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# Kinematic Enhancement of Non-Perturbative Corrections to Quarkonium Production

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## Abstract

In this letter we address issues involved in quarkonium production near the boundaries of phase space. It is shown that higher-order non-perturbative contributions are enhanced in this kinematic region and lead to a breakdown of the non-relativistic (NRQCD) expansion. This breakdown is a consequence of sensitivity to the kinematics of soft gluon radiation and to the difference between partonic and hadronic phase space. We show how these large corrections can be resummed giving the dominant contribution to the cross section. The resummation leads to the introduction of non-perturbative, universal distribution functions. We discuss the importance of these shape functions for several observables, in particular the energy distribution of photo-produced  $J/\psi$  close to the endpoint.

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Non-relativistic effective field theory (NRQCD) [1] for quarkonium decays and production has shed new light on many aspects of the experimental data. In particular, the inclusion of color-octet decay and production channels rectified some of the main theoretical and phenomenological deficiencies of the color-singlet model and could explain the so-called ‘ $\psi'$ -anomaly’ in  $p\bar{p}$  collisions at the Tevatron [2]. Despite this success, the verification of the universality of long-distance parameters in NRQCD through the comparison of different production processes turns out to be difficult due to significant theoretical uncertainties of various kinds. A large uncertainty stems from the treatment of the kinematics of the hadronization process, which is especially important near the boundary of phase space where keeping the leading order terms in the NRQCD expansion is not valid. Here we concern ourselves exactly with this problem. A partial resummation of the NRQCD expansion leads us to introduce universal shape functions that parameterize quarkonium formation at its kinematic limits. We discuss the effect of these shape functions on quarkonium production rates in a variety of production processes.

In the NRQCD approach the inclusive quarkonium production process factorizes into the production of a (heavy) quark-anti-quark pair at small relative momentum

$$\text{initial state} \rightarrow Q\bar{Q}[n] + \tilde{X}, \quad (1)$$

followed by the ‘hadronization’ of the  $Q\bar{Q}$  pair into a quarkonium  $H$  and light hadrons

$$Q\bar{Q}[n] \rightarrow H + X. \quad (2)$$

The cross section may be written as

$$d\sigma_H = \sum_n d\sigma_{Q\bar{Q}[n]+\tilde{X}} \langle \mathcal{O}_n^H \rangle, \quad (3)$$

where  $d\sigma_{Q\bar{Q}[n]+\tilde{X}}$  is the short distance cross section to produce a  $Q\bar{Q}$  state labeled by  $n$  plus  $\tilde{X}$ , and the general form of the NRQCD matrix element  $\langle \mathcal{O}_n^H \rangle$  is given by

$$\langle \mathcal{O}_n^H \rangle = \sum_X \langle 0 | \psi^\dagger \Gamma_n \chi | H + X \rangle \langle H + X | \chi^\dagger \Gamma'_n \psi | 0 \rangle. \quad (4)$$

$\Gamma_n$  ( $\Gamma'_n$ ) is a matrix in color and spin and may contain derivatives and, in principle, gluon and light quark fields.

The short-distance cross section is insensitive to quarkonium binding by construction and therefore can depend only on the heavy quark mass and kinematic invariants constructed from parton momenta. The quarkonium mass never enters explicitly, since

