\mathcal{M}}_{q\bar{q}\to[Q\bar{Q}(\kappa)]}|_c^2$ is the partonic scattering amplitude squared with the initial-state spin and color averaged and the spin-color state of the final-state heavy quark pair defined by the projection operators in Eqs. (13) and (14), and where subscript "c" again indicates the use of the contact term of the divergent gluon propagator of momentum p. Once more, this is equivalent to the removal of the gluonic pole contribution from the gluon with a short bar in Fig. 2, replacing the full propagator by the contact term, $G_c^{\rho\sigma}(p)$, Eq. (11). In Eq. (15), the last factor including the δ-function is from the two-particle phase space, with the differential element

d^3p/E_p moved to the left of the equation. The parton-level Mandelstam variables in Eq. (15) are defined as

$$\hat{s} = (p_1 + p_2)^2, \qquad \hat{t} = (p_1 - p)^2, \quad \text{and} \quad \hat{u} = (p_2 - p)^2, \tag{16}$$

with $\hat{s} + \hat{t} + \hat{u} = 0$ imposed by the δ-function. From Eq. (15), calculating the NLP partonic hard parts at $\mathcal{O}(\alpha_s^3)$ is equivalent to calculating the spin-color averaged partonic scattering matrix element squared with the fragmenting gluonic pole contribution removed.

For convenience, we introduce a slightly simplified partonic hard part, H, to isolate the common factors for all scattering channels,

$$E_p \frac{d\hat{\sigma}^{(3)}_{q+\bar{q}\to[Q\bar{Q}(\kappa)](p)}}{d^3p} \equiv \left[\frac{4\pi\alpha_s^3}{\hat{s}}\right] \frac{1}{\bar{u}u\bar{v}v} H_{q\bar{q}\to[Q\bar{Q}(\kappa)]}(\hat{s},\hat{t},\hat{u})\delta(\hat{s}+\hat{t}+\hat{u}), \tag{17}$$

where the functions H are defined by

$$H_{q\bar{q}\to[Q\bar{Q}(\kappa)]}(\hat{s},\hat{t},\hat{u}) = |\overline{\mathcal{M}}_{q\bar{q}\to[Q\bar{Q}(\kappa)]}|_c^2 \left[\frac{\bar{u}u\bar{v}v}{g_s^6}\right] \tag{18}$$

with coupling constant g_s. The factors u, $\bar{u}$, v and $\bar{v}$ are light-cone momentum fractions of heavy quark momenta P_Q and $P_{\bar{Q}}$ of the scattering amplitude and P'_Q and $P'_{\bar{Q}}$ in its complex conjugate, respectively [22],

$$P_Q = \frac{p}{2} + q_1 = up = \frac{1+\zeta_1}{2}p, \quad P_{\bar{Q}} = \frac{p}{2} - q_1 = \bar{u}p = \frac{1-\zeta_1}{2}p,$$
$$P'_Q = \frac{p}{2} + q_2 = vp = \frac{1+\zeta_2}{2}p, \quad P'_{\bar{Q}} = \frac{p}{2} - q_2 = \bar{v}p = \frac{1-\zeta_2}{2}p. \tag{19}$$

Here, alternate variables ζ_1 and ζ_2 represent the light-cone momentum fraction flow between the heavy quark pair in the scattering amplitude and its complex conjugate, respectively. Although the total momentum of the heavy quark pair in the amplitude and its complex conjugate is the same, $P_Q + P_{\bar{Q}} = P'_Q + P'_{\bar{Q}} = p$, the relative momenta between the pair, q_1 in the amplitude and q_2 in the complex conjugate amplitude, need not be the same. That is, ζ_1 (or u) does not have to equal ζ_2 (or v), while $u + \bar{u} = 1$ and $v + \bar{v} = 1$.

The expression in Eq. (18) is actually useful for calculating the hard parts of all partonic scattering channels, including quark-gluon and gluon-gluon scattering channels at $\mathcal{O}(\alpha_s^3)$.

B. Short-distance coefficient for a heavy quark pair in an axial-vector spin state

For calculating the short-distance coefficients, or hard parts of the partonic process, $q(p_1) + \bar{q}(p_2) \to [Q\bar{Q}(\kappa)](p) + g$ with $\kappa = a1$ and $a8$, we only need to consider two diagrams, (a) and (b) in Fig. 2. The other three diagrams in the figure vanish because of the γ_5 in the axial-vector spin projection operators in Eq. (13).

The only difference between producing a color-singlet and a color-octet heavy quark pair in an axial-vector spin state, $[Q\bar{Q}(a1)]$ vs $[Q\bar{Q}(a8)]$, is the color factor. For producing a color-singlet pair, we find that the four terms from the square of two diagrams (a) and (b) in Fig. 2 have the same color factor, which can be derived from the square of diagram (a), as shown in Fig. 5,

$$C^{[1]} = \left(\frac{1}{N_c}\right)^2 \sum_{A,B,D} \mathrm{Tr}[t^A t^B] \frac{1}{\sqrt{N_c}} \mathrm{Tr}[t^A t^D] \frac{1}{\sqrt{N_c}} \mathrm{Tr}[t^B t^D] = \frac{N_c^2 - 1}{8N_c^3}, \tag{20}$$

where $(1/N_c)^2$ is from the average of the initial-state quark and antiquark color, the $1/\sqrt{N_c}$ factor is from the definition of the color projection operator in Eq. (14), and all color indices are from the labels in Fig. 5. Unlike the color-singlet case, the color factor for producing a color-octet heavy quark pair in an axial-vector spin state is not the same for all four terms from the square of the two diagrams. From Fig. 5, we find for color factors $C^{[8]}_{ij^\dagger}$, with i and j labeling diagrams in the figure,

$$C^{[8]}_{aa^\dagger} = \left(\frac{1}{N_c}\right)^2 \sum_{A,B,D} \mathrm{Tr}[t^A t^B] \sqrt{2}\mathrm{Tr}[t^C t^A t^D] \sqrt{2}\mathrm{Tr}[t^C t^D t^B] = \left[\frac{N_c^2 - 1}{8N_c^3}\right](N_c^2 - 2), \tag{21}$$

where the $\sqrt{2}$ factor is from the definition of the color projection operator in Eq. (14), and generator t^C projects the octet state of the produced heavy quark pair, and is summed over. Similarly, we find the color factor for the other three terms from the squares of the diagrams (a) and (b) in Fig. 2:

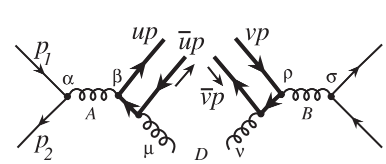

FIG. 5. Square of the diagram (a) in Fig. 2.

$$C^{[8]}_{ab^\dagger} = -\left[\frac{N_c^2-1}{4N_c^3}\right],$$
$$C^{[8]}_{ba^\dagger} = -\left[\frac{N_c^2-1}{4N_c^3}\right] = C^{[8]}_{ab^\dagger},$$
$$C^{[8]}_{bb^\dagger} = \left[\frac{N_c^2-1}{8N_c^3}\right](N_c^2-2) = C^{[8]}_{aa^\dagger}. \tag{22}$$

If we introduce two separate color factors,

$$\mathcal{C}_1 = \left[\frac{N_c^2-1}{8N_c}\right] \quad \text{and} \quad \mathcal{C}_2 = -\left[\frac{N_c^2-1}{4N_c^3}\right], \tag{23}$$

we have

$$C^{[8]}_{aa^\dagger} = C^{[8]}_{bb^\dagger} = \mathcal{C}_1 + \mathcal{C}_2 \quad \text{and} \quad C^{[8]}_{ab^\dagger} = C^{[8]}_{ba^\dagger} = \mathcal{C}_2. \tag{24}$$

For producing a color-singlet axial-vector heavy quark pair, $[Q\bar{Q}(a1)]$, the amplitude squared of diagram (a) in Fig. 2, as shown in Fig. 5, is given by

$$\begin{aligned}
&|\overline{\mathcal{M}}^{aa^\dagger}_{q\bar{q}\to[Q\bar{Q}(a1)]}|^2 \\
&= C^{[1]} g_s^6 \left(\frac{1}{2}\right)^2 \mathrm{Tr}[\gamma\cdot p_1 \gamma^\sigma \gamma\cdot p_2 \gamma^\alpha] \frac{(-g_{\alpha\beta})}{(p_1+p_2)^2} \frac{(-g_{\sigma\rho})}{(p_1+p_2)^2} \\
&\quad \times \mathrm{Tr}\left[\gamma\cdot p\gamma_5 \gamma^\beta \frac{\gamma\cdot(up-p_1-p_2)}{(up-p_1-p_2)^2}\gamma^\mu\right] \\
&\quad \times \mathrm{Tr}\left[\gamma\cdot p\gamma_5 \gamma^\nu \frac{\gamma\cdot(vp-p_1-p_2)}{(vp-p_1-p_2)^2}\gamma^\rho\right](-g_{\mu\nu}) \\
&= C^{[1]}\left[\frac{g_s^6}{\bar{u}\,\bar{v}}\right]\frac{4}{\hat{s}}\left[\frac{\hat{t}^2+\hat{u}^2}{\hat{s}^2}\right],
\end{aligned} \tag{25}$$

where the Feynman gauge was used for this gauge-invariant quantity. Similarly, we find the other three terms from the squares of the diagrams (a) and (b) in Fig. 2:

$$|\overline{\mathcal{M}}^{ab^\dagger}_{q\bar{q}\to[Q\bar{Q}(a1)]}|^2 = C^{[1]}\left[\frac{g_s^6}{\bar{u}v}\right]\frac{4}{\hat{s}}\left[\frac{\hat{t}^2+\hat{u}^2}{\hat{s}^2}\right], \tag{26}$$

$$|\overline{\mathcal{M}}^{ba^\dagger}_{q\bar{q}\to[Q\bar{Q}(a1)]}|^2 = C^{[1]}\left[\frac{g_s^6}{u\bar{v}}\right]\frac{4}{\hat{s}}\left[\frac{\hat{t}^2+\hat{u}^2}{\hat{s}^2}\right], \tag{27}$$

$$|\overline{\mathcal{M}}^{bb^\dagger}_{q\bar{q}\to[Q\bar{Q}(a1)]}|^2 = C^{[1]}\left[\frac{g_s^6}{uv}\right]\frac{4}{\hat{s}}\left[\frac{\hat{t}^2+\hat{u}^2}{\hat{s}^2}\right]. \tag{28}$$

Combining the four terms in Eqs. (25), (26), (27), and (28), and using an identity satisfied by the momentum fractions defined in Eq. (19),

$$\frac{1}{\bar{u}\,\bar{v}} + \frac{1}{\bar{u}v} + \frac{1}{u\bar{v}} + \frac{1}{uv} = \frac{1}{\bar{u}u\bar{v}v}, \tag{29}$$

we derive the spin-color averaged matrix element squared for the partonic channel, $q(p_1)+\bar{q}(p_2)\to[Q\bar{Q}(a1)](p)+g$, as

$$|\overline{\mathcal{M}}_{q\bar{q}\to[Q\bar{Q}(a1)]}|^2 = \left[\frac{g_s^6}{\bar{u}u\bar{v}v}\right]4C^{[1]}\left[\frac{\hat{t}^2+\hat{u}^2}{\hat{s}^3}\right], \tag{30}$$

where we have suppressed the subscript "c" for the squared matrix element, because no LP subtraction is necessary for these diagrams. From the definition of the modified hard part in Eq. (18), we have

$$H_{q\bar{q}\to[Q\bar{Q}(a1)]}(\hat{s},\hat{t},\hat{u}) = 4\left[\frac{N_c^2-1}{8N_c^3}\right]\left[\frac{\hat{t}^2+\hat{u}^2}{\hat{s}^3}\right]. \tag{31}$$

Since the spinor trace and the contraction of Lorentz indices are independent of the color, we derive the partonic scattering matrix element square for producing a $[Q\bar{Q}(a8)]$ pair as

$$|\overline{\mathcal{M}}^{aa^\dagger}_{q\bar{q}\to[Q\bar{Q}(a8)]}|^2 = C^{[8]}_{aa^\dagger}\left[\frac{g_s^6}{\bar{u}\,\bar{v}}\right]\frac{4}{\hat{s}}\left[\frac{\hat{t}^2+\hat{u}^2}{\hat{s}^2}\right], \tag{32}$$

$$|\overline{\mathcal{M}}^{ab^\dagger}_{q\bar{q}\to[Q\bar{Q}(a8)]}|^2 = C^{[8]}_{ab^\dagger}\left[\frac{g_s^6}{\bar{u}v}\right]\frac{4}{\hat{s}}\left[\frac{\hat{t}^2+\hat{u}^2}{\hat{s}^2}\right], \tag{33}$$

$$|\overline{\mathcal{M}}^{ba^\dagger}_{q\bar{q}\to[Q\bar{Q}(a8)]}|^2 = C^{[8]}_{ba^\dagger}\left[\frac{g_s^6}{u\bar{v}}\right]\frac{4}{\hat{s}}\left[\frac{\hat{t}^2+\hat{u}^2}{\hat{s}^2}\right], \tag{34}$$

$$|\overline{\mathcal{M}}^{bb^\dagger}_{q\bar{q}\to[Q\bar{Q}(a8)]}|^2 = C^{[8]}_{bb^\dagger}\left[\frac{g_s^6}{uv}\right]\frac{4}{\hat{s}}\left[\frac{\hat{t}^2+\hat{u}^2}{\hat{s}^2}\right]. \tag{35}$$

Combining all four terms together, recognizing

$$\begin{aligned}
&\frac{1}{\bar{u}\,\bar{v}}C^{[8]}_{aa^\dagger} + \frac{1}{\bar{u}v}C^{[8]}_{ab^\dagger} + \frac{1}{u\bar{v}}C^{[8]}_{ba^\dagger} + \frac{1}{uv}C^{[8]}_{bb^\dagger} \\
&\quad = \frac{1}{\bar{u}u\bar{v}v}\left[\frac{1}{2}(1+\zeta_1\zeta_2)\mathcal{C}_1 + \mathcal{C}_2\right],
\end{aligned} \tag{36}$$

and using $\mathcal{C}_1$ and $\mathcal{C}_2$ from Eq. (23), we obtain

$$H_{q\bar{q}\to[Q\bar{Q}(a8)]}(\hat{s},\hat{t},\hat{u}) = 2\left[\frac{N_c^2-1}{8N_c}\right]\left[1+\zeta_1\zeta_2-\frac{4}{N_c^2}\right]\left[\frac{\hat{t}^2+\hat{u}^2}{\hat{s}^3}\right], \tag{37}$$

where ζ_1 and ζ_2 are heavy quark momentum fractions defined in Eq. (19).

