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Fragmentation, factorization and infrared poles in heavy quarkonium production

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Abstract

We explore the role of soft gluon exchange in heavy quarkonium production at large transverse momentum. We find uncanceled infrared poles at NNLO that are not matched by conventional NRQCD matrix elements. We show, however, that gauge invariance and factorization require that conventional NRQCD production operators be modified to include non-Abelian phases or Wilson lines. With appropriately modified operators, factorization is restored at NNLO. We also argue that, in the absence of special cancellations, infrared poles at yet higher orders may require the inclusion of additional nonlocal operators, not present in the NRQCD expansion in relative velocity.

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1. Introduction

The production of heavy quarkonium offers a unique perspective into the process of hadronization, because the creation of the relevant valence partons, the heavy quarks, is essentially perturbative. Quarkonium production and decay have been the subject of a vast theoretical literature and of intensive experi-

mental study, in which the effective field theory non-relativistic QCD (NRQCD) [1] has played a guiding role. NRQCD offers a systematic formalism to separate dynamics at the perturbative mass scale of the heavy quarks from nonperturbative dynamics, through an expansion in relative velocity within the pair forming the bound state. In NRQCD, the description of the relevant nonperturbative dynamics is reduced to the determination of a limited number of QCD matrix elements, accessible from experiment and, in principle, lattice computation. A characteristic feature of the application of NRQCD to production processes is

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the indispensable role of color octet matrix elements, which describe the nonperturbative transition of quark pairs in adjoint representation into quarkonia through soft gluon emission.

An early success of NRQCD was to provide a framework for the striking Tevatron Run I data on high- p_T heavy quarkonium production [2], and it has been extensively applied to heavy quarkonia in both collider and fixed target experiments. A wide-ranging review of theory and experiment for quarkonium production and decay has been given recently in Ref. [3]. Much of the analysis has been based on a factorization formalism proposed in [1], which offers a systematic procedure for the application of NRQCD to quarkonium production. It is fair to say, however, that, in contrast to quarkonium decay, fully convincing arguments have not yet been given for NRQCD factorization as applied to high- p_T production processes [3,4]. This omission may or may not be related to the current lack of confirmation for its predictions on quarkonium polarization at high p_T [5].

In this Letter, we summarize progress toward the derivation of an appropriate factorization formalism for high- p_T quarkonia, illustrating our considerations with results on infrared emission at next-to-next-to-leading order (NNLO). At NNLO we find infrared divergences that do not fall precisely into the pattern suggested in Ref. [1]. These divergences may, however, be incorporated into color octet matrix elements by a technical redefinition that makes the latter gauge invariant. It is not clear whether this pattern extends beyond NNLO, and we conclude that NRQCD factorization must be examined further for production processes. In any case, all our results are consistent with the factorization of evolution logarithms in the ratio of momentum transfer to quark mass from non-perturbative matrix elements [1].

In the results presented below, the relevant infrared divergence is proportional to v^2 , where \vec{v} is the relative velocity of the heavy pair in the quarkonium rest frame. The rotational invariance of this result (in the quarkonium rest frame) makes it possible to match the long-distance behavior of an arbitrary cross section to an octet matrix element in a manner that does not depend on the directions of energetic final-state gluons. In other words, we may factorize the perturbative long-distance contributions from the short-distance cross section, and replace them with a universal nonpertur-

bative matrix element that has the same perturbative long-distance behavior, just as proposed in [1] and extended in [6]. We begin our discussion with a brief review of NRQCD factorization at high transverse momentum.