any non-perturbative effect is parametrized by one of the matrix elements  $\langle \mathcal{O}_n^H \rangle$ . As a further consequence of factorization, the momentum taken by the light hadronic final state  $X$  in (2) is neglected at lowest order in the velocity expansion [1]. This is consistent since the energies involved in (2) are small, of order  $m_Q v^2$ , in the  $Q\bar{Q}$  rest frame, and because the process is inclusive over the light hadronic final state. Thus, given that the difference between partonic and hadronic kinematics is higher order in  $v^2$ , shifting say a partonic to a hadronic endpoint, does not in general improve the accuracy of a calculation if other effects of the same order in the velocity expansion are left out. However, there are circumstances, namely near the boundaries of phase space, where effects higher order in  $v^2$  related to kinematics are enhanced and lead to a breakdown of the velocity expansion. In these cases it becomes necessary to include these effects in a systematic fashion. The breakdown of the velocity expansion is closely related to the fact that near the boundaries of phase space the details of the hadronization process (2) are probed at a scale smaller than  $m_Q v^2$ . This happens, for instance, for quarkonium production close to threshold,  $\hat{s} \rightarrow M_H^2$ , or in  $J/\psi$  photo-production close to the point where all the photon's energy is transferred to the  $J/\psi$  ( $z = E_{J/\psi}/E_\gamma \rightarrow 1$  in the proton rest frame). In these cases, to make the NRQCD expansion convergent, one must smear sufficiently (in  $\hat{s}$  and  $z$ , respectively) so as not to probe the details of hadronization. However, it is possible to reduce the necessary smearing region by resumming a class of leading twist operators into universal shape functions, thus extending the range of applicability of NRQCD. Resummations of related nature have been introduced to treat energy spectra in semileptonic or radiative  $B$  meson [3] and quarkonium [4] decays.

Each kinematic situation must be dealt with slightly differently, although the general idea is the same. Consider some general production process  $A + B \rightarrow H + \tilde{X}$ . To determine the matching coefficients  $d\sigma_{Q\bar{Q}[n]+\tilde{X}}$  at lowest order we calculate the inclusive rate in full QCD to produce a free quark anti-quark pair in a state  $n$ . The momenta of the quark and anti-quark are defined as

$$p_\mu = \frac{P_\mu}{2} + (\Lambda l_1)_\mu \quad \bar{p}_\mu = \frac{P_\mu}{2} + (\Lambda l_2)_\mu, \quad (5)$$

respectively.  $\Lambda$  is the Lorentz transformation which boosts from the frame where  $P_\mu$  is given by  $(2m_Q, \vec{0})$  to whatever frame one chooses for the calculation. In the  $P$ -rest frame  $l_i = (\sqrt{\vec{l}_i^2 + m_Q^2} - m_Q, \vec{l}_i)$  so that  $p^2 = \bar{p}^2 = m_Q^2$ . The production cross section is then expanded in the small momenta  $\vec{l}_i \sim O(m_Q v)$ , and powers of momentum are identified with derivatives acting on heavy quark fields in NRQCD. Thus, a factor of relative momentum  $l_{1i} - l_{2i}$  corresponds to  $(\psi^\dagger i \vec{D}_i \chi)$  and a factor of center-of-mass (cms)

momentum (of the  $Q\bar{Q}$  pair in the  $P$ -rest frame)  $l_{1i}+l_{2i}$  is identified with a total derivative  $iD_i(\psi^\dagger\chi)$ . Four-fermion operators with total derivatives on fermion bilinears are usually ignored since they are of higher order in the non-relativistic expansion than the relative momentum operators. They were first written down in [5] and were later shown to be of dynamical importance in radiative quarkonium decay near the endpoint [4, 6]. (Note that using the equations of motion  $l_{10}+l_{20}$  can be identified with the total time derivative  $iD_0(\psi^\dagger\chi)$ .)

It is precisely these cms-derivative operators that cause the leading singular contributions in the NRQCD expansion in a general situation of constrained phase space. The phase space measure for the process, initial state  $\rightarrow Q(p) + \bar{Q}(\bar{p}) + \tilde{X}$ , is given by

$$d\text{PS} = \frac{d^3P}{(2\pi)^3 2P_0} \prod_i \frac{d^3k_i}{(2\pi)^3 2k_0} \delta^4\left(\sum_l t_l - \sum k_i - (P + \Lambda(l_1 + l_2))\right), \quad (6)$$