C. Short-distance coefficient for a heavy quark pair production with vector spin

For producing a color-singlet heavy quark pair from quark-antiquark scattering at $\mathcal{O}(\alpha_s^3)$, only diagrams (a) and (b) in Fig. 2 contribute, since the other three diagrams can only produce the pair in a color-octet state. Since the color is independent of the spin state of the pair, the color factor for producing a color-singlet pair in a vector spin state is the same as $C^{[1]}$ in Eq. (20).

Similar to Eq. (25), we have from the diagram in Fig. 5

$$
\begin{aligned}
&|\overline{\mathcal{M}}^{aa^\dagger}_{q\bar{q}\to[Q\bar{Q}(v1)]}|^2 \\
&= C^{[1]} g_s^6 \left(\frac{1}{2}\right)^2 \mathrm{Tr}[\gamma\cdot p_1 \gamma^\sigma \gamma\cdot p_2 \gamma^\alpha] \frac{(-g_{\alpha\beta})}{(p_1+p_2)^2} \frac{(-g_{\sigma\rho})}{(p_1+p_2)^2} \\
&\quad \times \mathrm{Tr}\left[\gamma\cdot p \gamma^\beta \frac{\gamma\cdot(up-p_1-p_2)}{(up-p_1-p_2)^2}\gamma^\mu\right] \\
&\quad \times \mathrm{Tr}\left[\gamma\cdot p \gamma^\nu \frac{\gamma\cdot(vp-p_1-p_2)}{(vp-p_1-p_2)^2}\gamma^\rho\right](-g_{\mu\nu}) \\
&= C^{[1]}\left[\frac{g_s^6}{\bar{u}\,\bar{v}}\right]\frac{4}{\hat{s}}\left[\frac{\hat{t}^2+\hat{u}^2}{\hat{s}^2}\right], \qquad (38)
\end{aligned}
$$

which is the same as $|\overline{\mathcal{M}}^{aa^\dagger}_{q\bar{q}\to[Q\bar{Q}(a1)]}|^2$. In the same way, we find for the other three terms contributing to the production of a $[Q\bar{Q}(v1)]$ pair

$$|\overline{\mathcal{M}}^{ab^\dagger}_{q\bar{q}\to[Q\bar{Q}(v1)]}|^2 = -C^{[1]}\left[\frac{g_s^6}{\bar{u}v}\right]\frac{4}{\hat{s}}\left[\frac{\hat{t}^2+\hat{u}^2}{\hat{s}^2}\right], \qquad (39)$$

$$|\overline{\mathcal{M}}^{ba^\dagger}_{q\bar{q}\to[Q\bar{Q}(v1)]}|^2 = -C^{[1]}\left[\frac{g_s^6}{u\bar{v}}\right]\frac{4}{\hat{s}}\left[\frac{\hat{t}^2+\hat{u}^2}{\hat{s}^2}\right], \qquad (40)$$

$$|\overline{\mathcal{M}}^{bb^\dagger}_{q\bar{q}\to[Q\bar{Q}(v1)]}|^2 = C^{[1]}\left[\frac{g_s^6}{uv}\right]\frac{4}{\hat{s}}\left[\frac{\hat{t}^2+\hat{u}^2}{\hat{s}^2}\right], \qquad (41)$$

where the interference terms have the opposite sign compared to the corresponding terms for producing a $[Q\bar{Q}(a1)]$ pair, Eqs. (26) and (27). Combining Eqs. (38), (39), (40), and (41), we obtain

$$H_{q\bar{q}\to[Q\bar{Q}(v1)]}(\hat{s},\hat{t},\hat{u}) = 4\left[\frac{N_c^2-1}{8N_c^3}\right]\left[\frac{\hat{t}^2+\hat{u}^2}{\hat{s}^3}\right]\zeta_1\zeta_2, \qquad (42)$$

which differs from $H_{q\bar{q}\to[Q\bar{Q}(a1)]}(\hat{s},\hat{t},\hat{u})$ only by an overall factor of $\zeta_1\zeta_2$, and vanishes if the produced heavy quark and antiquark have the same momentum.

For the production of a color-octet heavy quark pair in a vector spin state from quark and antiquark scattering at $\mathcal{O}(\alpha_s^3)$, all five diagrams in Fig. 2 can contribute. With three more diagrams for producing a $[Q\bar{Q}(v8)]$ pair, each combination of the diagrams in the scattering amplitude and its complex conjugate has its unique color factor, labeled $C^{[8]}_{ij^\dagger}$ for diagram "i" multiplied by the complex conjugate diagram "j" with $i, j =$ (a), (b), (c), (d), and (e) in Fig. 2. We find, however, that all of these 25 color factors can be expressed in terms of the two color factors, $\mathcal{C}_1$ and $\mathcal{C}_2$, as defined in Eq. (23), and we present all of them in Table I. To normalize the color factor involving the three-gluon vertex, we take the following convention for the

TABLE I. Color factors for all combinations of diagrams in the scattering amplitude and its complex conjugate for the partonic process, $q+\bar{q}\to[Q\bar{Q}(v8)]+g$, expressed in terms of $\mathcal{C}_1$ and $\mathcal{C}_2$ defined in Eq. (23).

$C^{[8]}_{ij^\dagger}$	(a)	(b)	(c)	(d)	(e)
(a)	$\mathcal{C}_1+\mathcal{C}_2$	$\mathcal{C}_2$	$-\mathcal{C}_1$	$\mathcal{C}_1+\mathcal{C}_2$	$\mathcal{C}_2$
(b)	$\mathcal{C}_2$	$\mathcal{C}_1+\mathcal{C}_2$	$\mathcal{C}_1$	$\mathcal{C}_2$	$\mathcal{C}_1+\mathcal{C}_2$
(c)	$-\mathcal{C}_1$	$\mathcal{C}_1$	$2\mathcal{C}_1$	$-\mathcal{C}_1$	$\mathcal{C}_1$
(d)	$\mathcal{C}_1+\mathcal{C}_2$	$\mathcal{C}_2$	$-\mathcal{C}_1$	$\mathcal{C}_1+\mathcal{C}_2/2$	$\mathcal{C}_2/2$
(e)	$\mathcal{C}_2$	$\mathcal{C}_1+\mathcal{C}_2$	$\mathcal{C}_1$	$\mathcal{C}_2/2$	$\mathcal{C}_1+\mathcal{C}_2/2$

Feynman rule of the three-gluon vertex. For the three-gluon vertex of diagram (c) in Fig. 2, we let $-g_s f^{\mathrm{EAD}} = (-ig_s)(-if^{\mathrm{EAD}})$, and include the "$(-if^{\mathrm{EAD}})$" in the calculation of the color factor, while keeping "$(-ig_s)$" with the calculation of the rest of diagram. We follow the same convention for the three-gluon vertices in the complex conjugate of the scattering amplitude.

From our discussion leading to Eq. (18), we need to calculate the initial-state spin-color averaged scattering amplitude square, $|\overline{\mathcal{M}}_{q\bar{q}\to[Q\bar{Q}(v8)]}|^2_c$, for a quark and an antiquark to produce a heavy $[Q\bar{Q}(v8)]$ pair with the LP gluonic pole contribution removed. That is, we need to use the contact term of the gluon propagator for the gluon with a short bar and momentum p in Fig. 2. Although three particles are produced in the final state, the scattering process, $q(p_1)+\bar{q}(p_2)\to[Q\bar{Q}(v8)](p)+g(k)$, has effectively a "$2\to 2$" kinematics, and has three independent external momenta due to momentum conservation, $p_1+p_2=p+k$. With the use of the contact term for the gluon propagator, Eq. (11), $i\hat{n}^\mu\hat{n}^\nu/(p\cdot\hat{n})^2$, the calculated partonic hard parts for this production channel, $q(p_1)+\bar{q}(p_2)\to[Q\bar{Q}(v8)](p)+g(k)$, can depend on the ratios $p_1\cdot\hat{n}/p\cdot\hat{n}$ and $p_2\cdot\hat{n}/p\cdot\hat{n}$, if we choose p_1, p_2, and p as the three independent momentum vectors for this partonic subprocess.

In Eq. (11), the auxiliary vector $\hat{n}^\mu$ is defined to be conjugate to the heavy quark pair momentum p^μ, in the sense defined after Eq. (9). Since the squares of the diagrams in Fig. 2, $|\overline{\mathcal{M}}_{q\bar{q}\to[Q\bar{Q}(v8)]}|^2$, are Lorentz invariant, and the subtraction term that removes the LP contribution in Eq. (7) is Lorentz invariant, the NLP hard part defined in Eq. (18) is Lorentz invariant as well. That is, with the "$2\to 2$" kinematics, the NLP hard parts can be expressed in terms of the Mandelstam variables defined in Eq. (16), as can the ratios $p_1\cdot\hat{n}/p\cdot\hat{n}$ and $p_2\cdot\hat{n}/p\cdot\hat{n}$. Since the inner products, $p_1\cdot\hat{n}$, $p_2\cdot\hat{n}$, and $p\cdot\hat{n}$, are Lorentz scalars, we can evaluate them in any Lorentz frame. The most convenient choice of $\hat{n}^\mu$ makes the gluon polarization in Eq. (9) transverse in the center of mass frame of the parton-parton scattering, in which the heavy quark pair moves along the z-axis, and the unobserved final-state parton of momentum $k^\mu = p_1^\mu + p_2^\mu - p^\mu$ with $k^2=0$ moves along the $-z$-axis, back-to-back to the p^μ. In this frame, the unobserved final-state parton momentum k^μ should be exactly proportional to the auxiliary vector $\hat{n}^\mu$. Since the contact term of the gluon propagator is invariant when the vector $\hat{n}^\mu$ is rescaled, we can write the contact term of the gluon propagator of momentum p in this frame as

$$\frac{i\hat{n}^\mu \hat{n}^\nu}{(p\cdot\hat{n})^2} = \frac{ik^\mu k^\nu}{(p\cdot k)^2}. \tag{43}$$

Thus, we can replace $\hat{n}^\mu$ by k^μ for our calculation of the NLP hard parts in this frame. The Lorentz-invariant ratios involving the $\hat{n}^\mu$ vector can be then expressed in terms of the Mandelstam variables as

$$\frac{p_1\cdot\hat{n}}{p\cdot\hat{n}} = \frac{-\hat{u}}{\hat{s}}, \qquad \frac{p_2\cdot\hat{n}}{p\cdot\hat{n}} = \frac{-\hat{t}}{\hat{s}}. \tag{44}$$

The Lorentz invariance of these ratios and of the scattering amplitude ensures that the NLP hard parts evaluated in this frame are valid in all other Lorentz frames, including the center-of-mass frame of the colliding hadrons or the lab frame. This simplification is specific to the $2\to 2$ subprocess that characterizes this calculation of the NLP cross section at LO.