2. NRQCD in fragmentation

We discuss for definiteness the production of the J/ψ and related heavy quarkonium states H in leptonic or hadronic collisions, $A + B \rightarrow H(p_T) + X$. To leading power in m_c/p_T , which we assume to be a small parameter, production proceeds through gluon fragmentation. According to conventional factorization theorems [7], we have (keeping only the gluon)

$$\begin{aligned} d\sigma_{A+B \rightarrow H+X}(p_T) &= d\hat{\sigma}_{A+B \rightarrow g+X}(p_T/z\mu) \otimes D_{H/g}(z, m_c, \mu) \\ &\quad + \mathcal{O}(m_c^2/p_T^2), \end{aligned} \quad (1)$$

where generally we pick the factorization scale μ to be of the order of p_T . In this expression, the convolution in the momentum fraction z is denoted by \otimes , and we have absorbed all information on the initial state into $d\hat{\sigma}_{A+B \rightarrow g+X}$. If we also assume NRQCD factorization, we have in addition to (1),

$$d\sigma_{A+B \rightarrow H+X}(p_T) = \sum_n d\hat{\sigma}_{A+B \rightarrow c\bar{c}[n]+X}(p_T) \langle \mathcal{O}_n^H \rangle, \quad (2)$$

where the \mathcal{O}_n^H are NRQCD operators, classified by powers of relative velocity and characterized by the various rotational and color transformation properties of the $c\bar{c}$ state $[n]$. Assuming both (1) and (2) to hold, we conclude that the gluon fragmentation function is related to the NRQCD matrix element by [8]

$$D_{H/g}(z, m_c, \mu) = \sum_n d_{g \rightarrow c\bar{c}[n]}(z, \mu, m_c) \langle \mathcal{O}_n^H \rangle, \quad (3)$$

where $d_{g \rightarrow c\bar{c}[n]}(z, \mu, m_c)$ describes the evolution of an off-shell gluon into a quark pair in state $[n]$, including logarithms of μ/m_c .

In the following, we will study the fragmentation function itself, concentrating on infrared divergences at NNLO. First, however, we make some observations

concerning the gauge transformation properties of NRQCD color octet matrix elements.

3. Gauge invariance and Wilson lines

Production operators for state H were introduced in Ref. [1] in the form

$$\mathcal{O}_n^H(0) = \chi^\dagger \mathcal{K}_n \psi(0) (a_H^\dagger a_H) \psi^\dagger \mathcal{K}'_n \chi(0), \quad (4)$$

where a_H^\dagger is the creation operator for state H , and where \mathcal{K}_n and \mathcal{K}'_n involve products of color and spin matrices, and at higher dimensions of covariant derivatives. Although the heavy (anti)quark fields (χ) ψ are all at the same space–time point (here 0), the operator \mathcal{O}_n^H is not truly local, because the operator a_H creates particle H for out states, in the far future. In particular, operator-valued gauge transformations do not commute with the product $a_H^\dagger a_H$ in general.

A consequence of nonlocality is that the right-hand side of Eq. (4) is not gauge invariant in perturbation theory unless the individual product $\psi^\dagger \mathcal{K}'_n \chi(0)$ and $\chi^\dagger \mathcal{K}_n \psi(0)$ are separately invariant. This is the case when the \mathcal{K}_n 's specify color singlets, but not when they specify color octets. A related issue arises in the field-theoretic definitions of fragmentation functions [9], such as $D_{H/g}$ in Eq. (1). It is resolved by supplementing the bi-local products of fields by non-Abelian phase operators, or Wilson lines: $\Phi_l[x, A] = \exp[-ig \int_0^\infty d\lambda l \cdot A(x + \lambda l)]$. In contrast to parton distributions, moments of fragmentation functions do not result in expectation values of local operators [10], and the corresponding Wilson lines are not guaranteed to cancel identically. For a color octet combination, the gauge field A^μ is given in adjoint representation, just as for a gluon fragmentation function, for which the operator $\Phi_l(x)_{ab}$ multiplies the gauge covariant field strength $F_b^{\mu\nu}$. To be definite, and for convenience in relating NRQCD operators to the gluon fragmentation function, we will choose l as a lightlike vector in the minus direction: $l^\mu = \delta_{\mu-}$.