where the  $t_l$  are the incoming momenta and  $k_i$  are the momenta of final state particles other than the  $Q\bar{Q}$  pair. The matching strategy then tells us to expand this delta-function, as well as the amplitude squared, in powers of the momenta  $l_1$  and  $l_2$ . The delta-function depends explicitly on the cms momentum  $\vec{l}_1 + \vec{l}_2$  and implicitly on the relative momentum through the zero-components of  $l_i$ . The expansion of the delta-function results in a series in  $v^2$ , but with increasingly singular distributions at the boundary of partonic phase space defined by the delta-function with  $l_i$  set to zero. Normally, the phase space is integrated with a smooth function, and the terms coming from the expansion of the delta function converge rapidly, provided  $v^2$  is small. However, if the weighting function has support mainly in a region of order  $\epsilon m_Q$  near the boundary of phase space, the expansion parameter is  $v^2/\epsilon$ . Thus  $\epsilon \gg v^2$  is required for convergence. On the other hand, resumming the leading terms  $(v^2/\epsilon)^n$  to all orders allows us to take  $\epsilon \sim v^2$ . Provided that the squared amplitude for the production process is non-singular at the boundary of phase space, the resummation of the leading singular contributions is easily accomplished. Note that even after resummation we can not consider  $\epsilon \ll v^2$ , because all subleading terms  $v^{2m}(v^2/\epsilon)^n$  become important as well in this region. Since the details depend on the particular kinematic situation, we shall show how this works in several processes of topical interest.

Let us begin by considering the case of gluon fragmentation into  $\psi$  ( $J/\psi$  or  $\psi'$ ) through a  $Q\bar{Q}$  pair in a  $^3S_1$  color-octet state, which is now regarded as the dominant source of direct  $\psi$  production at large transverse momentum in hadron collisions [2]. The octet  $Q\bar{Q}$  pair evolves non-perturbatively into the  $\psi$ , a process necessarily accompanied

by soft gluon radiation. At lowest order in  $v^2$  the momentum of the soft gluon radiation can be neglected and the fragmentation function is given by

$$D_{\psi/g}(\hat{z}, 2m_c) = \frac{\pi\alpha_s(2m_c)}{24m_c^3}\delta(1-\hat{z})\langle\mathcal{O}_8^\psi(^3S_1)\rangle. \quad (7)$$

The hat reminds us that the variable  $\hat{z} = P_+/k_+$  is defined in terms of the light-cone +-components of parton momenta, that is,  $P_+$  refers to  $P$  in (5) rather than the  $\psi$ -momentum.  $k$  is the momentum of the fragmenting gluon. As noted in [7] this fragmentation function is folded with a gluon production cross section, which, for a given value of the  $\psi$  transverse momentum, is a rapidly varying function of  $\hat{z}$ . To be precise

$$\frac{d\sigma}{dp_t} = \int_{\hat{z}_{min}}^1 \frac{d\hat{z}}{\hat{z}} K(\hat{z}, p_t) D_{\psi/g}(\hat{z}, p_t), \quad (8)$$

where  $K(\hat{z}, p_t) \sim \hat{z}^5$  in the region  $p_t \sim 15$  GeV. Consequently, the integral (8) depends sensitively on the shape of the fragmentation function near  $\hat{z} = 1$  and neglecting the kinematics of soft gluon emission is not a good approximation. Intuitively, one expects soft gluon radiation to soften the fragmentation function<sup>1</sup> (7) and therefore to reduce  $d\sigma/dp_t$  [7]. However, this intuition relies on interpreting  $\hat{z}$  as the quarkonium +-momentum fraction, different from the definition of  $\hat{z}$  given above.

Now the existence of cms momentum  $l = l_1 + l_2$  in the matching relations can be interpreted in the quarkonium rest frame as recoil of the  $Q\bar{Q}$  pair against the emitted soft gluons. Indeed, since the matrix element for  $g^* \rightarrow Q\bar{Q}$  is evidently non-singular at  $\hat{z} = 1$ , the leading singular contributions to the coefficient functions of higher-dimension operators in the NRQCD expansion simply follow from (6). After integrating over phase space except for the +-direction, this leads to the shift

$$\delta(1-\hat{z}) \rightarrow \delta(1-\hat{z}-\Lambda_{+\mu}l^\mu/P_+). \quad (9)$$

In terms of operators in the NRQCD expansion, expanding the modified delta-function in  $\Lambda_{+\mu}l^\mu/P_+ = l_+/(2m_Q)$ , we obtain the series

$$D_{\psi/g}(\hat{z}, 2m_c) = \frac{\pi\alpha_s(2m_c)}{24m_c^3} \sum_m \frac{1}{m!} \delta^{(m)}(1-\hat{z}) \sum_X \langle 0 | \psi^\dagger \sigma_i T^A \chi | \psi + X \rangle \langle \psi + X | (in \cdot \hat{D})^m (\chi^\dagger \sigma_i T^A \psi) | 0 \rangle, \quad (10)$$