With the Feynman diagrams in Fig. 2, spin projection operators in Eq. (13), the contact gluon propagator in Eq. (43), and the calculated color factors in Table I, it is straightforward to derive the hard parts for the partonic production channel, $q(p_1)+\bar{q}(p_2)\to[Q\bar{Q}(v8)](p)+g(k)$. Since all color factors from combinations of the diagrams in Fig. 2 and its complex conjugate can be expressed in terms of two color factors, $\mathcal{C}_1$ and $\mathcal{C}_2$, as shown in Table I, we express our calculated short-distance hard part of this channel as

$$H_{q\bar{q}\to[Q\bar{Q}(v8)]}(\hat{s},\hat{t},\hat{u}) = 2\left[\frac{N_c^2-1}{8N_c}\right]\mathcal{H}_1(\hat{s},\hat{t},\hat{u}) + 4\left[-\frac{N_c^2-1}{4N_c^3}\right]\mathcal{H}_2(\hat{s},\hat{t},\hat{u}), \tag{45}$$

where we find that

$$\begin{aligned}\mathcal{H}_1 &= \frac{\hat{t}^2+\hat{u}^2}{\hat{s}^3}[(1+\zeta_1\zeta_2)\zeta_1\zeta_2+4(1-\zeta_1^2)(1-\zeta_2^2)] \\ &\quad + \frac{\hat{t}^2-\hat{u}^2}{\hat{s}^3}[(1-\zeta_1\zeta_2)(\zeta_1+\zeta_2)] \\ &\quad - \frac{(\hat{t}-\hat{u})^2}{\hat{s}^3}[\zeta_1^2(1-\zeta_2^2)+\zeta_2^2(1-\zeta_1^2)], \\ \mathcal{H}_2 &= \frac{\hat{t}^2+\hat{u}^2}{\hat{s}^3}[\zeta_1\zeta_2] + \frac{\hat{t}^2-\hat{u}^2}{\hat{s}^3}[\zeta_1(1-\zeta_2^2)+\zeta_2(1-\zeta_1^2)] \\ &\quad + \frac{1}{\hat{s}}[(1-\zeta_1^2)(1-\zeta_2^2)].\end{aligned} \tag{46}$$

This result for the $(v8)$ heavy pair color-spin configuration, together with Eqs. (31), (37) and (42) for the $(a1)$, $(a8)$ and $(v1)$ configurations, respectively, gives the full $\mathcal{O}(\alpha_s^3)$ contribution to heavy pair production in the light pair channel. The partonic short-distance hard part for producing a heavy quark pair in a tensor spin state from the scattering of a light quark pair vanishes at the order of α_s^3. This is simply because the tensor spin projection operator in Eq. (13) has an even number of Dirac γ matrices, and the trace of an odd number of γ-matrices vanishes.

Using essentially the same methods described in this section, we have calculated the NLP short-distance hard parts for other partonic scattering channels at $\mathcal{O}(\alpha_s^3)$, including $q+g\to[Q\bar{Q}(\kappa)]+q$, $g+q\to[Q\bar{Q}(\kappa)]+q$, and $g+g\to[Q\bar{Q}(\kappa)]+g$, with the produced heavy quark pair in all possible spin-color states. The complete results of perturbatively calculated hard parts for all partonic scattering channels are presented in the Appendix.

III. PREDICTIVE POWER AND CONNECTION TO NRQCD

Even with the first nontrivial order of partonic hard parts calculated in this paper, and additional future improvement of the hard parts with higher-order perturbative corrections, the predictive power of the QCD collinear factorization formalism in Eq. (1) for heavy quarkonium production still relies on knowledge of the nonperturbative, but universal, heavy quarkonium fragmentation functions: $D_{f\to H}(z,\mu_F^2;m_Q)$ and $\mathcal{D}_{[Q\bar{Q}(\kappa)]\to H}(z,u,v,\mu_F^2;m_Q)$. As derived in Ref. [22], these universal heavy quarkonium FFs satisfy a closed set of evolution equations that determines their dependence on the factorization scale, μ_F. The first nontrivial order of all evolution kernels is also available in Ref. [22]. Higher-order corrections to these evolution kernels could be systematically calculated in perturbation theory. That is, we are able, in principle, to derive all heavy quarkonium FFs at any factorization scale μ_F with a set of input distributions at an initial factorization scale, $\mu_0 \gtrsim 2m_Q$, at which the power-suppressed contribution in $1/\mu_F^2$ is compatible with the leading logarithmic contribution in $\ln\mu_F^2$. Like all other QCD factorization formalisms, the predictive power of the factorization formula for heavy quarkonium production in Eq. (1) thus depends on a set of nonperturbative input FFs (as well as the input PDFs for hadronic collisions). Since both the short-distance partonic hard parts and the evolution kernels of these FFs are perturbatively calculated, it is the FFs at input scale μ_0 that are the most sensitive to the detailed properties of the heavy quarkonia produced, including their spin and angular momenta. If we were to follow the procedure familiar for light parton PDFs and FFs, we would need to extract heavy quarkonium nonperturbative input FFs from experimental data or possible lattice QCD calculations, similar to the extraction of light hadron, such as pion or proton, FFs.

However, unlike the light hadron FFs, heavy quarkonium FFs at the input scale $\mu_0 \gtrsim 2m_Q$ depend on a large perturbative scale—the heavy quark mass, $m_Q \sim \mathcal{O}(\mu_0) \gg \Lambda_{\rm QCD}$. Even more importantly, this perturbative scale is substantially separated from the momentum scale needed for the binding of heavy quarkonium, $m_Q v$ and any other nonperturbative scales of the bound state. With such a clear separation of momentum scales, NRQCD is a natural effective theory of QCD to separate the dynamics of the fragmentation process at the perturbative scale $\mu_0 \sim \mathcal{O}(m_Q)$ from the physics at the scale $m_Q v$ and below. Appealing to NRQCD factorization for this production process as a very plausible conjecture, we can, at least as a reasonable model, express all heavy quarkonium FFs in terms of the universal NRQCD long-distance matrix elements (LDMEs) with perturbatively calculated functional dependence on the momentum fractions, z, ζ_1, and ζ_2. In this approach, all input heavy quarkonium FFs are expanded in terms of the LDMEs, according to their effective powers in heavy quark velocity v in the heavy quark pair's rest frame. These LDMEs are the same as those used in light parton FFs to heavy quarkonia, so that this approach has the attractive feature of introducing no new nonperturbative parameters relative to those that are already in the LP expansion [31]. The perturbatively calculated coefficient for each LDME is further expanded in terms of the power of the strong coupling constant $\alpha_s(\mu_0)$. With the small value of the velocity, v, the perturbative expansion of all heavy quarkonium FFs can be expressed in terms of a very small number of universal LDMEs for each physical quarkonium state to enhance the predictive power of the QCD factorization formalism in Eq. (1) tremendously.

A. NRQCD factorization and input fragmentation functions

The NRQCD factorization approach to heavy quarkonium production was proposed to express the inclusive cross section for the direct production of a quarkonium state H as a sum of "short-distance" coefficients times NRQCD LDMEs [2],

$$\sigma^H(p_T, m_Q) = \sum_{[Q\bar{Q}(n)]} \hat{\sigma}_{[Q\bar{Q}(n)]}(p_T, m_Q, \mu_\Lambda)\langle 0|\mathcal{O}^H_{[Q\bar{Q}(n)]}(\mu_\Lambda)|0\rangle, \quad (47)$$

where p_T is the transverse momentum of produced heavy quarkonium, and $\mu_\Lambda \sim \mathcal{O}(m_Q)$ is the ultraviolet cutoff of the NRQCD effective theory, or equivalently the factorization scale of the factorization formalism. When the physical scale $p_T \gg m_Q$, it was demonstrated in Ref. [22] that the perturbative expansion of the short-distance coefficient functions, $\hat{\sigma}_{[Q\bar{Q}(n)]}(p_T, m_Q, \mu_\Lambda)$ in Eq. (47), in powers of α_s is not always stable, since high orders in α_s can be enhanced by the powers of p_T/m_Q, as well as powers of large logarithms in $\ln(p_T/m_Q)$. The QCD factorization formalism in Eq. (1) was in fact proposed to reorganize both of these large power and logarithmic enhancements.

With the input factorization scale, $\mu_0 \sim \mathcal{O}(m_Q)$, and the large momentum scale separation between μ_0 and all other nonperturbative scales of the heavy quarkonium, we propose as above and as a conjecture, to use NRQCD factorization for calculating the heavy quarkonium FFs at the input scale μ_0 as

$$D_{f\to H}(z, \mu_0^2; m_Q) = \sum_{[Q\bar{Q}(n)]} \hat{d}_{f\to[Q\bar{Q}(n)]}(z, \mu_0^2; m_Q, \mu_\Lambda)\langle \mathcal{O}^H_{[Q\bar{Q}(n)]}(\mu_\Lambda)\rangle \quad (48)$$

for the heavy quarkonium FFs from a single parton of flavor $f = q, \bar{q}, g$, and

$$\mathcal{D}_{[Q\bar{Q}(\kappa)]\to H}(z, u, v, \mu_0^2; m_Q) = \sum_{[Q\bar{Q}(n)]} \hat{d}_{[Q\bar{Q}(\kappa)]\to[Q\bar{Q}(n)]}(z, u, v, \mu_0^2; m_Q, \mu_\Lambda)\langle \mathcal{O}^H_{[Q\bar{Q}(n)]}(\mu_\Lambda)\rangle \quad (49)$$

for the heavy quarkonium FFs from a perturbatively produced heavy quark pair of the spin-color state κ defined in Sec. II. In Eq. (48), $\hat{d}_{f\to[Q\bar{Q}(n)]}(z, \mu_0^2; m_Q, \mu_\Lambda)$ is the perturbatively calculable short-distance coefficient function for an off-shell parton of flavor f to evolve into a nonrelativistic heavy quark pair represented by $[Q\bar{Q}(n)]$ with n expressed in terms of the standard spectroscopic notation, ${}^{2S+1}L_J^{[1,8]}$, according to the spin S, orbital angular momentum L, and total angular momentum J, as well as the color state ([1] for singlet and [8] for octet) of the pair. Similarly, $\hat{d}_{[Q\bar{Q}(\kappa)]\to[Q\bar{Q}(n)]}(z, u, v, \mu_0^2; m_Q, \mu_\Lambda)$ are the short-distance coefficient functions for an off-shell perturbatively produced heavy quark pair with the spin-color quantum number κ to evolve into the same nonrelativistic heavy quark pair state $[Q\bar{Q}(n)]$.

Since the short-distance coefficient functions, $\hat{d}_{f\to[Q\bar{Q}(n)]}(z, \mu_0^2; m_Q, \mu_\Lambda)$ in Eq. (48), and $\hat{d}_{[Q\bar{Q}(\kappa)]\to[Q\bar{Q}(n)]}(z, u, v, \mu_0^2; m_Q, \mu_\Lambda)$ in Eq. (49), are not sensitive to the details of the produced heavy quarkonium H, they can be calculated systematically by projecting the factorization formalisms in Eqs. (48) and (49) on a pair of nonrelativistic heavy quarks of mass m_Q. Note that the heavy quarkonium fragmentation functions defined in both Eqs. (48) and (49) are boost invariant along the direction of heavy quarkonium momentum p^μ. Let $[Q\bar{Q}(c)]$ be such a state with c expressed in terms of the standard spectroscopic notation. The corresponding projection operators for such a nonrelativistic heavy quark pair are given in Appendix A of

Ref. [26], or in the references therein. By expanding both sides of the factorization formulas in Eqs. (48) and (49) order-by-order in powers of α_s, the short-distance coefficient functions can be perturbatively extracted by calculating both sides in perturbation theory.

For example, by expanding the factorization formula in Eq. (49) for producing a nonrelativistic heavy quark pair, $[Q\bar{Q}(^1S_0^{[8]})]$, to zeroth order in power of α_s, we have [26]

$$\mathcal{D}^{(0)}_{[Q\bar{Q}(\kappa)]\to[Q\bar{Q}(^1S_0^{[8]})]}(z,u,v) = \hat{d}^{(0)}_{[Q\bar{Q}(\kappa)]\to[Q\bar{Q}(^1S_0^{[8]})]}(z,u,v), \tag{50}$$

where the superscript "(0)" indicates the zeroth order in powers of α_s, the dependence on the heavy quark mass and factorization scales are suppressed, and the normalization of NRQCD LDMEs, $\langle\mathcal{O}^{[Q\bar{Q}(^1S_0^{[8]})]}_{[Q\bar{Q}(n)]}(0)\rangle^{(0)} = 1$ with $n = {}^1S_0^{[8]}$, is used. The perturbatively produced heavy quark pair states, $[Q\bar{Q}(\kappa)]$, are defined in terms of relativistic heavy quark field operators in QCD with the vector, axial-vector, and tensor spin states and singlet and octet color states, along with the projection operators defined in Ref. [22]. On the other hand, the NRQCD states of a heavy quark pair are defined in terms of nonrelativistic heavy quark fields of NRQCD. As a result, there can be nontrivial matching coefficients even at zeroth order in α_s. With our definition of heavy quarkonium FFs and the normalization of NRQCD LDMEs, we have, for example,

$$\hat{d}^{(0)}_{[Q\bar{Q}(a8)]\to[Q\bar{Q}(^1S_0^{[8]})]}(z,u,v) = \frac{1}{N_c^2-1}\frac{1}{2m_Q}\delta(1-z)\delta(2u-1)\delta(2v-1), \tag{51}$$

where $u = (1-\zeta_1)/2$ and $v = (1-\zeta_2)/2$. A complete list of the zeroth-order short-distance coefficient functions can be found in Ref. [26].