Our gauge invariant redefinition of production operators in octet representation is now found by the replacement (which we refer to as a gauge completion)

$$\begin{aligned} \mathcal{O}_n^H(0) \rightarrow & \chi^\dagger \mathcal{K}_{n,c} \psi(0) \Phi_l^\dagger[0, A]_{cb} (a_H^\dagger a_H) \\ & \times \Phi_l[0, A]_{ba} \chi^\dagger \mathcal{K}'_{n,a} \psi(0), \end{aligned} \quad (5)$$

where we have exhibited the color indices of the octets. In perturbation theory, the Wilson lines generate propagators of the form $i/(l \cdot k + i\epsilon)$ when they carry gluon momentum k , and the gluons couple to the Wilson line at vertices $g_s l^\mu C_{abc}$, with C_{abc} structure constants. These are precisely the same as the propagators and vertices of the eikonal approximation for the emission and absorption of soft gluons by an energetic gluon of momentum l^μ . We will use this correspondence below.

It is worth noting that the replacement (5) is not really necessary if gauge dependence in the matrix elements and coefficient functions is infrared safe. This appears to be an implicit assumption in the discussion of Ref. [1]. As we shall see, however, although gauge dependence is certainly free of infrared singularities at next-to-leading order, at NNLO this is no longer the case.

4. Eikonal approximation for $g \rightarrow H$

For this discussion, we study the perturbative expansion of the fragmentation function for $g \rightarrow c\bar{c}[n_0] + X$ with $c\bar{c}[n_0] = c(P/2 + q)\bar{c}(P/2 - q)$, a pair with total momentum P and relative momentum q , always projected onto a color singlet state. We can, of course, further project various spin and orbital angular momentum states $[n]$ as in Eq. (3).

Beyond lowest order, the computation of these diagrams tests NRQCD factorization, Eq. (3), which is verified to the extent that we can absorb, that is match, any infrared divergences into the perturbative expansion of NRQCD matrix elements \mathcal{O}_n^H [11]. We will be interested in gluons whose energies are much below m_c . For NRQCD factorization to hold these soft gluons must factorize from the higher energy radiation that generates logarithms of p_T/m_c .¹

Because we need only the infrared structure of the diagrams from gluons of very low momentum, we may suppress overall color and combinatorial factors, as well as momentum factors that depend only on the scale of m_c , including the LO fragmentation of the parent gluon, which is off-shell by $\mu^2 \geq 4m_c^2$, into the quark pair.

¹ We will show elsewhere that this is indeed the case.

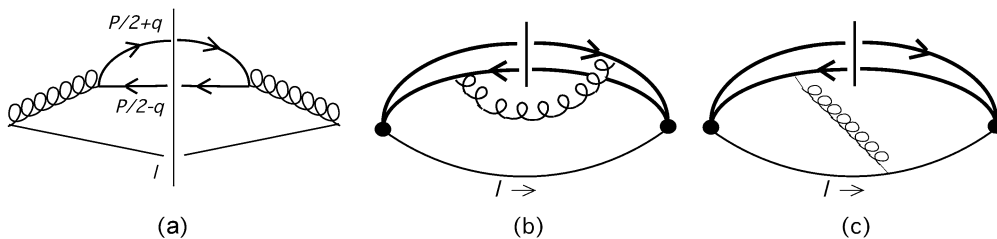


Fig. 1. (a) Lowest-order fragmentation function for $g \rightarrow c\bar{c}$. There are no interactions on the eikonal quark pair or the Wilson line that corresponds to an eikonal gluon of four-velocity l . (b), (c) Representative NLO contributions to $g \rightarrow c\bar{c}$ fragmentation in eikonal approximation. In these figures the parent gluon is contracted to a point, represented by the dark circle, because it is off-shell by order m_c .

Fig. 1(a) shows the lowest-order diagram $g \rightarrow c\bar{c}$, and Fig. 1(b), (c) show typical contributions with single soft gluon emission in the fragmentation function, all in cut diagram notation. Both Fig. 1(b) and (c) represent a class of four diagrams, in which gluons are attached to one of the two lines of the quark pair in the amplitude and its complex conjugate. In each diagram we may treat the quarks in eikonal approximation, in effect replacing them with time-like Wilson lines, whose propagators and vertices are given by $i/(\beta \cdot k + i\epsilon)$ and $-ig_s T_a \beta^\mu$, respectively, for quarks, with T_a a color generator in fundamental representation and β^μ the time-like quark four-velocity. The corresponding approximation for antiquarks simply changes the sign at the vertex.