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<sup>1</sup>This softening occurs before the onset of Altarelli-Parisi evolution that further softens the fragmentation function at the scale  $p_t$ .

where  $n$  is the light like vector  $(1, 0, 0, -1)$ ,  $\hat{D} = D/(2m_c)$  and  $\delta^{(m)}(1 - \hat{z})$  denotes the  $m$ 'th derivative of the delta-function. The first term in the sum reproduces (7). Introducing the shape function

$$F_\psi[{}^3S_1^{(8)}](y_+) = \sum_X \langle 0 | \psi^\dagger \sigma_i T^A \chi | \psi + X \rangle \langle \psi + X | \delta(y_+ - in \cdot \hat{D}) (\chi^\dagger \sigma_i T^A \psi) | 0 \rangle, \quad (11)$$

we rewrite (10) as

$$D_{\psi/g}(\hat{z}, 2m_c) = \frac{\pi\alpha_s(2m_c)}{24m_c^3} \int dy_+ \delta(1 - \hat{z} - y_+) F_\psi[{}^3S_1^{(8)}](y_+). \quad (12)$$

Note that  $F_\psi[{}^3S_1^{(8)}](y_+)$  is a non-perturbative distribution function that can not be calculated except within models. But the factorization as expressed by (11) and (12) implies that such shape functions are process-independent. Moreover,  $F_\psi[{}^3S_1^{(8)}](y_+)$  has support mainly for  $|y_+| < v^2$ . We assume  $m_Q v \gg m_Q v^2 \sim \Lambda_{QCD}$  for NRQCD power counting, in which case a cms-derivative acting on a quark bilinear scales as  $m_Q v^2$ , the momentum of dynamical gluons in NRQCD.<sup>2</sup> It is suggestive to interpret  $F_\psi[{}^3S_1^{(8)}](y_+)$  as the probability for soft gluons to carry off a light-cone momentum fraction  $y_+$  in the hadronization of the color-octet  $Q\bar{Q}$  pair. Although useful, this interpretation is not quite exact, because, as will be seen in more detail below, such distribution functions are non-trivial even for color-singlet  $Q\bar{Q}$  states, when no soft gluon emission is required. In such cases, the shape functions account for the difference between quark and quarkonium masses and the corresponding difference in the definition of kinematic variables.

The  $\psi$  production rate at fixed  $p_t$  follows from integrating the fragmentation function with a function that roughly varies as  $\hat{z}^4$ , see (8). Eq. (10) implies that the NRQCD expansion parameter is then  $4v^2 \sim 1$  rather than  $v^2$ . Inclusion of the effects due to the shape function  $F_\psi[{}^3S_1^{(8)}](y_+)$  can therefore alter the  $\psi$  production cross section of order unity, an effect that should be kept in mind when  $\langle \mathcal{O}_8^\psi({}^3S_1) \rangle$  extracted from Tevatron data [9] is compared with the extraction from another production process. Unfortunately, without a non-perturbative calculation of the shape function, no detailed prediction is possible. We note that the prediction that the  $\psi$  is transversely polarized at large  $p_t$  [10] in hadron collisions remains unaffected by the resummation procedure described here. (For perturbative corrections to this prediction see [11].)

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<sup>2</sup>In the construction of [8] this can be seen from the fact that the matrix element with  $n$  cms derivatives vanishes unless one inserts an  $n$ 'th multipole operator resulting in an additional  $1/c^n$  factor above those coming from naive dimensional analysis.