Beyond the LO in α_s, the partonic FFs to a nonrelativistic heavy quark pair on the left-hand side of the factorization formulas in both Eqs. (48) and (49) have several types of perturbative divergences, as do the NRQCD LDMEs to a nonrelativistic heavy quark pair on the right-hand side of these equations. With the finite heavy quark mass, m_Q, the partonic FFs on the left-hand side of Eqs. (48) and (49) have no CO divergence. The UV divergence associated with the composite operators defining the FFs are systematically removed by the UV counterterms (UVCT), required as a necessary part of the definition of these FFs, while the UV divergences associated with the virtual loop diagrams are taken care of by the standard renormalization of QCD perturbation theory. The factorization scheme, associated with the cancellation of the UV divergence between the partonic FFs and the UVCT, should be chosen to be the same as the factorization scheme used to calculate the short-distance partonic hard parts of the QCD collinear factorization formalism in Eq. (1). For calculating the partonic FFs for producing a heavy quark pair in a nonrelativistic S-wave state, the IR divergence associated with contributions from individual Feynman diagrams completely cancels at any given order of α_s after we sum up all contributions at this order. However, for calculating the partonic FFs of producing a heavy quark pair in a nonrelativistic P-wave or higher orbital angular momentum state, IR divergences (as well as what is often referred to as the rapidity divergence [32–36] in the context of transverse-momentum-dependent factorization formalism [37]) cannot be completely canceled by summing over contributions from all diagrams [27]. Instead, IR divergences (and the rapidity divergences) should be canceled by corresponding divergences in the NRQCD LDMEs on the rhs of the factorization formalism, as required by factorization. In addition to the UV and IR divergences, the partonic FFs for producing a pair of heavy quarks have Coulomb divergences from the exchange of soft gluons between the pair. The Coulomb divergence of the partonic FFs on the lhs of Eqs. (48) and (49) should be exactly canceled by the Coulomb divergence of the NRQCD LDMEs on the rhs to ensure the validity of the factorization. Although there is no formal proof for the NRQCD factorization formalisms in Eqs. (48) and (49), the NLO calculation of the short-distance hard parts for both the single parton and heavy quark pair FFs in Refs. [26,27] confirms that all UV, IR (as well as rapidity), and Coulomb divergences are completely canceled to leave all hard parts at this order infrared safe (IRS). NRQCD factorization effectively predicts the functional dependence of the heavy quarkonium FFs in terms of momentum fractions: z, u, and v (or equivalently z, ζ_1 and ζ_2), and NRQCD LDMEs up to the approximation to truncate the perturbative expansion in powers of α_s and v in Eqs. (48) and (49) [28].

It is the input FFs that are the most sensitive to the characteristics of the individual heavy quarkonia produced in high-energy scattering, since both the short-distance partonic hard parts in the QCD collinear factorization formalism in Eq. (1) and the evolution kernels of the FFs are perturbatively calculated and completely universal for the production of any heavy quarkonium states. The input FFs determine the difference in the production of various states, including their spin and polarization dependencee, as well as the normalization of their production rates. The QCD factorization in Eq. (1) assures that these input FFs are universal regardless of whether the heavy quarkonium state is produced in hadron-hadron, lepton-hadron or lepton-lepton collisions. In summary, input FFs are essential for understanding the characteristic differences between all heavy quarkonium states produced.

B. Relation between QCD factorization and NRQCD factorization

The NRQCD factorization for the input FFs in Eqs. (48) and (49) is independent of the QCD collinear factorization in Eq. (1). The two factorizations have their own power counting and perturbative expansions. The QCD factorization is valid up to the first-power corrections in the $1/p_T^2$ expansion of the cross section, while the short-distance hard parts and evolution kernels of FFs can be systematically improved by calculating higher-order corrections in powers of α_s. As noted above, although the NRQCD factorization has not been fully proved perturbatively for high orders in powers α_s and v, explicit NLO calculation up to v^4 in LDMEs verifies the factorization. In order to best compare with experimental data, it is important to get the most accurate calculations from each factorization series, and in particular, the NRQCD factorization for the input FFs to test the universality of these functions.

If the NRQCD factorization for the input FFs in Eqs. (48) and (49) is valid to all orders in α_s and the relative heavy quark velocity v, the validity of the QCD collinear factorization formalism for heavy quarkonium production in Eq. (1) effectively ensures that the NRQCD factorization for the production cross section in Eq. (47) is valid at least for the LP and NLP terms in the $1/p_T$ expansion. In addition, the QCD factorization formalism reorganizes the perturbative expansion of NRQCD factorization by resumming all powers of $\ln(p_T/m_Q)$. However, this equivalence between QCD factorization and NRQCD factorization does not say anything about the validity of the NRQCD factorized cross section in Eq. (47) beyond the NLP terms.

In terms of QCD collinear factorization in Eq. (1), all partonic hard parts for production cross sections and evolution kernels of the FFs are calculated with the heavy quark mass neglected. The heavy quark mass dependence of the NRQCD factorization for the production cross section can be systematically included by the following perturbative matching formalism:

$$E_P\frac{d\sigma_{A+B\to H+X}}{d^3P}(P,m_Q)\equiv E_P\frac{d\sigma^{\text{QCD}}_{A+B\to H+X}}{d^3P}(P,m_Q=0) + E_P\frac{d\sigma^{\text{NRQCD}}_{A+B\to H+X}}{d^3P}(P,m_Q\neq 0) - E_P\frac{d\sigma^{\text{QCD-Asym}}_{A+B\to H+X}}{d^3P}(P,m_Q=0), \tag{52}$$

where σ^{QCD} is given in Eq. (1) with the input FFs calculated in NRQCD factorization, σ^{NRQCD} is given by Eq. (47) with only the LP and NLP terms in the $1/p_T$ expansion, and the "asymptotic" $\sigma^{\text{QCD-Asym}}$ is defined to be the same as σ^{QCD} with the FFs expanded to a fixed order in both α_s and v to match the order used to calculate σ^{NRQCD}. If the NRQCD factorization formalism in Eq. (47) is valid beyond the NLP, the σ^{NRQCD} in Eq. (52) should include terms beyond the NLP. In Eq. (52), the first term on the rhs is more reliable for large p_T, while the second term is more suited for the low-p_T region, and the third term effectively removes the double counting at any given fixed order in powers of α_s. Consequently, the combined formula in Eq. (52) could be consistent with experimental measurement of heavy quarkonium cross sections for a wider range of $p_T(> m_Q)$.

C. An example

In this subsection, we provide an explicit example to demonstrate how the very large and complex NLO contribution to the heavy quarkonium production calculated in the color-singlet model (also in NRQCD) can be reproduced by a much simpler and fully analytic LO calculation in terms of QCD factorization, Eq. (1) with the FFs calculated in NRQCD. The same comparison for other partonic production channels can be found in Ref. [28].

From the QCD factorization formalism in Eq. (1) and the NRQCD factorization formalisms in Eqs. (48) and (49), we found that the LO contribution to the production of a color-singlet spin-1 heavy quark pair, $[Q\bar{Q}(^3S_1^{[1]})]$, which matches to a physical heavy quarkonium H by a NRQCD LDME, $\langle\mathcal{O}^H_{[Q\bar{Q}(^3S_1^{[1]})]}\rangle$, is given by the combination of producing a color-octet heavy quark pair, which fragments into a color-singlet and spin-1 NRQCD state, $[Q\bar{Q}(^3S_1^{[1]})]$. At the order of α_s, only the pair in a vector $[Q\bar{Q}(v8)]$ or an axial-vector $[Q\bar{Q}(a8)]$ spin state can fragment into the spin-1 NRQCD state.[1] The LO partonic hard parts at $\mathcal{O}(\alpha_s^3)$ for producing a heavy quark pair in both $[Q\bar{Q}(v8)]$ and $[Q\bar{Q}(a8)]$ perturbative states are given in the Appendix found from the detailed derivation given in Sec. II. The $\mathcal{O}(\alpha_s)$ heavy quarkonium FFs, $\mathcal{D}^{(1)}_{[Q\bar{Q}(\kappa)]\to[Q\bar{Q}(^3S_1^{[1]})]\to H}$ with $\kappa = a8,\ v8$, can be calculated by using Eq. (49).

At the order of α_s, the relevant Feynman diagrams for calculating the heavy quarkonium FFs, $\mathcal{D}^{(1)}_{[Q\bar{Q}(\kappa)]\to[Q\bar{Q}(^3S_1^{[1]})]\to H}$ with $\kappa = a8,\ v8$, in NRQCD are given in Fig. 6, where the amplitude and its complex conjugate are combined together in the cut diagram notation. As in the standard NRQCD calculation, the momenta of the heavy quark and antiquark (upper lines of the diagrams) are fixed at $p/2$, and Dirac indices of these lines are contracted with an NRQCD singlet spin-1 projection operator [26]. The only difference for the fragmentation between a vector $[Q\bar{Q}(v8)]$ and an axial-vector $[Q\bar{Q}(a8)]$ state is that the lower fragmenting heavy quark and antiquark lines in Fig. 6 are contracted with different projection operators, as defined in Eq. (13). We obtain

[1]The contribution from the vector spin state, $[Q\bar{Q}(v8)]$, was not included in our previous short paper (Ref. [21]).

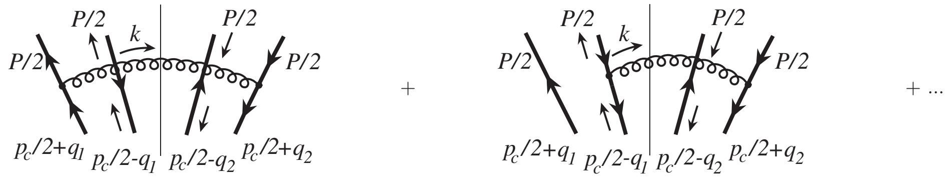

FIG. 6. Leading-order Feynman diagrams representing the fragmentation of a heavy quark pair to another heavy quark pair.

$$\mathcal{D}^{\rm CR}_{[Q\bar{Q}(v8)]\to[Q\bar{Q}(^3S_1^{[1]})]\to H}(z,u,v,\mu^2;m_Q) = \frac{1}{2N_c^2}\frac{\langle\mathcal{O}^H_{[Q\bar{Q}(^3S_1^{[1]})]}\rangle}{3m_Q}\times\frac{\alpha_s}{2\pi}\Delta_-(u,v)\frac{z}{1-z}\left[\ln(r(z)+1)+(1-4z+2z^2)\left(1-\frac{1}{1+r(z)}\right)\right], \tag{53}$$

$$\mathcal{D}^{\rm CR}_{[Q\bar{Q}(a8)]\to[Q\bar{Q}(^3S_1^{[1]})]\to H}(z,u,v,\mu^2;m_Q) = \frac{1}{2N_c^2}\frac{\langle\mathcal{O}^H_{[Q\bar{Q}(^3S_1^{[1]})]}\rangle}{3m_Q}\times\frac{\alpha_s}{2\pi}\Delta_+(u,v)z(1-z)\left[\ln(r(z)+1)+\left(1-\frac{1}{1+r(z)}\right)\right] \tag{54}$$

for the fragmentation of a $[Q\bar{Q}(v8)]$ state and of a $[Q\bar{Q}(a8)]$ state, respectively. In Eqs. (53) and (54), the superscript "CR" indicates the use of a cutoff regularization scheme for the logarithmic UV divergence, the function $r(z)\equiv z^2\mu^2/(4m_Q^2(1-z)^2)$, and $\Delta_\pm(u,v)$ are defined as

$$\Delta_+(u,v) = \frac{1}{4}\left[\delta\left(u-\frac{z}{2}\right)+\delta\left(\bar{u}-\frac{z}{2}\right)\right]\left[\delta\left(v-\frac{z}{2}\right)+\delta\left(\bar{v}-\frac{z}{2}\right)\right],$$
$$\Delta_-(u,v) = \frac{1}{4}\left[\delta\left(u-\frac{z}{2}\right)-\delta\left(\bar{u}-\frac{z}{2}\right)\right]\left[\delta\left(v-\frac{z}{2}\right)-\delta\left(\bar{v}-\frac{z}{2}\right)\right]. \tag{55}$$

As explained in Sec. III A, UV counterterms are needed to calculate the FFs perturbatively in order to renormalize the composite operators that define these heavy quarkonium FFs. In deriving Eqs. (53) and (54), we renormalized the UV divergence by a cutoff μ^2 on the transverse momentum integration, dk_T^2, which is directly connected to the virtuality of the fragmenting heavy quark pair. The heavy quark mass, m_Q, effectively removes the potential CO divergence.

The perturbatively calculated FFs in Eqs. (53) and (54) are not unique due to the renormalization of the perturbative UV divergence. Just like the light hadron FFs, the exact expression of heavy quarkonium FFs depend on the factorization scheme, which is a direct consequence of the renormalization ambiguity for removing the perturbative UV divergence. For a comparison, we also list here the same FFs calculated with dimensional regularization and the $\overline{\rm MS}$ renormalization scheme [26,27]:

$$\mathcal{D}^{\rm DR}_{[Q\bar{Q}(v8)]\to[Q\bar{Q}(^3S_1^{[1]})]\to H}(z,u,v,\mu^2;m_Q) = \frac{1}{2N_c^2}\frac{\langle\mathcal{O}^H_{[Q\bar{Q}(^3S_1^{[1]})]}\rangle}{3m_Q}\times\frac{\alpha_s}{2\pi}\Delta_-(u,v)\frac{z}{1-z}\left[\ln\left(\frac{\mu^2}{4(1-z)^2m_Q^2}\right)+(1-4z+2z^2)\right], \tag{56}$$

$$\mathcal{D}^{\rm DR}_{[Q\bar{Q}(a8)]\to[Q\bar{Q}(^3S_1^{[1]})]\to H}(z,u,v,\mu^2;m_Q) = \frac{1}{2N_c^2}\frac{\langle\mathcal{O}^H_{[Q\bar{Q}(^3S_1^{[1]})]}\rangle}{3m_Q}\times\frac{\alpha_s}{2\pi}\Delta_+(u,v)z(1-z)\left[\ln\left(\frac{\mu^2}{4(1-z)^2m_Q^2}\right)-1\right], \tag{57}$$

for the fragmentation of a $[Q\bar{Q}(v8)]$ state and a $[Q\bar{Q}(a8)]$ state, respectively. In Eqs. (56) and (57) the superscript "DR" indicates the use of dimensional regularization. The difference between the FFs in Eqs. (53) and (54) and those in Eqs. (56) and (57) reflects the factorization scheme dependence of the perturbatively calculated FFs, which should lead to differences in fitted values of the NRQCD LDMEs—for example, the value of $\langle \mathcal{O}^H_{[Q\bar{Q}(^3S_1^{[1]})]}\rangle$ in these equations.

