Kinematic effects in radiative quarkonia decays

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Nonrelativistic QCD (NRQCD) predicts color octet contributions to be significant not only in many production processes of heavy quarkonia but also in their radiative decays. We investigate the photon energy distributions in these processes in the end point region. There the velocity expansion of NRQCD breaks down which requires a resummation of an infinite class of color octet operators to so-called shape functions. We model these nonperturbative functions by the emission of a soft gluon cluster in the initial state. We found that the spectrum in the end point region is poorly understood if the values for the color octet matrix elements are taken as large as indicated from NRQCD scaling rules. Therefore the end point region should not be taken into account for a fit of the strong coupling constant at the scale of the heavy quark mass.

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I. INTRODUCTION

Since the discovery of the J/ψ [1] and the Υ [2] heavy quarkonia decays are one of the most interesting laboratories for investigations within the framework of perturbative QCD. In particular these bound states of a heavy quark Q and its antiparticle $\overline{Q}$ have been examined to extract the value of the strong coupling constant α_s at the scale of the heavy quark mass m_Q.

Early theoretical analyses starting from the calculation of the total rates in leptonic and inclusive hadronic decays [3] were done in the color singlet model (CSM). It *assumes* the quark-antiquark pair being in the same quantum state $n = {}^{2S+1}L_J^{(C)}$ on the partonic level as the corresponding quarkonium on the hadronic level. In particular the $Q\overline{Q}$ pair has to be in a color singlet state ($C=1$) when it annihilates. As a consequence of this requirement the underlying partonic process in the radiative decay $H\to\gamma X$ of a quarkonium H in the ground state ${}^3S_1$ is the annihilation of the heavy $Q\overline{Q}$ pair into a photon and at least two gluons. This process was calculated first in [4].

Great theoretical progress in the understanding of bound states of heavy $Q\overline{Q}$ systems has been achieved by nonrelativistic quantum chromodynamics (NRQCD) [5]. In this *theory* quarkonia decays are factorized into two step processes: the short-distance annihilation of a $Q\overline{Q}$ pair with fixed total spin S, orbital angular momentum L, and total angular momentum J and its preceding long-distance transition into this state. While the partonic subprocess can be calculated perturbatively to definite order in α_s the nonperturbative subprocess $H\to Q\overline{Q}[n]+$ *soft degrees of freedom* is parametrized by NRQCD matrix elements. They are the NRQCD counterparts of the wave function at the origin in the color singlet model and give the probability for finding the quark-antiquark pair in the quantum state n at the moment of annihilation. In principle the values of these parameters are unknown and must be fitted to experimental data [6] or computed on the lattice [7]. Nevertheless NRQCD provides scaling rules which, e.g., predict color octet matrix elements being suppressed by powers of the non-relativistic velocity v with respect to the leading order color singlet matrix element. This typical velocity of the heavy (anti)quark inside the quarkonium simultaneously serves as expansion parameter of the effective field theory. As a result NRQCD describes a decay rate by an infinite sum over matrix elements of four fermion operators with Wilson coefficients which on their part are expansions in α_s.

Taking only the leading order in v/c the NRQCD result coincides with the one of the CSM. However, subleading terms in the velocity expansion could be still important numerically: In radiative decays the partonic kernel of a color octet contribution is enhanced by an inverse power of $\alpha_s(m_Q)$ with respect to the leading order color singlet mode. While the leading term needs two hard gluons in the final state [cf. Fig. 1(a)] a $Q\overline{Q}$ pair in a color octet state can annihilate into a photon and a single gluon [cf. Fig. 1(b)]. Thus one may also take into account the subleading terms in v/c.

The photon energy spectrum in the hard subprocess $Q\overline{Q}[n]\to\gamma X$ of radiative decays has been calculated in next-to-leading order perturbative QCD for both the color singlet mode [8] and the color octet modes [9]. Another perturbative contribution may become important in the upper end point region ($z=2E_\gamma/M_H\to 1$) of the spectrum. Due to an imperfect cancellation between terms stemming from real and virtual emission of soft gluons one could expect potentially large logarithms $\ln(1-z)$ to all orders of the perturbation theory. A resummation of these logarithms would then give rise to a Sudakov suppression $\sim\exp\{-\alpha_s\ln^2(1-z)\}$. Though an earlier analysis [10] claimed such a Sudakov damping factor in the color singlet mode, a more recent work [11]

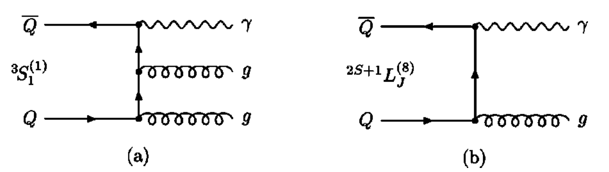

FIG. 1. Direct contributions to the radiative decay of a $Q\overline{Q}$ pair: on the left (a) one of six color singlet diagrams, on the right (b) one of two diagrams per color octet mode.