Our second example concerns the total hadro-production cross section of a quarkonium  $H$  at fixed target energies. In this case we write the cross section as

$$\sigma_H = \sum_{i,j} \int_0^1 dx_1 dx_2 f_{i/A}(x_1) f_{j/B}(x_2) \hat{\sigma}(ij \rightarrow H + \tilde{X}), \quad (13)$$

The sum extends over all partons in the colliding hadrons and  $f_{i/A}$ , etc. denote the corresponding parton distribution functions. The parton cross section  $\hat{\sigma}$  is a distribution that is weighted with the parton densities. Let us consider the leading parton process  $i + j \rightarrow Q(p) + \bar{Q}(\bar{p})$ . Since its matrix element is again non-singular at the boundaries of phase space, it is sufficient to retain  $l_i$  in (6) and to set  $l_i = 0$  in the matrix element, in order to obtain the most singular coefficient functions to all orders in  $v^2$ . The parton cross section may then be written as

$$\hat{\sigma}(ij \rightarrow H) = \frac{\pi^3 \alpha_s^2 (2m_Q)}{(2m_Q)^3} \sum_n C^{ij}[n] \sum_X \langle 0 | \psi^\dagger \Gamma_n \chi | H + X \rangle \langle H + X | \delta(x_1 x_2 s - 4m_Q^2 - 2(k_i + k_j) \cdot \Lambda l) \chi^\dagger \Gamma'_n \psi | 0 \rangle, \quad (14)$$

where  $k_{i,j}$  are the four-momenta of the incoming partons,  $s$  the hadron center-of-mass energy and  $l = iD$ . The sum over  $n$  extends over all possible operators and is truncated according to the non-relativistic power counting rules. For the two most important production channels in  $S$ -wave quarkonium production  $C^{gg}[^1S_0^{(8)}] = 5/12$ ,  $C^{gg}[^3P_0^{(8)}] = 35/(12m_Q^2)$  [12, 13]. Using  $2(k_i + k_j) \cdot \Lambda l \approx 2P \cdot \Lambda l = 4m_Q l^0$  and expanding the delta-function gives the series of higher-dimension operators

$$\hat{\sigma}(ij \rightarrow H) = \frac{\pi^3 \alpha_s^2 (2m_Q)}{(2m_Q)^3 s} \sum_n C^{ij}[n] \sum_m \frac{1}{m!} \delta^{(m)}(x_1 x_2 - \frac{4m_Q^2}{s}) \sum_X \langle 0 | \psi^\dagger \Gamma_n \chi | H + X \rangle \langle H + X | \left( \frac{8m_Q^2 i \hat{D}_0}{s} \right)^m (\chi^\dagger \Gamma'_n \psi) | 0 \rangle, \quad (15)$$

which accounts for all most singular contributions at  $x_1 x_2 = 4m_Q^2/s$ . As previously,  $\hat{D} = D/(2m_Q)$ . Note that as opposed to (10), the higher-dimension operators involve time rather than +-derivatives. Accordingly we define a shape function in energy fraction  $y_E$

$$F_H[n](y_E) = \sum_X \langle 0 | \psi^\dagger \Gamma_n \chi | H + X \rangle \langle H + X | \delta(y_E - i \hat{D}_0) (\chi^\dagger \Gamma'_n \psi) | 0 \rangle. \quad (16)$$

We emphasize that  $F_H[n](y_E)$  and  $F_H[n](y_+)$  in (11) are different non-perturbative distributions. Up to the caveat mentioned above,  $F_H[n](y_E)$  can be interpreted, in the

quarkonium rest frame, as the distribution of energy fraction taken by soft gluons during the transition from the short-distance heavy quark pair in a state  $n$  into the quarkonium  $H$ .

Consider now the case where the  $Q\bar{Q}$  pair is in the same color-singlet state as the quarkonium  $H$ . Up to corrections suppressed in  $v^2$ , we can use the vacuum saturation approximation and drop the sum over  $X$  in (16). The derivative  $iD_0$  produces a factor of the binding energy and we obtain

$$F_H[n](y_E) = \delta\left(y_E - \frac{M_H - 2m_Q}{2m_Q}\right) \langle 0|\psi^\dagger\Gamma_n\chi|H\rangle\langle H|\chi^\dagger\Gamma'_n\psi|0\rangle, \quad (17)$$

where  $M_H$  is the quarkonium mass. Consequently, the  $y_E$ -integral that enters the production cross section (see (20) below) can be done:

$$\int dy_E F_H[n](y_E) \delta(x_1x_2s - 4m_Q^2 - 8m_Q^2y_E) = \delta(x_1x_2s - 4m_Q^2 - 4m_Q(M_H - 2m_Q)) \cdot \langle 0|\psi^\dagger\Gamma_n\chi|H\rangle\langle H|\chi^\dagger\Gamma'_n\psi|0\rangle. \quad (18)$$