From Eq. (55), it is clear that $\Delta_+(u,v)$ and $\Delta_-(u,v)$ have different symmetry properties under the transformation of $u\leftrightarrow\bar{u}=1-u$ or $v\leftrightarrow\bar{v}=1-v$, or equivalently, $\zeta_1\leftrightarrow-\zeta_1$ or $\zeta_2\leftrightarrow-\zeta_2$: $\Delta_+(u,v)$ is symmetric, while $\Delta_-(u,v)$ is antisymmetric. That is, when the relative momentum fraction of the heavy quark pair in the amplitude or in its complex conjugate reverses its direction, the calculated FF, $\mathcal{D}^{(1)}_{[Q\bar{Q}(a8)]\to[Q\bar{Q}(^3S_1^{[1]})]\to H}(z,u,v,\mu^2;m_Q)$, which is proportional to $\Delta_+(u,v)$, is symmetric, while $\mathcal{D}^{(1)}_{[Q\bar{Q}(v8)]\to[Q\bar{Q}(^3S_1^{[1]})]\to H}(z,u,v,\mu^2;m_Q)$ is antisymmetric. This symmetry property effectively requires that under the same transformation, only the symmetric part of partonic hard parts for producing a $[Q\bar{Q}(a8)]$ pair, or the antisymmetric part of partonic hard parts for producing a $[Q\bar{Q}(v8)]$ pair, can give a nonvanishing contribution to the production cross section at this order. For example, the LO QCD factorization contribution from Eq. (1) to hadronic J/ψ production via a color-singlet $[Q\bar{Q}(^3S_1^{[1]})]$ channel can be symbolically given by

$$d\sigma_{A+B\to J/\psi}=\sum_{ab}\phi_{A\to a}\otimes\phi_{B\to b}\otimes\Big[d\hat{\sigma}^A_{ab\to[Q\bar{Q}(v8)]}\otimes\mathcal{D}^{(1)}_{[Q\bar{Q}(v8)]\to[Q\bar{Q}^3S_1^{[1]})]\to J/\psi}+d\hat{\sigma}^S_{ab\to[Q\bar{Q}(a8)]}\otimes\mathcal{D}^{(1)}_{[Q\bar{Q}(a8)]\to[Q\bar{Q}(^3S_1^{[1]})]\to J/\psi}\Big],\tag{58}$$

where $\sum_{a,b}$ sums over all possible initial-state parton flavors, and the superscripts "A" and "S" represent the "antisymmetric" and "symmetric" properties of the partonic hard parts under the transformation $\zeta_1\leftrightarrow-\zeta_1$ or $\zeta_2\leftrightarrow-\zeta_2$.

The relation between the partonic cross sections $d\hat{\sigma}$ and the short-distance hard parts, H, is given in Eq. (17). The complete results for short-distance hard parts at $\mathcal{O}(\alpha_s^3)$ are listed in the Appendix, and their derivation was given in Sec. II. The symmetric part for producing a color-octet axial-vector pair, $[Q\bar{Q}(a8)]$, was derived in one of our previous papers on the subject [21], and is summarized here:

$$H^S_{q\bar{q}\to[Q\bar{Q}(a8)]g}=\frac{(N_c^2-4)(N_c^2-1)}{4N_c^3}\left[\frac{(\hat{t}^2+\hat{u}^2)}{\hat{s}^3}\right],\tag{59}$$

$$H^S_{gq\to[Q\bar{Q}(a8)]q}=\frac{(N_c^2-4)}{4N_c^2}\left[\frac{(\hat{s}^2+\hat{u}^2)}{-\hat{t}^3}\right],\tag{60}$$

$$H^S_{gg\to[Q\bar{Q}(a8)]g}=\frac{(N_c^2-4)}{N_c^2-1}\left[\frac{(-\hat{s}\,\hat{t}-\hat{t}\,\hat{u}-\hat{u}\,\hat{s})^3}{(\hat{s}\,\hat{t}\,\hat{u})^3}\right],\tag{61}$$

where the superscript "S" indicates keeping only the symmetric terms of the hard parts under the transformation of $\zeta_1\leftrightarrow-\zeta_1$ or $\zeta_2\leftrightarrow-\zeta_2$.

For the production of a color-octet vector pair, $[Q\bar{Q}(v8)]$, we need only the hard parts that are antisymmetric under the transformation of $\zeta_1\leftrightarrow-\zeta_1$ or $\zeta_2\leftrightarrow-\zeta_2$. That is, only the terms that are of odd powers in both ζ_1 and ζ_2 are relevant. From Eqs. (45) and (46), we obtain

$$H^A_{q\bar{q}\to[Q\bar{Q}(v8)]g}=\frac{(N_c^2-4)(N_c^2-1)}{4N_c^3}\left[\frac{(\hat{t}^2+\hat{u}^2)}{\hat{s}^3}\right]\zeta_1\zeta_2\tag{62}$$

$$=\zeta_1\zeta_2H^S_{q\bar{q}\to[Q\bar{Q}(a8)]g},\tag{63}$$

where the superscript "A" indicates keeping the antisymmetric terms when $\zeta_1\leftrightarrow-\zeta_1$ or $\zeta_2\leftrightarrow-\zeta_2$. From the Appendix, we find that the relation in Eq. (63) is actually true for all partonic scattering channels at $\mathcal{O}(\alpha_s^3)$,

$$H^A_{ab\to[Q\bar{Q}(v8)]c}=(u-\bar{u})(v-\bar{v})H^S_{ab\to[Q\bar{Q}(a8)]c},\tag{64}$$

where the identities $u-\bar{u}=\zeta_1$ and $v-\bar{v}=\zeta_2$ are used, and a, b and c, run over all possible parton flavors: quark, antiquark and gluon.

In Fig. 7, we compare the NLO results of J/ψ production (solid line), calculated in terms of the color-singlet model (a special case of NRQCD), with the LO results of QCD factorization (dashed line). Both results are for J/ψ production multiplied by the branching ratio to a $\mu^+\mu^-$ pair and evaluated at the Tevatron energy $\sqrt{S}=1.96$ TeV and in the central rapidity region with $|y|<0.6$. The NLO results of the CSM calculation are from Ref. [38]. The LO QCD factorization results were generated by using Eq. (1), or more precisely, Eq. (58), for proton-antiproton collisions with the LO partonic hard parts and the perturbative FFs calculated in this section *without* evolution (or resummation). We set the factorization scale μ_F equal to the renormalization scale μ, and $\mu_F=\mu=p_T$. To be consistent with our factorized LO calculations, we used CTEQ6L1 parton distribution functions [39] and the one-loop

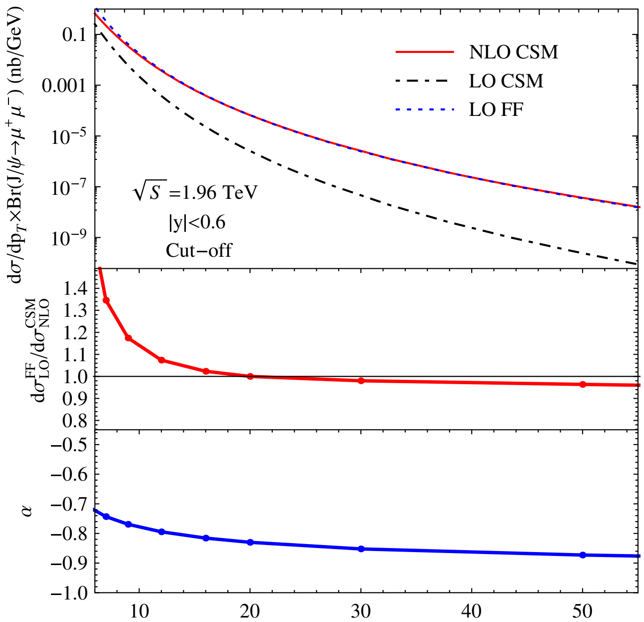

FIG. 7 (color online). Upper panel: Comparison of LO QCD factorization results with FFs calculated in the "CR"—the cutoff regularization and renormalization scheme (solid line) with the LO (dot-dashed line) and NLO (dashed line) results calculated in CSM. Middle panel: Ratio of LO QCD factorization results over NLO CSM results. Lower panel: Polarization parameter evaluated with the LO QCD factorization formalism and FFs given in Eqs. (68) and (69).

expression for α_s with $n_f = 5$ active flavors and $\Lambda^{(5)}_{\rm QCD} = 165$ MeV. In addition, we set the charm quark mass $m_Q = 1.5$ GeV, and NRQCD LDME, $\langle \mathcal{O}^{J/\psi}_{[Q\bar{Q}(^3S_1^{[1]})]}\rangle = 1.32\ \mathrm{GeV}^3$. From the upper and central panels of Fig. 7, we find that our LO contribution to the production cross section, which is effectively a NLP contribution from the QCD factorization formalism in Eq. (1), gives a nice description of the very complicated NLO CSM results when the J/ψ's p_T is sufficiently large. In addition, as shown in Ref. [28], the QCD factorization formalism in Eq. (1) with fully analytical LO short-distance hard parts and fully analytical NLO FFs calculated in NRQCD, without higher-order resummation or evolution, can reproduce the state-of-the-art, numerical NLO NRQCD results, channel by channel for $p_T \gtrsim 10$ GeV.

In Fig. 7, we have also plotted the LO results of the CSM (dot-dashed line), which is much more than an order of magnitude smaller than the NLO results of the CSM calculation. This is exactly caused by the order-p_T^2/m_Q^2 power enhancement that the NLO has over the LO in the CSM calculation (the same issue appears in NRQCD calculations as well) [22]. That is, the expansion of CSM in powers of α_s is not perturbatively reliable because some of the higher-order terms are enhanced by large powers and/or logarithms of such large powers [22]. Although the LO QCD factorization results (solid line) are from the NLP terms ($\sim\mathcal{O}(1/p_T^6)$) of the QCD factorization formalism, they are still power enhanced in comparison to the LO CSM results, which are actually of the $\mathcal{O}(1/p_T^8)$ [22]. The key difference between the QCD factorization formalism in Eq. (1) and the NRQCD factorization formalism in Eq. (47) is that all perturbatively calculated short-distance hard parts and evolution kernels of the QCD factorization formalism are evaluated at a *single* hard scale so that they are free of any large higher-order enhancement from the power of large momentum ratios or the logarithms of such large ratios.

IV. HEAVY QUARKONIUM POLARIZATION

Understanding the polarization of produced heavy quarkonia is critically important for determining the true QCD dynamics, as well as the mechanism of production. In terms of the QCD factorization formalism in Eq. (1), as pointed out earlier in this paper, all hadronic properties of the heavy quarkonia, including their spin and polarizations, are only sensitive to the FFs at the input scale $\mu_0 \gtrsim 2m_Q$, since all perturbatively calculated partonic hard parts and evolution kernels of FFs are insensitive to the details of the produced states. In this section, we adapt the same NRQCD factorization conjecture to evaluate the input FFs to a polarized heavy quarkonium state. We introduce the basic method for calculating these input FFs, and present a complete example for the calculation of the input FFs to a polarized J/ψ via a polarized color-singlet and spin-1 nonrelativistic heavy quark pair ($^3S_1^{[1]}$). A complete set of polarized heavy quarkonium FFs, and their derivation in detail, calculated to NLO in the NRQCD factorization approach, including all possible partonic scattering channels at this order, can be found in Refs. [26,27,29].

If we keep only the LP term in QCD collinear factorization, Eq. (1), for the production of a heavy quarkonium at $p_T \gg m_Q$, the hard partonic collision produces a single, energetic virtual parton state at the short-distance scale $\sim\mathcal{O}(1/p_T)$, followed by a fragmentation process to generate a physical J/ψ, represented by the FFs of the produced single parton. Although the single-parton FFs to a heavy quarkonium are nonperturbative, their factorization scale dependence is given by the DGLAP evolution equations with perturbatively calculated evolution kernels (expanded in powers of α_s). The DGLAP equations evolve the fragmentation process, initiated by the energetic parton, *perturbatively*, to the input scale, $\mu_0 \gtrsim 2m_Q$ or a distance scale $\sim\mathcal{O}(1/2m_Q)$, where a heavy quark pair emerges from the fragmenting parton, and the pair eventually fragments into a heavy quarkonium nonperturbatively. The polarization of the produced heavy quarkonium from this LP production chain is determined by the polarization of the fragmenting parton at the input scale, and the dynamics behind the emergence of the heavy quark pair from the fragmenting parton, as well as the emergence of the heavy quarkonium from the heavy quark pair.