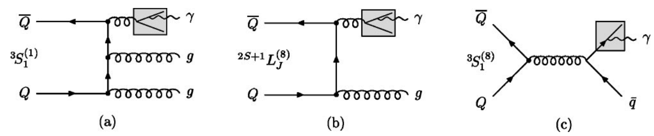

FIG. 2. Fragmentation contributions to the radiative decay of a $Q\bar{Q}$ pair: color singlet contribution (a); color octet contribution (b) and (c). The non-perturbative subprocesses inside the gray boxes are described by the gluon (a) + (b) and the quark (c) fragmentation function respectively.

predicts such Sudakov factors in the color octet channels only while the logarithms should cancel order by order α_s in the color singlet mode.

Besides these perturbative contributions several non-perturbative effects have been investigated as well. They become important near the phase space boundaries where the photon energy fraction z is small or close to 1, respectively. For low values of z there is a large fragmentation contribution caused by the collinear emission of a photon from a light (anti)quark in the final state. Examples for such processes are diagrammed in Fig. 2. They have been investigated in [12] for the color singlet mode and in [9] for the color octet channels.

At the upper end point of the spectrum two different sources for non-perturbative effects exist. The first one is the phase space effect associated with the hadronization of massless gluons into massive final states. This effect usually is considered by a parton shower Monte Carlo thereby generating a non-zero invariant mass for the outgoing gluon(s) [13]. Another method based on the introduction of an effective gluon mass [14] could obtain the appropriate phase space suppression by fitting the values of the effective gluon mass to data of radiative J/ψ [15] and Υ [16,17] decays independently [18].

In this article we concentrate on another non-perturbative effect contributing to the upper endpoint of the spectrum. In this region NRQCD operators connected to the center-of-mass (cms) movement of the $Q\bar{Q}$ pair inside the quarkonium could become significant even though they are subleading in the sense of the naive NRQCD power counting [19,20]. It has been shown in [20] explicitly that the NRQCD velocity expansion breaks down near the end point. The reason for this breakdown is the kinematical enhancement of the cms operators. In the end point region the expansion parameter is v^2/ϵ rather than v^2 where $\epsilon = 1 - E_\gamma/m_Q$ is a measure for the distance from the end point. Thus the velocity expansion works fine only for photon energies that are significantly further away from the end point than $\Delta E_\gamma \sim m_Q v^2$. However, the range of applicability of NRQCD can be extended to higher values for E_γ by the resummation of an infinite class of operators into so-called shape functions [20].[1] Thereafter the shape function improved spectrum holds up to a resolution of $\Delta E_\gamma \sim m_Q v^2$.

The shape function formalism yields different shape functions for the different quantum states n of the quark-antiquark pair ($Q\bar{Q}[n]$). In the leading color singlet case the shape function is nothing else than a *number*, namely the corresponding NRQCD matrix element. In the color octet modes the shape functions are real *functions* reflecting the phase space dependence of the soft gluon radiation. Thus the partonic spectrum of the relevant channels $n = \{{}^1S_0^{(8)}, {}^3P_J^{(8)}, {}^3S_1^{(8)}\}$ which is proportional to $\delta(E_\gamma - m_Q)$ is smeared out to a quite broad peak.

As mentioned above their contribution may be as large as the one from the leading order. If we compare the total rates of the leading color singlet and a subleading color octet term we get

$$\Gamma_1 : \Gamma_8 = \frac{\alpha_s(m_Q)}{4\pi} : v^4 = \mathcal{O}(1). \tag{1}$$

Thus it is worth modeling the non-perturbative shape functions to estimate their influence on the photon energy distribution. For the construction of the model we keep close to a model successfully used for shape functions in quarkonium production [22]. In this case the shape functions which originally were defined in [23] have been modeled by soft gluon emission from the final state. Inspired by the success in describing the J/ψ production in B decays and in the photoproduction channel we take over the physically simple picture of radiating off soft gluons from the heavy (anti)quark.