Since  $M_H^2 = 4m_Q^2 + 4m_Q(M_H - 2m_Q) + O(v^4)$ , we see that the sole effect of the distribution function in the vacuum saturation approximation is to shift the unphysical partonic boundary of phase space to the hadronic one. The inclusion of sub-leading terms would complete the transmutation

$$\delta(x_1x_2s - 4m_Q^2) \rightarrow \delta(x_1x_2s - M_H^2). \quad (19)$$

As we previously mentioned, performing this resummation does not in general improve the accuracy of the calculation, given that other contributions of the same order in  $v^2$  have been left out. However, if the corrections from the expansion of the delta-function are enhanced because the dominant contribution to the cross section comes from a region close to the boundary of phase space, then we have indeed improved the situation. Introducing the variable  $\tau = x_1x_2$  and the parton luminosities  $L_{ij}(\tau) = \int_\tau^1 dx/x f_{i/A}(x)f_{j/B}(\tau/x)$ , the hadro-production cross section can be expressed as

$$\sigma_H = \frac{\pi^3\alpha_s^2(2m_Q)}{(2m_Q)^3} \sum_{i,j} \int_0^1 d\tau L_{ij}(\tau) \sum_n C^{ij}[n] \int dy_E F_H[n](y_E) \delta(\tau s - 4m_Q^2 - 8m_Q^2y_E). \quad (20)$$

At high energies  $s \gg 4m_Q^2$ , the gluon-gluon fusion channel dominates and we see that the partonic cross section is weighted by a gluon luminosity, that, because of the small- $x$



behaviour of the gluon distribution, increases rapidly as  $\tau$  decreases. Thus, a systematic shift in  $\tau$  due to an asymmetric shape function  $F_H[n](y_E)$  (such as the example (17) above) can affect the magnitude of the total cross section in an important way. Indeed, one finds in the leading order in  $v^2$  predictions that the difference between quark and quarkonium masses in the phase space delta-function introduces a normalization uncertainty of up to a factor two for  $\psi'$  and  $\chi$  production. As noted in [12], the effect should be even more pronounced in color-octet mechanisms as, due to soft gluon radiation, the final state invariant mass is always larger than  $M_H^2$ .

As our final, and perhaps most interesting, example we examine photo-production of  $J/\psi$ , in particular the  $z$ -distribution, where  $z = p \cdot P_{J/\psi} / p \cdot k_\gamma$  and  $p$  is the proton momentum.<sup>3</sup> ( $z = E_{J/\psi} / E_\gamma$  in the proton rest frame.) To exclude higher-twist contributions from diffractive  $J/\psi$  production, which can not be accommodated in the leading-twist NRQCD factorization formalism, it is preferable to consider inelastic  $J/\psi$  production and to impose  $z < 0.9$  and  $P_t > 1$  GeV. Inelastic  $J/\psi$  photo-production is often perceived as a problem for the NRQCD theory of onium production, because the color-octet contributions to this process rise rapidly with  $z$  [14], which is not supported by the data. On the other hand octet production is accompanied by gluon radiation, which carries away an energy fraction of order  $v^2$  and makes it highly unlikely to reach a value of  $z$  close to one [12]. Technically, the necessary smearing of the energy distribution is again achieved through a shape function, as we shall see, although the situation is slightly more complicated for the  $2 \rightarrow 3$  parton processes than for the  $2 \rightarrow 2$  parton processes considered before.