The vertical lines in Fig. 1(b) and (c) represent the quark pair final state, including a projection onto a color singlet configuration. The full fragmentation function is found by cutting the remaining lines in all possible ways. When the gluon is cut in Fig. 1(b), in particular, the resulting diagrams have an uncanceled infrared pole in dimensional regularization, beginning at order $v^2 \sim \vec{q}^2/m_c^2$ when the gluon momentum $k \rightarrow 0$. This gluonic contribution, however, which involves only interactions between the pair, may be matched straightforwardly to a color octet matrix element, with which it shares an identical topology [8, 11].

The divergent part of Fig. 1(b) may be isolated by evaluating the four relevant diagrams in eikonal approximation and then expanding them in $v = q/m_c$. Alternately, we may expand the momentum-space integrand, isolating the v^2 term before the integration. In $D = 4 - 2\epsilon$ dimensions, and in the quark pair rest frame, the latter approach leads readily to an expression in terms of the total and relative momenta P

($P^2 = m_H^2$) and q , respectively,

$$\begin{aligned} \Sigma^{(1b)}(P, q) &= 16 g^2 \mu^{2\epsilon} \int \frac{d^D k}{(2\pi)^{D-1}} \\ &\times \delta(k^2) [q_\nu (P \cdot k) - (q \cdot k) P_\nu] \\ &\times [q^\nu (P \cdot k) - (q \cdot k) P^\nu] \frac{1}{[(P \cdot k)^2]^2} \\ &= \frac{16 \alpha_s}{3 \pi} \frac{\vec{q}^2}{P^2 - \epsilon} + \dots, \end{aligned} \quad (6)$$

where we have exhibited the infrared pole, regularized for $\epsilon < 0$. This infrared pole, along with an appropriate color trace, appears at NLO as a multiplicative factor times the lowest-order fragmentation function, as found, for example, in Refs. [6, 12].

In the integral, the terms in square brackets correspond to the lowest-order vertices for the operator $q^\alpha F_{\alpha\beta} P^\beta$, with F the field strength. In the quarkonium rest frame, this corresponds to an electric dipole transition from octet to singlet color states [8]. An advantage of this expansion is that, because the field strength decouples from scalar polarized lines, all singularities associated with gluon momenta collinear to l^μ vanish on a diagram-by-diagram basis, and double poles in ϵ are entirely absent in the calculation. By the same token, the integral in (6) is gauge invariant in the polarization sum for the final-state gluon of Fig. 1(b).

Finally, in Fig. 1(c), the soft gluon connects the pair to the Wilson line. In covariant gauges, this diagram has double and single infrared/collinear poles in dimensional regularization. These poles, however, cancel against analogous contributions from the corresponding virtual diagram. Imaginary parts of the virtual diagrams, of course, cancel in the fragmentation

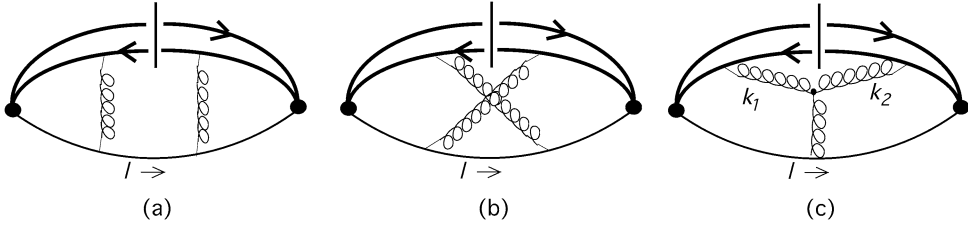


Fig. 2. Representative NNLO contributions to $g \rightarrow c\bar{c}$ fragmentation in eikonal approximation.

function, which is real. In practical terms, the contribution of Fig. 1(c) plus its virtual counterpart contributes solely to the perturbative factor $d_{g \rightarrow c\bar{c}[n]}(z, \mu, m_c)$ in Eq. (3).