We will proceed as follows: First we will recapitulate the result of underlying partonic process $Q\bar{Q}[n] \to \gamma + g$ and $Q\bar{Q}[n] \to \gamma + g + g$ for $n = {}^{2S+1}L_J^{(C)} \in \{{}^1S_0^{(8)}, {}^3P_J^{(8)}, {}^3S_1^{(8)}\}$ and $n = {}^3S_1^{(1)}$ respectively. Moreover, we will show to what extent fragmentation contributions must be taken into account. Afterwards the construction and application of our shape function model in the decay mode is given. Finally we discuss the results of the numerical evaluation of the semi-inclusive decay $\Upsilon(1S) \to \gamma +$ *light hadrons*.

II. THE PARTONIC CALCULATION

Within NRQCD the photon energy spectrum in the semi-inclusive decay $H \to \gamma X$ of a quarkonium is represented by the operator product expansion

$$\frac{d\Gamma}{d\hat{z}} = \sum_n \mathcal{C}[n] \langle H | \mathcal{O}[n] | H \rangle. \tag{2}$$

Here the Wilson coefficient $\mathcal{C}[n]$ is calculable perturbatively and gives the differential rate $d\Gamma_n/d\hat{z}$ in the decay of a $Q\bar{Q}$ pair with quantum numbers n into a photon and light hadrons X. Note that in conventional NRQCD the photon energy is normalized on the quark rather than on the quarkonium mass: $\hat{z} = E_\gamma/m_Q$.

A. Direct contributions

Equation (2) includes not only the contributions from the direct production of a photon (Fig. 1) but also the production via fragmentation (Fig. 2). We will come to this point later.

[1] These shape functions are conceptually similar to the shape functions used in B meson decays [21].

We first deal with the direct channels. The leading term in the non-relativistic expansion is the color singlet mode displayed in diagram 1(a). It has been calculated perturbatively up to $\mathcal{O}(\alpha_s)$ [8]. For the sake of simplicity we restrict ourselves on the tree level contribution. It is [4]

$$\mathcal{C}_\gamma^{\rm dir}[{}^3S_1^{(1)}](\hat{z}) = \frac{32e_Q^2\alpha_{\rm em}(m_Q)\alpha_s^2(m_Q)}{27m_Q^2}\left[\frac{2-\hat{z}}{\hat{z}}+\frac{\hat{z}(1-\hat{z})}{(2-\hat{z})^2} + 2\frac{1-\hat{z}}{\hat{z}^2}\ln(1-\hat{z}) - 2\frac{(1-\hat{z})^2}{(2-\hat{z})^3}\ln(1-\hat{z})\right]. \tag{3}$$

The subleading terms $\mathcal{O}(v^4)$ in the velocity expansion arise from Feynman diagrams like Fig. 1(b), where ${}^{2S+1}L_J^{(C)} = {}^1S_0^{(8)}$, ${}^3P_0^{(8)}$, or ${}^3P_2^{(8)}$. They are perturbatively enhanced in comparison to the color singlet channel $[\mathcal{O}(\alpha_s)$ versus $\mathcal{O}(\alpha_s^2)]$. Due to their two body kinematics the photon spectrum is fixed to a definite energy value:

$$\mathcal{C}_\gamma^{\rm dir}[n](\hat{z}) = \frac{1}{2(2m_Q)}\frac{1}{8\pi}H[Q\overline{Q}[n]\to\gamma g](2m_Q)\,\delta(1-\hat{z}). \tag{4}$$

The spin and color averaged squares $H[Q\overline{Q}[n]\to\gamma g](2m_Q)$ of the amplitudes for the three relevant channels are (again we take only leading terms in α_s) [9]

$$H[Q\overline{Q}[{}^1S_0^{(8)}]\to\gamma g](2m_Q) = \frac{256\pi^2 e_Q^2\alpha_{\rm em}(m_Q)\alpha_s(m_Q)}{2m_Q}, \tag{5a}$$

$$H[Q\overline{Q}[{}^3P_0^{(8)}]\to\gamma g](2m_Q) = \frac{768\pi^2 e_Q^2\alpha_{\rm em}(m_Q)\alpha_s(m_Q)}{2m_Q}, \tag{5b}$$

$$H[Q\overline{Q}[{}^3P_2^{(8)}]\to\gamma g](2m_Q) = \frac{1024\pi^2 e_Q^2\alpha_{\rm em}(m_Q)\alpha_s(m_Q)}{5(2m_Q)}. \tag{5c}$$