In this whole LP production chain of a heavy quarkonium at high p_T, no heavy quark pair was produced in the fragmentation process all the way down to the input scale $\mu_0 \gtrsim 2m_Q$, at which the logarithmic contribution in terms of $\ln(\mu_0/(2m_Q))$ is comparable with the corrections in powers of $2m_Q/\mu_0$. More precisely, the heavy quark pair, necessary for the production of the heavy quarkonium, is only produced as a part of the input FFs. When the available phase space for radiation is much smaller than the mass of heavy quarks, the polarization of the J/ψ should be very much the same as the polarization of the heavy quark pair, which is more or less the same as the polarization of the "final" parton, most often a gluon that splits into the pair. Since a virtual gluon of invariant mass much less than its momentum is likely to be transversely polarized, the LP QCD factorization formalism for the production naturally predicts that J/ψ produced at a high p_T is transversely polarized, which is also consistent with the prediction of the NRQCD factorization formalism [1]. However, almost all data on the polarization of high-p_T J/ψ as well as Υ, produced at Tevatron and the LHC energies, do not favor the dominance of transverse polarization at the current values of p_T; instead, they are consistent with no strong polarization. This is in fact an outstanding puzzle whose solution must be crucial for understanding the true mechanism of heavy quarkonium production in high-energy collisions.

If the NLP term in the QCD factorization formalism in Eq. (1) is important, which seems to be the case [9,28,31,40], heavy quark pairs produced at all distance scales from $\mathcal{O}(1/p_T)$ to $\mathcal{O}(1/2m_Q)$ could contribute to the production of heavy quarkonia significantly, and the knowledge of heavy quarkonium FFs from a heavy quark pair at the input scale μ_0 is then crucial for understanding the polarization of produced heavy quarkonia. In the following, we use an example to describe the calculations of these input FFs to a polarized J/ψ. More details for fragmentation via other NRQCD states can be found in Ref. [29].

Like the perturbative NRQCD calculation for the unpolarized heavy quarkonium FFs, as discussed in the previous section, we use the same Feynman diagrams in Fig. 6 for calculating the FFs to a polarized heavy quarkonium, but with different spin projection operators to identify the polarization states of the produced heavy quark pair (the upper lines in Fig. 6). For a heavy quark pair moving in the $+z$-direction, we can write $p^\mu = p\cdot\hat{n}\bar{n}^\mu + p^2/(2p\cdot\hat{n})\hat{n}^\mu$, with two auxiliary vectors, $\bar{n}^\mu = (\bar{n}^+,\bar{n}^-,\bar{\mathbf{n}}_\perp) = (1,0,\mathbf{0}_\perp)$ and $\hat{n}^\mu = (0,1,\mathbf{0}_\perp)$, and we define the polarization vector for a longitudinally polarized spin-1 heavy quark pair,

$$\epsilon^\mu_{\lambda=0} = \frac{1}{\sqrt{p^2}}\left[p\cdot\hat{n}\bar{n}^\mu - \frac{p^2}{2p\cdot\hat{n}}\hat{n}^\mu\right], \tag{65}$$

with $p\cdot\epsilon_0 = 0$ and $\epsilon_0^2 = -1$. From $\epsilon^\mu_{\lambda=0}$, we can derive the following spin polarization tensors in this frame, which is effectively the S-helicity frame [41],

$$\mathcal{P}_L^{\mu\nu}(p) \equiv \epsilon_0^{*\mu}\epsilon_0^\nu = \frac{1}{p^2}\left[p\cdot\hat{n}\bar{n}^\mu - \frac{p^2}{2p\cdot\hat{n}}\hat{n}^\mu\right]\left[p\cdot\hat{n}\bar{n}^\nu - \frac{p^2}{2p\cdot\hat{n}}\hat{n}^\nu\right],$$
$$\mathcal{P}_T^{\mu\nu}(p) \equiv \frac{1}{2}\sum_{\lambda=\pm1}\epsilon_\lambda^{*\mu}\epsilon_\lambda^\nu = \frac{1}{2}[-g^{\mu\nu} + \bar{n}^\mu\hat{n}^\nu + \hat{n}^\mu\bar{n}^\nu] = \frac{1}{2}[\mathcal{P}^{\mu\nu}(p) - \mathcal{P}_L^{\mu\nu}(p),], \tag{66}$$

for producing a longitudinally and transversely polarized spin-1 heavy quark pair of momentum p, respectively. The tensor $\mathcal{P}^{\mu\nu}(p)$ in Eq. (66) is defined as

$$\mathcal{P}^{\mu\nu}(p) = \sum_{\lambda=0,\pm1}\epsilon_\lambda^{*\mu}\epsilon_\lambda^\nu = -g^{\mu\nu} + \frac{p^\mu p^\nu}{p^2}, \tag{67}$$

which is the polarization tensor for an unpolarized spin-1 heavy quark pair of total momentum p, which was used for calculating the unpolarized input FFs in the last section.

Similar to those unpolarized input FFs, presented in Eqs. (53), (54), (56) and (57), we derive the input FFs to a polarized heavy quarkonium H via a color-singlet spin-1 NRQCD heavy quark pair, by using the polarization tensors in Eq. (66),

$$\mathcal{D}^{L,\mathrm{CR}}_{[Q\bar{Q}(v8)]\to[Q\bar{Q}(^3S_1^{[1]})]\to H}(z,u,v,\mu^2;m_Q)$$
$$= \frac{1}{2N_c^2}\frac{\langle\mathcal{O}^H_{[Q\bar{Q}(^3S_1^{[1]})]}\rangle}{3m_Q}\Delta_-(u,v)\times\frac{\alpha_s}{2\pi}\frac{z}{1-z}\left[\ln(r(z)+1) - \left(1-\frac{1}{1+r(z)}\right)\right],$$
$$\mathcal{D}^{T,\mathrm{CR}}_{[Q\bar{Q}(v8)]\to[Q\bar{Q}(^3S_1^{[1]})]\to H}(z,u,v,\mu^2;m_Q)$$
$$= \frac{1}{2N_c^2}\frac{\langle\mathcal{O}^H_{[Q\bar{Q}(^3S_1^{[1]})]}\rangle}{3m_Q}\Delta_-(u,v)\times\frac{\alpha_s}{2\pi}z(1-z)\left[1-\frac{1}{1+r(z)}\right], \tag{68}$$

for the fragmentation of a $[Q\bar{Q}(v8)]$ state, and [21]

$$\mathcal{D}^{L,\mathrm{CR}}_{[Q\bar{Q}(a8)]\to[Q\bar{Q}(^3S_1^{[1]})]\to H}(z,u,v,\mu^2;m_Q) = \frac{1}{2N_c^2}\frac{\langle\mathcal{O}^H_{[Q\bar{Q}(^3S_1^{[1]})]}\rangle}{3m_Q}\Delta_+(u,v)\times\frac{\alpha_s}{2\pi}z(1-z)\left[\ln(r(z)+1)-\left(1-\frac{1}{1+r(z)}\right)\right],$$
$$\mathcal{D}^{T,\mathrm{CR}}_{[Q\bar{Q}(a8)]\to[Q\bar{Q}(^3S_1^{[1]})]\to H}(z,u,v,\mu^2;m_Q) = \frac{1}{2N_c^2}\frac{\langle\mathcal{O}^H_{[Q\bar{Q}(^3S_1^{[1]})]}\rangle}{3m_Q}\Delta_+(u,v)\times\frac{\alpha_s}{2\pi}z(1-z)\left[1-\frac{1}{1+r(z)}\right] \quad (69)$$

for the fragmentation of a $[Q\bar{Q}(a8)]$ state. Comparing with those unpolarized input FFs derived in the last section, it is clear that the relation $\mathcal{D}(p)=2\mathcal{D}^T(p)+\mathcal{D}^L(p)$ is satisfied. Similarly, in a dimensional regularization and $\overline{\mathrm{MS}}$ renormalization scheme, we have

$$\mathcal{D}^{L,\mathrm{DR}}_{[Q\bar{Q}(v8)]\to[Q\bar{Q}(^3S_1^{[1]})]\to H}(z,u,v,\mu^2;m_Q) = \frac{1}{2N_c^2}\frac{\langle\mathcal{O}^H_{[Q\bar{Q}(^3S_1^{[1]})]}\rangle}{3m_Q}\Delta_-(u,v)\times\frac{\alpha_s}{2\pi}\frac{z}{1-z}\left[\ln\left(\frac{\mu^2}{4(1-z)^2m_Q^2}\right)-1\right],$$
$$\mathcal{D}^{T,\mathrm{DR}}_{[Q\bar{Q}(v8)]\to[Q\bar{Q}(^3S_1^{[1]})]\to H}(z,u,v,\mu^2;m_Q) = \frac{1}{2N_c^2}\frac{\langle\mathcal{O}^H_{[Q\bar{Q}(^3S_1^{[1]})]}\rangle}{3m_Q}\Delta_-(u,v)\times\frac{\alpha_s}{2\pi}z(1-z) \quad (70)$$

for the fragmentation of a $[Q\bar{Q}(v8)]$ state, and

$$\mathcal{D}^{L,\mathrm{DR}}_{[Q\bar{Q}(a8)]\to[Q\bar{Q}(^3S_1^{[1]})]\to H}(z,u,v,\mu^2;m_Q) = \frac{1}{2N_c^2}\frac{\langle\mathcal{O}^H_{[Q\bar{Q}(^3S_1^{[1]})]}\rangle}{3m_Q}\Delta_+(u,v)\times\frac{\alpha_s}{2\pi}z(1-z)\left[\ln\left(\frac{\mu^2}{4(1-z)^2m_Q^2}\right)-3\right],$$
$$\mathcal{D}^{T,\mathrm{DR}}_{[Q\bar{Q}(a8)]\to[Q\bar{Q}(^3S_1^{[1]})]\to H}(z,u,v,\mu^2;m_Q) = \frac{1}{2N_c^2}\frac{\langle\mathcal{O}^H_{[Q\bar{Q}(^3S_1^{[1]})]}\rangle}{3m_Q}\Delta_+(u,v)\times\frac{\alpha_s}{2\pi}z(1-z) \quad (71)$$

for the fragmentation of a $[Q\bar{Q}(a8)]$ state. In Eqs. (68), (69), (70), and (71) above, we have assumed that the NRQCD LDME for an unpolarized spin-1 heavy quark pair to an unpolarized heavy quarkonium H, $\langle\mathcal{O}^H_{[Q\bar{Q}(^3S_1^{[1]})]}\rangle$, is the same as that for a polarized spin-1 heavy quark pair to a polarized heavy quarkonium H in the same polarization state.

In the polarized input FFs in Eqs. (68), (69), (70), and (71), it is interesting to note the following feature: the FFs to a longitudinally polarized heavy quark pair are enhanced by a logarithmic term, $\ln(r(z)+1)\approx\ln(1/(1-z)^2)+\cdots$, as $z\to 1$, while those to a transversely polarized pair are not. This is a natural result of the UV power counting, because only the $p\cdot\hat{n}\bar{n}^\mu$ term of the longitudinal polarization vector, ϵ_0^μ in Eq. (65), which leads to an equivalent spin contraction $\gamma\cdot p$ for the produced heavy quark pair, picks up the leading logarithmic UV divergence of the diagrams in Fig. 6 when the fragmenting heavy quark pair is in a vector or axial-vector spin state (contracted by $\gamma\cdot\hat{n}$ or $\gamma\cdot\hat{n}\gamma_5$). While the UV divergence, when the transverse momentum of the radiated gluon $k_\perp^2\to\infty$, is renormalized leading to the logarithmic factorization scale μ^2 dependence of the FFs, the opposite limit when $k_\perp^2\to 0$ corresponding to $z\to 1$ gives the logarithmic enhancement of the FFs to a longitudinally polarized heavy quark pair. That is, a perturbatively produced color-octet heavy quark pair, in either a vector or an axial vector spin state, is more likely to fragment into a longitudinally polarized color-singlet spin-1 NRQCD heavy quark pair when the momentum fraction z, carried by the NRQCD heavy quark pair, is large.

From the QCD factorization formalism in Eq. (1), the hadronic cross section for heavy quarkonium production at large p_T is proportional to a convolution of two PDFs and one FF for each partonic scattering channel. With two steeply falling PDFs as a function of parton momentum fraction x, the hadronic production cross section is dominated by the phase space where the momentum fractions x of colliding partons are small while the produced outgoing hadron momentum fraction z is large [42]. That is, the heavy quarkonium produced by the fragmentation of a perturbatively produced heavy quark pair via a color-singlet and spin-1 NRQCD heavy quark pair is likely to be longitudinally polarized. To demonstrate this feature quantitatively, we define the polarization parameter,

$$\alpha(p) \equiv \frac{\sigma^T_{A+B\to J/\psi(p)} - \sigma^L_{A+B\to J/\psi(p)}}{\sigma^T_{A+B\to J/\psi(p)} + \sigma^L_{A+B\to J/\psi(p)}}, \qquad (72)$$

where $\sigma^T_{A+B\to J/\psi(p)}$ and $\sigma^L_{A+B\to J/\psi(p)}$ are the cross sections for producing a transversely and a longitudinally polarized J/ψ of momentum p, respectively, and are given by the same factorized expressions in Eq. (58) with the FFs replaced by corresponding FFs to a transversely (or longitudinally) polarized J/ψ in Eq. (68) [or in Eq. (69)]. In the bottom panel of Fig. 7, we have plotted the polarization parameter $\alpha(p)$ for J/ψ production as a function of its p_T. It is clear from Fig. 7 that most J/ψ's produced through spin-1 and color-singlet heavy quark pairs are longitudinally polarized [21]. Like the cross section shown in Fig. 7, the polarization parameter α, calculated by using the QCD factorization formalism at the LO and with the calculated FFs, completely reproduces the NLO CSM calculation in Ref. [43]. Having the complete set of input FFs to a polarized heavy quarkonium [29], which are universal, it should be straightforward in terms of the QCD factorization formalism in Eq. (1) to evaluate the production rate for both transversely and longitudinally polarized heavy quarkonia in high-energy hadron-hadron, hadron-lepton, and lepton-lepton scatterings, and to test the QCD factorization formalism and our understanding of the mechanism responsible for the heavy quarkonium production, which we leave for future work.