We note that the infrared behavior of all of the diagrams of Fig. 1 is common between the fragmentation function and a generic cross section in which a high- p_T gluon of momentum l recoils against the heavy quark pair. Indeed, the same cancellation mechanism for the infrared divergences of Fig. 1(c) is referred to specifically in Ref. [1] as an essential step in the justification of NRQCD factorization for production cross sections. To the extent that all the infrared poles of diagrams that do not share the topology of NRQCD matrix elements cancel, the matching of perturbative infrared poles with those of the effective theory is ensured. The result of this cancellation is referred to as topological factorization [8]. The same considerations that lead to the inclusion of non-Abelian phases to the fragmentation function, however, suggest that the cancellation of nonfactored soft gluons may be nontrivial, and should be checked beyond NLO. Of course, a full NNLO calculation of either cross sections or fragmentation functions would be daunting. Fortunately, the analysis of the relevant infrared behavior at NNLO requires only the eikonal approximation, and is therefore a much more manageable, although still extensive, task, to which we now turn.

5. Fragmentation function at NNLO

We can readily generalize our NLO discussion to NNLO. Once again, because we are interested in gluons whose energies are much less than m_c , we can adopt the eikonal approximation, and neglect all dynamics at the scale of the quark masses. In NRQCD, these approximations are relevant to gluons of order

$m_c v$, with v the relative velocity, but of course in the perturbative calculation the gluon momentum goes to zero. We note that for octet-singlet transitions at NNLO, we need not include virtual gluon exchange between the quark and antiquark, except for diagrams that are already topologically factorized. As a result, we will not need to consider violations of the eikonal approximation from momentum regions at or below the scale $m_c v^2$, or the resulting $1/v$ singular behavior.

Representative diagrams for the fragmentation function are shown in Fig. 2. The full infrared fragmentation function is again generated by taking all allowed cuts of the remaining lines of each such diagram.

We are concerned only with diagrams that connect octet to singlet quark states, and which are not topologically factorized, since these are the potential sources of nonfactoring behavior in both the fragmentation function and related cross sections. We recall once more that the familiar argument for NRQCD factorization is based on the conjecture that all infrared regions in these diagrams cancel after this limited sum over cuts [1]. In fact, we shall see that this is the case at NNLO only if we employ the gauge-completed definitions for NRQCD matrix elements, as in Eq. (5).

As at NLO, we will concern ourselves here with infrared behavior at order v^2 , which may be computed by evaluating each diagram in eikonal approximation and then expanding their sum in q/P , or by expanding the diagrams first, as in Eq. (6). Noting that the two approaches give the same answer, we summarize the results here, and provide details of the calculations elsewhere [13].

The individual classes of diagrams in Fig. 2(a) and (b), for which two gluons are exchanged between the quarks and the Wilson line, satisfy the infrared cancellation conjecture of Ref. [1], by summing over the possible cuts and connections to quark and antiquark lines, as do diagrams that have three gluon-eikonal

vertices on the quark pair and one on the Wilson line. For the class of diagrams related to Fig. 2(c), however, with a three-gluon interaction, this cancellation fails. Expanding again to second order in the relative momentum q , the full contribution from Fig. 2(c), found by cutting the gluon line k_1 and the Wilson line can be written by analogy to Eq. (6) as