Before addressing this issue, let us briefly comment on the  $2 \rightarrow 2$  parton processes in photo-production, which are kinematically restricted to  $\hat{z} = p \cdot P / p \cdot k_\gamma = 1$  and  $P_t = 0$ . We emphasize again that the calculation in NRQCD refers to partonic variables like  $\hat{z}$  with  $P$  defined in (5) rather than  $z$ . If we are interested in the total cross section then the analysis goes through almost exactly as in the case of hadro-production. In fact the same shape function (16) enters. However, the total cross section is of marginal interest experimentally. More interesting are the differential distributions. For the gluon fusion process

$$\frac{d\sigma_H}{d\hat{z}d^2P_t} = \frac{\pi^3 \alpha_s (2m_Q) \alpha_{em}}{\hat{z} (2m_Q)^3} \int_0^1 dx f_{g/P}(x) \int dy_E dy_+ d^2\rho_t \sum_n C^g[n] F_H[n](y_E, y_+, \vec{\rho}_t)$$

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<sup>3</sup>Because we will be concerned with the large- $z$  region, we do not consider resolved photon interactions in the following.

$$\delta(sx - 4m_Q^2 - 8m_Q^2 y_E) \delta(1 - \hat{z} - y_+) \delta^{(2)}(\vec{P}_t - \vec{\rho}_t), \quad (21)$$

where

$$F_H[n](y_E, y_+, \vec{\rho}_t) = \sum_X \langle 0 | \psi^\dagger \Gamma_n \chi | H + X \rangle \langle H + X | \delta(y_+ - in \cdot \hat{D}) \delta(y_E - i\hat{D}^0) \delta(\vec{\rho}_T - i\vec{D}_T) (\chi^\dagger \Gamma'_n \psi) | 0 \rangle. \quad (22)$$

Such a multi-dimensional distribution is much too complicated to be useful in practice, and we do not pursue it further here. Qualitatively, this distribution causes smearing in  $\hat{z}$  and transverse momentum over a region (for  $Q = c$ )

$$\delta\hat{z} \approx v^2 \approx 0.25 - 0.3, \quad \delta P_t \approx m_c v^2 \approx 0.5 \text{ GeV}. \quad (23)$$

Unless the endpoint region is averaged over an interval of this size, the NRQCD expansion fails to be convergent, even if the above distribution function is taken into account. Smearing over a range much larger than (23), makes the corrections considered here irrelevant and one can return to the ordinary velocity expansion. Note that because of the sizeable smearing in  $\hat{z}$ , part of the  $2 \rightarrow 2$  parton contributions that are normally considered to be localized at  $z = 1$  actually leaks into the inelastic region  $z < 0.9$ . This leakage can be eliminated by a transverse momentum cut  $P_t \gg m_c v^2$ . Note also that the smearing in the transverse direction is of the same order of magnitude as the smearing caused by intrinsic transverse momentum of the gluon in the proton.

Let us return now to inelastic photo-production of quarkonium and consider  $\gamma + g \rightarrow Q(p) + \bar{Q}(\bar{p}) + g(k)$ . It is straightforward to obtain

$$\begin{aligned} \frac{d\sigma}{d\hat{z}} &= \int_{P_{t,min}^2} dP_t^2 \int_0^1 dx S(x, \hat{z}, P_t^2) \sum_X \langle 0 | \psi^\dagger \Gamma_n \chi | H + X \rangle \\ &\quad \langle H + X | \delta \left( s(1 - \hat{z})x - \frac{M^2(1 - \hat{z}) + P_t^2}{\hat{z}} - 2k \cdot \Lambda iD \right) (\chi^\dagger \Gamma'_n \psi) | 0 \rangle, \quad (24) \\ S(x, \hat{z}, P_t^2) &= \frac{1}{16\pi \hat{z} x s} f_{g/p}(x) |\mathcal{M}_n|^2, \end{aligned}$$

where  $s$  is the cms energy,  $M = 2m_Q$ , and  $\mathcal{M}_n$  is the matrix element to produce the  $Q\bar{Q}$  pair in a state  $n$ . If we neglect the covariant derivative  $D$  in the delta-function, the standard kinematic relations for the inelastic processes considered in [14] are recovered. To proceed, we have to extract the dependence of  $2k \cdot \Lambda D$  on  $\hat{z}$  and  $P_t$ . To this end we