There have been many proposals to resolve the polarization puzzle of heavy quarkonum polarization [1], and many of them are within the NRQCD factorization approach [9,31,40]. By adjusting the value of NRQCD LDMEs so that the two leading power production channels, via $[Q\bar{Q}({}^3S_1^{[8]})]$ and $[Q\bar{Q}({}^3P_J^{[8]})]$ states, which likely produce the transversely polarized J/ψ, are canceled between them, it is possible to leave the production dominated by the channel with an unpolarized $[Q\bar{Q}({}^1S_0^{[8]})]$ state. As demonstrated in Ref. [31], the contribution from this channel for the relevant p_T region cannot be reproduced by the QCD factorized fragmentation restricted to LP. Instead, as demonstrated in Ref. [28], the contribution from the $[Q\bar{Q}({}^1S_0^{[8]})]$ channel from the state-of-the-art NLO NRQCD calculation is completely reproduced by the LO contribution from QCD factorization in Eq. (1), evaluated with heavy quarkonium FFs calculated in NRQCD, and is found to be dominated by the NLP contribution for the most relevant p_T range of the existing data. It seems likely, then, that the NLP contribution to heavy quarkonium production is crucial for resolving the outstanding puzzles of heavy quarkonium polarization at the current collision energies.

In terms of the QCD factorization formalism in Eq. (1), there are two major sources of NLP contributions that could generate heavy quarkonium polarization different from that at the LP. One is directly from the NLP term of the factorization formalism, or more specifically, from the heavy quark pair FFs to a heavy quarkonium, and the other is indirectly from the LP term due to the NLP corrections to the evolution equations of the single-parton FFs to a heavy quarkonium [22].

The direct contribution to heavy quarkonium polarization should come from the knowledge of input FFs to a polarized heavy quarkonium, since the partonic hard parts are insensitive to the details of the hadronic states produced. Like the color-singlet contribution discussed in this section, longitudinally polarized heavy quarkonia at large p_T can be naturally estimated using the model FFs of Refs. [26,27,29], in this direct NLP contribution.

As required by the consistency of QCD factorization at NLP accuracy, which was pointed out in Ref. [22], the DGLAP evolution equation for the factorization scale dependence of the single-parton FFs to a heavy quarkonium needs to be modified to include an NLP correction. This modification takes into account the power-suppressed contribution to the evolution of single-parton FFs, in which a single parton evolves into a heavy quark pair, in addition to its evolution to other single partons at LP. The pair subsequently evolves into a heavy quarkonium via the heavy quark pair FFs. While the LP evolution of the single-parton FFs leads to a dominance of transverse polarization, the NLP correction to the evolution of single-parton FFs could lead to more longitudinally polarized heavy quarkonia. It is clear that both the direct and the indirect NLP contributions to heavy quarkonium production from the QCD factorization formalism in Eq. (1) reduce the dominance of transversely polarized heavy quarkonia, as predicted by the purely LP fragmentation contribution to heavy quarkonium production. It is therefore critically important to evaluate the production rate of polarized heavy quarkonia in high-energy scattering in terms of the QCD factorization formalism in Eq. (1) using the heavy quarkonium FFs calculated in the NRQCD factorization approach [26,27,29].

V. SUMMARY AND CONCLUSIONS

We have calculated, in terms of the QCD collinear factorization formalism in Eq. (1), a complete set of short-distance partonic hard parts at $\mathcal{O}(\alpha_s^3)$ for the NLP contribution to hadronic heavy quarkonium production at large transverse momentum p_T at collider energies. This new factorization formalism organizes the production cross section of heavy quarkonia at large p_T in terms of a power expansion of $1/p_T$, with both the LP and NLP contributions factorized into convolutions of perturbatively calculable short-distance partonic hard parts and the universal but nonperturbative heavy quarkonium FFs [22]. Like all QCD factorization formalisms, the short-distance partonic hard parts are insensitive to the details of the hadrons produced. The short-distance hard parts at LP are the same as the hard parts for LP hadronic production of light hadrons, and are available in the literature for both LO and NLO at $\mathcal{O}(\alpha_s^2)$ and $\mathcal{O}(\alpha_s^3)$, respectively [25]. Our calculated LO partonic hard parts to the NLP contribution at $\mathcal{O}(\alpha_s^3)$, in principle, depend on the separation of LP from the NLP contribution to the cross section from the same partonic scattering diagrams. In practice, as discussed in Sec. II, we introduce a gluon contact term to remove the LP contribution analytically in our calculation at $\mathcal{O}(\alpha_s^3)$.

With the short-distance partonic hard parts calculated in this paper and the evolution kernels for the scale dependence of FFs calculated in Ref. [22], the predictive power of the QCD factorization formalism for heavy quarkonium production still depends on our knowledge of heavy quarkonium FFs at an input scale μ_0. Because of the large heavy quark mass, $m_Q \gg \Lambda_{\rm QCD}$, and the clear separation of momentum scales between the perturbative scales, $\mu_0 \gtrsim m_Q$, and the nonperturbative scales of the input FFs, such as heavy quark momentum $\sim m_Q v$, and energy $\sim m_Q v^2$, we have proposed, as a conjecture or model, to use NRQCD factorization to evaluate the heavy quarkonium FFs at the input scale. Then, the large number of unknown heavy quarkonium FFs from either a single parton or a heavy quark pair can be factorized into perturbatively calculable functional dependence on momentum fractions, z, ζ_1 and ζ_2, at the NRQCD factorization scale $\mu_\Lambda \sim m_Q \sim \mathcal{O}(\mu_0)$, which can be combined with a few universal NRQCD LDMEs organized in terms of their effective powers in heavy quark velocity v. This increases the predictive power of the QCD factorization formalism, as well as its testability. Since the QCD factorization of the production cross section and the NRQCD factorization of the universal FFs at the input scale are two independent factorizations, using different expansion parameters and power counting, we can improve overall predictive power or accuracy on the production cross section by increasing the perturbative accuracy of each perturbative expansion.

If the NRQCD factorization for the universal input FFs is proved to be valid, the QCD factorization approach with calculated FFs in NRQCD is effectively equal to the NRQCD factorization for the first two powers of the $1/p_T$ expansion of the production cross section, although the QCD factorization and NRQCD factorization organize their perturbative expansions of the cross section differently. The QCD factorization includes all-order resummation of $\ln(p_T^2/m_Q^2)$-type large logarithmic contributions at high p_T, and is more suited for heavy quarkonium production in the high-p_T region, while the NRQCD factorization, including the explicit heavy quark mass dependence, is better for the production at $p_T \gtrsim m_Q$. We proposed a matching equation in Eq. (52) to expand the coverage of the factorization formalism for heavy quarkonium production at collider energies.

Understanding the polarization of produced heavy quarkonia in high-energy scattering is a major challenge for the NRQCD factorization formalism. We demonstrated that the QCD collinear factorization including the NLP contribution associated with short-distance heavy pair production has potentially both direct and indirect ways to suppress the dominance of transverse polarization predicted by the LP fragmentation contribution. Since short-distance coefficients are insensitive to hadron properties, the universal FFs at the input scale are largely responsible for the polarization of produced heavy quarkonia, while the NLP corrections to the evolution equations of single-parton FFs may also be very important to reduce the dominance of transverse polarization. The input FFs to a polarized heavy quarkonium state, both longitudinal and transverse, are now calculated in the NRQCD factorization approach [26,27,29]. With the partonic short-distance hard parts calculated in this paper, the evolution kernels of heavy quarkonium FFs calculated in Ref. [22], and input FFs to a polarized heavy quarkonium, we are now in a position to evaluate, consistently, QCD predictions for the polarization of heavy quarkonia produced in high-energy scatterings. By calculating partonic hard parts for heavy quarkonium production in e^+e^- and lepton-hadron collisions, and using the existing universal evolution kernels and input FFs, it is completely possible to perform a QCD global analysis of all data on heavy quarkonium production to test our understanding on how heavy quarkonia are really produced, forty years since the first heavy quarkonium, J/ψ, was discovered [44,45].

ACKNOWLEDGMENTS

We thank G. T. Bodwin, E. Braaten, and H. Zhang for helpful discussions. This work was supported in part by the U.S. Department of Energy under Contracts No. DE-AC02-06NA25396 and No. DE-AC02-98CH10886, and Grant No. DE-FG02-93ER-40762, and the National Science

Foundation under Grants No. PHY-0969739 and No. PHY-1316617.

APPENDIX: PARTONIC HARD PARTS

In this appendix, we summarize the partonic hard parts for the NLP contribution to heavy quarkonium production from all partonic scattering channels, $i(p_1) + j(p_2) \to [Q\bar{Q}(\kappa)](p) + k(p_3)$, for hadronic collisions. We define the hard part, $H_{ij\to[Q\bar{Q}(\kappa)]}$, in terms of the invariant partonic cross section,

$$E_p \frac{d\hat{\sigma}_{ij\to[Q\bar{Q}(\kappa)]}}{d^3p} = \frac{4\pi\alpha_s^3}{\hat{s}} \frac{1}{\bar{u}u\bar{v}v} H_{ij\to[Q\bar{Q}(\kappa)]}\delta(\hat{s}+\hat{t}+\hat{u}), \tag{A1}$$

with Mandelstam variables defined as

$$\hat{s} = (p_1+p_2)^2 = (p+p_3)^2,$$
$$\hat{t} = (p_2-p_3)^2 = (p-p_1)^2,$$
$$\hat{u} = (p_1-p_3)^2 = (p-p_2)^2.$$

As discussed in Sec. II, the partonic hard parts at NLP depend on the subtraction of the LP contribution from the partonic scattering, and the corresponding choice of the regularization. The following results are calculated by using the gluon contact term to remove the LP contribution at this order analytically. The dependence on the auxiliary vector $\hat{n}^\mu$, which defines the gluon contact term, is kept explicit, in the form of $p\cdot\hat{n} \equiv p^+$ for any momentum vector p. More discussion on the definition and the choice of $\hat{n}^\mu$ can be found in Sec. II.

(1) *Quark-antiquark scattering:*

$$H_{q\bar{q}\to[Q\bar{Q}(a1)]g} = \frac{N_c^2-1}{2N_c^3}\frac{\hat{t}^2+\hat{u}^2}{\hat{s}^3}, \tag{A2}$$

$$H_{q\bar{q}\to[Q\bar{Q}(v1)]g} = \frac{N_c^2-1}{2N_c^3}\frac{\hat{t}^2+\hat{u}^2}{\hat{s}^3}\zeta_1\zeta_2, \tag{A3}$$

$$H_{q\bar{q}\to[Q\bar{Q}(a8)]g} = \frac{N_c^2-1}{4N_c}\frac{\hat{t}^2+\hat{u}^2}{\hat{s}^3}\left(\frac{N_c^2-4}{N_c^2}+\zeta_1\zeta_2\right), \tag{A4}$$

$$\begin{aligned}H_{q\bar{q}\to[Q\bar{Q}(v8)]g} = {}& \frac{N_c^2-1}{4N_c}\frac{\hat{t}^2+\hat{u}^2}{\hat{s}^3}\left(\frac{N_c^2-4}{N_c^2}+\zeta_1\zeta_2\right)\zeta_1\zeta_2 \\ & -\frac{N_c^2-1}{4N_c}\left\{2\left(\frac{1}{\hat{u}}\frac{p_1^+}{p^+}+\frac{1}{\hat{t}}\frac{p_2^+}{p^+}\right)\left(\frac{\hat{t}^2+\hat{u}^2}{\hat{s}^2}-\frac{1}{N_c^2}\right)(1-\zeta_1^2)(1-\zeta_2^2)\right. \\ & +\frac{1}{2}\left[\left(\frac{1}{\hat{t}}\frac{p_1^+}{p^+}-\frac{1}{\hat{u}}\frac{p_2^+}{p^+}\right)\frac{\hat{t}^2+\hat{u}^2}{\hat{s}^2}-\left(\frac{1}{\hat{t}}-\frac{1}{\hat{u}}\right)\right] \\ & \left.\times\left[\frac{\hat{t}-\hat{u}}{\hat{s}}(\zeta_1^2+\zeta_2^2-2\zeta_1^2\zeta_2^2)+\frac{N_c^2-4}{N_c^2}(\zeta_1+\zeta_2)(1-\zeta_1\zeta_2)\right]\right\}.\end{aligned} \tag{A5}$$