$$\begin{aligned} \Sigma^{(2c)}(P, q, l) &= -16i g^4 \mu^{4\epsilon} \int \frac{d^D k_1}{(2\pi)^D} \frac{d^D k_2}{(2\pi)^D} 2\pi \delta(k_1^2) l^\lambda \\ &\times V_{\nu\mu\lambda}[k_1, k_2] [q^\mu (P \cdot k_1) - (q \cdot k_1) P^\mu] \\ &\times [q^\nu (P \cdot k_2) - (q \cdot k_2) P^\nu] \\ &\times \frac{1}{[P \cdot k_1 + i\epsilon]^2 [P \cdot k_2 - i\epsilon]^2} \\ &\times \frac{1}{[k_2^2 - i\epsilon][(k_2 - k_1)^2 - i\epsilon][l \cdot (k_1 - k_2) - i\epsilon]}, \end{aligned} \quad (7)$$

where $V_{\nu\mu\lambda}[k_1, k_2]$ represents the momentum part of the three-gluon coupling. As in Eq. (6), we have suppressed color factors and momentum dependence at the scale m_c .

As observed above, the field-strength vertices eliminate collinear singularities on a diagram-by-diagram basis. The leading singularities in (7) and related diagrams are therefore never worse than $1/\epsilon^2$. Summing over all such contributions, however, we find a non-canceling real infrared pole in the fragmentation function, which may be written in invariant form as

$$\Sigma^{(2)}(P, q, l) = \alpha_s^2 \frac{4}{3\epsilon} \left[\frac{(P \cdot q)^2}{P^4} - \frac{q^2}{P^2} \right]. \quad (8)$$

In the rest frame of heavy-quarkonium ($\vec{P} = 0$), this becomes simply

$$\Sigma(P, q, l) = \alpha_s^2 \frac{4}{3\epsilon} \frac{\vec{q}^2}{4m_c^2} = \alpha_s^2 \frac{1}{3\epsilon} \frac{\vec{v}^2}{4}, \quad (9)$$

where \vec{v} is the relative velocity of the heavy quark pair. We will give the extension of this result to all powers in v elsewhere [13].

Eq. (9) shows explicitly the breakdown of the simplest topological factorization of infrared dependence at NNLO. Its presence implies that infrared poles would appear in coefficient functions at NNLO and beyond when the factorization is carried out with octet NRQCD matrix elements defined in the conventional

manner, Eq. (4). On the other hand, when defined according to its gauge-completed form (5), each octet NRQCD matrix element itself generates precisely the same pole terms given in (9). Thus, at least at NNLO and to order v^2 , NRQCD factorization can accommodate these corrections. We note, however, that at this order the NNLO correction is independent of the direction l of the Wilson line, while Lorentz invariance alone would seem to allow a correction of the form $(q \cdot l)^2/P^2$. The presence of poles with this coefficient could indicate problems with factorization, that is, with matching the poles of the fragmentation function to those of the perturbative cross section. These could arise when the integration over q is not rotationally invariant, as might happen for polarized final states, and/or final states with gluons of energies of order m_c in the rest frame of H , since their directions are arbitrary. We are unable at this stage to rule out the occurrence of such terms at higher orders in the strong coupling, or in higher powers of v^2 .

6. Summary and future studies

We have discussed the gauge invariance properties of color octet matrix elements in NRQCD as they appear in fragmentation functions. Gauge invariance and factorization require that they include non-Abelian phase operators to match otherwise nonfactoring infrared divergences beginning at NNLO.

We have shown that at NNLO there are infrared (not collinear) poles from fragmentation diagrams that are not topologically equivalent to conventional NRQCD operators. We have observed that rotational invariance in the quarkonium rest frame is an important consistency condition for the possibility of NRQCD factorization in terms of the gauge-completion of NRQCD operators. Should rotational invariance fail at higher orders, we anticipate that it will be necessary to complement the NRQCD classification of nonperturbative parameters for quarkonium production with matrix elements of additional operators, involving nonlocal products of the field strengths encountered above.

Finally, although our explicit calculations are carried out in the eikonal approximation for gluons of energies far below m_c , it is not difficult to verify that these gluons do not interfere with the generation of

standard evolution for the $g \rightarrow H$ fragmentation functions. The arguments for this result will be given elsewhere, along with details of the calculations described above.

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