note that

$$\sum_X \langle 0 | \psi^\dagger \Gamma_n \chi | H + X \rangle \langle H + X | (iD_{\mu_1}) \dots (iD_{\mu_m}) (\chi^\dagger \Gamma'_n \psi) | 0 \rangle = A_m[n] w_{\mu_1} \dots w_{\mu_m} + g_{\mu_i \mu_j}\text{-terms} \quad (25)$$

in a frame where the  $Q\bar{Q}$ -pair moves with four-velocity  $w$ . Since  $k$  is a light-like four-vector, terms involving the metric tensor  $g_{\mu_i \mu_j}$  do not contribute and we obtain, in the rest frame of  $P$  (see (5)),

$$\sum_X \langle 0 | \psi^\dagger \Gamma_n \chi | H + X \rangle \langle H + X | (2k \cdot \Lambda iD)^m (\chi^\dagger \Gamma'_n \psi) | 0 \rangle = A_m[n] (2k_{rest}^0)^m. \quad (26)$$

Using

$$2k_{rest}^0 = \frac{2P \cdot k}{M} = \frac{M^2(1 - \hat{z})^2 + P_t^2}{M\hat{z}(1 - \hat{z})}, \quad (27)$$

we can write (24) as

$$\frac{d\sigma}{d\hat{z}} = \int_{P_{t,min}^2} dP_t^2 \int_0^1 dx \int dy_+ S(x, \hat{z}, P_t^2) F_H[n](y_+) \delta\left(s(1 - \hat{z})x - \frac{M^2(1 - \hat{z}) + P_t^2}{\hat{z}} - \frac{M^2(1 - \hat{z})^2 + P_t^2}{\hat{z}(1 - \hat{z})}y_+\right), \quad (28)$$

where the shape function  $F_H[n](y_+)$  is defined as in (11), generalized to an arbitrary  $Q\bar{Q}$  state  $n$ . Now let us examine the delta-function. For any non-zero  $P_t$  we see that the expansion parameter close to  $\hat{z} = 1$  is  $y_+/(1 - \hat{z}) \sim v^2/(1 - \hat{z})$ . Thus, the NRQCD expansion breaks down for  $1 - \hat{z} \sim O(v^2)$ , because higher-order terms in  $v^2$  grow more and more rapidly as  $\hat{z} \rightarrow 1$ .<sup>4</sup> Consequently, the NRQCD factorization approach makes no prediction in the endpoint region and the discrepancy between leading order predictions [14] and data in this region does not allow us to draw any conclusion on the relevance of color-octet contributions to photo-production. If one averages the  $\hat{z}$ -distribution over a sufficiently large region containing the endpoint, the octet mechanisms contribute significantly to this average. However, the characteristic shape information is then lost and one has to deal with the more difficult and uncertain question of whether the absolute

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<sup>4</sup>The integral over  $\hat{z}$  still exists, because for any fixed  $P_t$ ,  $\hat{z}$  can never reach one. However,  $1 - \hat{z}_{max} = O(M^2/s, P_t^2/s)$  is very small in a high energy collision. We also mention that in the case considered here, the expansion of the partonic amplitude in  $l_1$  and  $l_2$  can also produce terms more singular in  $1/(1 - \hat{z})$  in higher orders in  $l_i$ .

magnitude of the cross section requires the presence of octet contributions and whether their magnitude is consistent with other production processes. Almost identical remarks apply to the endpoint region in the  $J/\psi$  energy distribution in the process  $B \rightarrow J/\psi + X$  or  $e^+e^- \rightarrow J/\psi + X$ .

In conclusion, we have shown how the NRQCD expansion of quarkonium production processes breaks down in regions of phase space, where the prediction is sensitive either to the difference between parton and hadron kinematics or to momentum carried away by light hadrons in the hadronization process (2). The amount of smearing which is necessitated by this breakdown can be reduced by introducing universal shape functions in NRQCD as illustrated in this letter. Being universal, these functions could in principle be extracted from one production process and used for another. However, the existence of such functions for every  $Q\bar{Q}$  state  $n$  at short distances, together with functions in different variables (such as  $y_+$  and  $y_E$ ) makes this difficult in practice. At this stage it seems worthwhile to use the operator expressions for the shape functions to invent phenomenological models for these functions, which are consistent with the properties of NRQCD.

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