In Eq. (A5), the term proportional to $\zeta_1\zeta_2$ comes from the contribution of (a) + (b) in Fig. 2, and the term proportional to $(\zeta_1+\zeta_2)(1-\zeta_1\zeta_2)$ comes from the contribution of interference between (a) + (b) and (c) + (d) + (e) in Fig. 2. It is straightforward to check charge conjugation symmetry:

$$H_{q\bar{q}\to[Q\bar{Q}(\kappa)]g}(p_1,p_2,p_3,\zeta_1,\zeta_2) = H_{q\bar{q}\to[Q\bar{Q}(\kappa)]g}(p_2,p_1,p_3,-\zeta_1,-\zeta_2). \tag{A6}$$

Results for $\bar{q}q$ initial states can be obtained from results of $q\bar{q}$ initial states by exchanging p_1 and p_2:

$$\begin{aligned}H_{\bar{q}q\to[Q\bar{Q}(\kappa)]g}(p_1,p_2,p_3,\zeta_1,\zeta_2) &= H_{q\bar{q}\to[Q\bar{Q}(\kappa)]g}(p_2,p_1,p_3,\zeta_1,\zeta_2) \\ &= H_{q\bar{q}\to[Q\bar{Q}(\kappa)]g}(p_1,p_2,p_3,-\zeta_1,-\zeta_2).\end{aligned} \tag{A7}$$

(2) *Quark-gluon and gluon-quark scattering:* Similarly, results for qg, $\bar{q}g$, gq and $g\bar{q}$ initial states are given by the following crossing relationships:

$$H_{qg\to[Q\bar{Q}(\kappa)]q}(p_1,p_2,p_3,\zeta_1,\zeta_2) = -\frac{N_c}{N_c^2-1}H_{q\bar{q}\to[Q\bar{Q}(\kappa)]g}(p_1,-p_3,-p_2,\zeta_1,\zeta_2), \tag{A8}$$

$$H_{\bar{q}g\to[Q\bar{Q}(\kappa)]\bar{q}}(p_1,p_2,p_3,\zeta_1,\zeta_2) = -\frac{N_c}{N_c^2-1}H_{q\bar{q}\to[Q\bar{Q}(\kappa)]g}(p_1,-p_3,-p_2,-\zeta_1,-\zeta_2), \tag{A9}$$

$$H_{gq\to[Q\bar{Q}(\kappa)]q}(p_1,p_2,p_3,\zeta_1,\zeta_2) = -\frac{N_c}{N_c^2-1}H_{q\bar{q}\to[Q\bar{Q}(\kappa)]g}(p_2,-p_3,-p_1,\zeta_1,\zeta_2), \tag{A10}$$

$$H_{g\bar{q}\to[Q\bar{Q}(\kappa)]\bar{q}}(p_1,p_2,p_3,\zeta_1,\zeta_2) = -\frac{N_c}{N_c^2-1}H_{q\bar{q}\to[Q\bar{Q}(\kappa)]g}(p_2,-p_3,-p_1,-\zeta_1,-\zeta_2), \tag{A11}$$

where the overall color factor accounts for differences of averaging over initial color states. We give the results for gq initial states explicitly:

$$H_{gq\to[Q\bar{Q}(a1)]q} = -\frac{1}{2N_c^2}\frac{\hat{u}^2+\hat{s}^2}{\hat{t}^3}, \tag{A12}$$

$$H_{gq\to[Q\bar{Q}(v1)]q} = -\frac{1}{2N_c^2}\frac{\hat{u}^2+\hat{s}^2}{\hat{t}^3}\zeta_1\zeta_2, \tag{A13}$$

$$H_{gq\to[Q\bar{Q}(a8)]q} = -\frac{1}{4}\frac{\hat{u}^2+\hat{s}^2}{\hat{t}^3}\left(\frac{N_c^2-4}{N_c^2}+\zeta_1\zeta_2\right), \tag{A14}$$

$$\begin{aligned} H_{gq\to[Q\bar{Q}(v8)]q} = &-\frac{1}{4}\frac{\hat{u}^2+\hat{s}^2}{\hat{t}^3}\left(\frac{N_c^2-4}{N_c^2}+\zeta_1\zeta_2\right)\zeta_1\zeta_2 \\ &+\frac{1}{4}\left\{2\left(\frac{1}{\hat{s}}\frac{p_2^+}{p^+}-\frac{1}{\hat{u}}\frac{p_3^+}{p^+}\right)\left(\frac{\hat{u}^2+\hat{s}^2}{\hat{t}^2}-\frac{1}{N_c^2}\right)(1-\zeta_1^2)(1-\zeta_2^2)\right. \\ &+\frac{1}{2}\left[\left(\frac{1}{\hat{u}}\frac{p_2^+}{p^+}+\frac{1}{\hat{s}}\frac{p_3^+}{p^+}\right)\frac{\hat{u}^2+\hat{s}^2}{\hat{t}^2}-\left(\frac{1}{\hat{u}}-\frac{1}{\hat{s}}\right)\right] \\ &\left.\times\left[\frac{\hat{u}-\hat{s}}{\hat{t}}(\zeta_1^2+\zeta_2^2-2\zeta_1^2\zeta_2^2)+\frac{N_c^2-4}{N_c^2}(\zeta_1+\zeta_2)(1-\zeta_1\zeta_2)\right]\right\}. \end{aligned} \tag{A15}$$

(3) *Gluon-gluon scattering:*

$$H_{gg\to[Q\bar{Q}(a1)]g} = \frac{2}{N_c^2-1}\frac{S_2^4}{S_3^3}, \tag{A16}$$

$$H_{gg\to[Q\bar{Q}(v1)]g} = \frac{2}{N_c^2-1}\frac{S_2^4}{S_3^3}\zeta_1\zeta_2, \tag{A17}$$

$$H_{gg\to[Q\bar{Q}(a8)]g} = \frac{N_c^2}{N_c^2-1}\frac{S_2^4}{S_3^3}\left[\frac{N_c^2-4}{N_c^2}+\left(1-5\frac{S_3^2}{S_2^3}\right)\zeta_1\zeta_2\right], \tag{A18}$$

$$
\begin{aligned}
H_{gg\to[Q\bar{Q}(v8)]g} = & \frac{N_c^2}{N_c^2-1}\frac{S_2^4}{S_3^3}\left[\frac{N_c^2-4}{N_c^2}+\left(1-5\frac{S_3^2}{S_2^3}\right)\zeta_1\zeta_2\right]\zeta_1\zeta_2 \\
& -\frac{N_c^2}{N_c^2-1}\frac{S_2}{S_3^2}\left\{2\left(\hat{t}^3\frac{p_1^+}{p^+}+\hat{u}^3\frac{p_2^+}{p^+}-\hat{s}^3\frac{p_3^+}{p^+}\right)(1-\zeta_1^2)(1-\zeta_2^2)\right. \\
& +\frac{1}{2}\left[-3\left(\hat{t}^3\frac{p_1^+}{p^+}+\hat{u}^3\frac{p_2^+}{p^+}-\hat{s}^3\frac{p_3^+}{p^+}\right)+\frac{2S_2^2}{S_3}\left(\hat{t}^2\frac{p_1^+}{p^+}+\hat{u}^2\frac{p_2^+}{p^+}-\hat{s}^2\frac{p_3^+}{p^+}\right)-4S_3\right] \\
& \left.\times(\zeta_1^2+\zeta_2^2-2\zeta_1^2\zeta_2^2)\right\}, \qquad \text{(A19)}
\end{aligned}
$$

where we have used the method described in Ref. [46] to write these expressions in symmetric form, with symmetric variables defined as

$$
\begin{aligned}
S_2 &= -\hat{s}\,\hat{t} - \hat{t}\,\hat{u} - \hat{u}\,\hat{s}, \\
S_3 &= \hat{s}\,\hat{t}\,\hat{u}. \qquad \text{(A20)}
\end{aligned}
$$

---

[1] N. Brambilla et al., Eur. Phys. J. C 71, 1534 (2011).
[2] G. T. Bodwin, E. Braaten, and G. P. Lepage, Phys. Rev. D 51, 1125 (1995); 55, 5853 (1997).
[3] E. Braaten, S. Fleming, and T. C. Yuan, Annu. Rev. Nucl. Part. Sci. 46, 197 (1996).
[4] M. Krämer, Prog. Part. Nucl. Phys. 47, 141 (2001).
[5] A. Petrelli, M. Cacciari, M. Greco, F. Maltoni, and M. L. Mangano, Nucl. Phys. B514, 245 (1998).
[6] Y.-Q. Ma, K. Wang, and K.-T. Chao, Phys. Rev. Lett. 106, 042002 (2011).
[7] M. Butenschoen and B. A. Kniehl, Phys. Rev. Lett. 106, 022003 (2011).
[8] K. Wang, Y.-Q. Ma, and K.-T. Chao, Phys. Rev. D 85, 114003 (2012).
[9] B. Gong, L.-P. Wan, J.-X. Wang, and H.-F. Zhang, Phys. Rev. Lett. 112, 032001 (2014).
[10] A. A. Affolder et al. (CDF Collaboration), Phys. Rev. Lett. 85, 2886 (2000).
[11] A. Abulencia et al. (CDF Collaboration), Phys. Rev. Lett. 99, 132001 (2007).
[12] D. Acosta et al. (CDF Collaboration), Phys. Rev. Lett. 88, 161802 (2002).
[13] V. Abazov et al. (D0 Collaboration), Phys. Rev. Lett. 101, 182004 (2008).
[14] S. Chatrchyan et al. (CMS Collaboration), Phys. Rev. Lett. 110, 081802 (2013).
[15] H. Han et al., arXiv:1410.8537.
[16] M. Butenschoen and B. A. Kniehl, Phys. Rev. D 84, 051501 (2011).
[17] G. T. Bodwin et al., arXiv:1307.7425.
[18] G. C. Nayak, J.-W. Qiu, and G. F. Sterman, Phys. Rev. D 72, 114012 (2005).
[19] G. C. Nayak, J.-W. Qiu, and G. F. Sterman, Phys. Rev. D 74, 074007 (2006).
[20] Z.-B. Kang, J.-W. Qiu, and G. Sterman, Nucl. Phys. Proc. Suppl. Ser. 214, 39 (2011).
[21] Z.-B. Kang, J.-W. Qiu, and G. Sterman, Phys. Rev. Lett. 108, 102002 (2012).
[22] Z.-B. Kang, Y.-Q. Ma, J.-W. Qiu, and G. Sterman, Phys. Rev. D 90, 034006 (2014).
[23] S. Fleming, A. K. Leibovich, T. Mehen, and I. Z. Rothstein, Phys. Rev. D 86, 094012 (2012).
[24] S. Fleming, A. K. Leibovich, T. Mehen, and I. Z. Rothstein, Phys. Rev. D 87, 074022 (2013).
[25] F. Aversa, P. Chiappetta, M. Greco, and J. Guillet, Nucl. Phys. B327, 105 (1989).
[26] Y.-Q. Ma, J.-W. Qiu, and H. Zhang, Phys. Rev. D 89, 094029 (2014).
[27] Y.-Q. Ma, J.-W. Qiu, and H. Zhang, Phys. Rev. D 89, 094030 (2014).
[28] Y.-Q. Ma, J.-W. Qiu, G. Sterman, and H. Zhang, Phys. Rev. Lett. 113, 142002 (2014).
[29] H. Zhang, Ph.D. thesis, Stony Brook University, August 2014.
[30] J.-W. Qiu, Phys. Rev. D 42, 30 (1990).
[31] G. T. Bodwin, H. S. Chung, U.-R. Kim, and J. Lee, Phys. Rev. Lett. 113, 022001 (2014).
[32] J. Collins, Proc. Sci., LC2008 (2008) 028.
[33] J.-y. Chiu, A. Fuhrer, A. Hoang, R. Kelley, and A. Manohar, Phys. Rev. D 79, 053007 (2009).
[34] T. Becher and G. Bell, Phys. Lett. B 713, 41 (2012).
[35] J.-Y. Chiu, A. Jain, D. Neill, and I. Z. Rothstein, J. High Energy Phys. 05 (2012) 084.
[36] M. G. Echevarria, A. Idilbi, and I. Scimemi, Int. J. Mod. Phys. Conf. Ser. 25, 1460005 (2014).
[37] J. C. Collins and D. E. Soper, Nucl. Phys. B193, 381 (1981).
[38] J. M. Campbell, F. Maltoni, and F. Tramontano, Phys. Rev. Lett. 98, 252002 (2007).

[39] J. Pumplin, J. Pumplin, D. R. Stump, J. Huston, H-L. Lai, P. Nadolsky, and Wu-Ki. Tung, J. High Energy Phys. 07 (2002) 012.
[40] K.-T. Chao, Y-Q. Ma, H-S. Shao, K. Wang, and Yu-Jie. Zhang, Phys. Rev. Lett. **108**, 242004 (2012).
[41] C. Lam and W.-K. Tung, Phys. Rev. D **18**, 2447 (1978).
[42] E. L. Berger, J.-W. Qiu, and X.-f. Zhang, Phys. Rev. D **65**, 034006 (2002).
[43] B. Gong and J.-X. Wang, Phys. Rev. Lett. **100**, 232001 (2008).
[44] J. Aubert *et al.* (E598 Collaboration), Phys. Rev. Lett. **33**, 1404 (1974).
[45] J. Augustin *et al.* (SLAC-SP-017 Collaboration), Phys. Rev. Lett. **33**, 1406 (1974).
[46] Y.-Q. Ma, Phys. Rev. D **87**, 034001 (2013).