B. Fragmentation contributions

Let us turn to the fragmentation contributions now. The corresponding processes are associated with diagrams like the ones in Fig. 2. There the photon does not stem directly from the annihilation of the heavy quark-antiquark pair but from the fragmentation of a gluon or a light (anti)quark in the final state. Nevertheless we can keep the form of Eq. (2) to describe these contributions, since this subprocess is independent from the initial state effects parametrized in the NRQCD matrix elements. The Wilson coefficient is then obtained by the folding

$$\mathcal{C}_\gamma^{\rm frag}[n](\hat{z}) = \sum_{a=g,q,\bar{q}}\int_{\hat{z}}^1\frac{d\hat{x}}{\hat{x}}\,\mathcal{C}_a^{\rm dir}[n](\hat{x},\mu^2)D_{a\to\gamma}(\hat{z}/\hat{x},\mu^2) \tag{6}$$

of the fragmentation function $D_{a\to\gamma}$ and the coefficient $\mathcal{C}_a^{\rm dir}[n]$ which is the perturbative part of the NRQCD decay rate of a $Q\overline{Q}$ pair with quantum numbers n into a particle $a\in\{g,q,\overline{q}\}$ and other light degrees of freedom. The integration variable $\hat{x}$ indicates the energy of the particle a normalized on the heavy quark mass: $\hat{x}=E_a/m_Q$.

Since the fragmentation takes place at a scale far below the heavy quark mass m_Q it can be factorized from the hard subprocess. This is denoted by the factorization scale μ in Eq. (6). As usual one may derive a renormalization group equation from the μ independence of $\mathcal{C}_\gamma^{\rm frag}[n]$ to shift potentially large logarithms between $\mathcal{C}_a^{\rm dir}[n]$ and $D_{a\to\gamma}$.

Though the fragmentation functions are non-perturbative objects a naive estimate for their order of magnitude is obtained from counting coupling constants and collinear singularities coming up in a perturbative calculation. For that we look at the subprocesses highlighted by gray boxes in Fig. 2. The coupling of the photon to a light (anti)quark is proportional to $\alpha_{em}(m_Q)$. For $D_{q\to\gamma}$ the leading term comes from the kinematic region where the photon and the (anti)quark are collinear. Thus one gets a factor $\ln(Q^2/Q_0^2)$ where $Q^2\sim m_Q^2$ from the phase space integration with a collinear cutoff parameter Q_0 of order $\Lambda_{\rm QCD}$. Accordingly one gets $\alpha_{em}(m_Q)\alpha_s(m_Q)\ln^2(Q^2/Q_0^2)$ for the gluon fragmentation function. Here the logarithm appears quadratically because quark, antiquark, and photon can become collinear simultaneously in this case.

The logarithms $\ln(Q^2/Q_0^2)$ could become so large that they could compensate the perturbative α_s suppression and thus confuse the perturbation series dramatically. This is seen in a easy way from the running of the strong coupling constant. At leading order the renormalization group equation yields

$$\alpha_s(\mu^2) = \frac{\alpha_s(\mu_0^2)}{1+\alpha_s(\mu_0^2)\dfrac{\beta_0}{4\pi}\ln\left(\dfrac{\mu^2}{\mu_0^2}\right)} \tag{7}$$

with $\beta_0=(33-2n_f)/3$ if n_f fermions are active. As long as μ is far above a typical hadronic scale $\mu_0\sim\Lambda_{\rm QCD}$ one can neglect the constant in the denominator. Hence

$$\alpha_s(\mu^2)\ln(\mu^2/\mu_0^2)\sim\mathcal{O}(1). \tag{8}$$

Based on this relation we receive fragmentation contributions with magnitudes comparable to the direct ones. This become clear if we rewrite the fragmentation functions in the *leading logarithmic approximation*. Then they have the form [24]

$$D_{a\to\gamma}(\xi,Q^2) = \frac{2}{\beta_0}\frac{\alpha_{\rm em}(Q^2)}{\alpha_s(Q^2)}f_a(\xi) \tag{9}$$

where f_a is a phenomenological function of the fraction $\xi=E_\gamma/E_a$ of the photon and the parton energy. In case of comparable functions f_a for the different partons a the α_s in the denominator cancels the additional α_s in the hard subprocess of the fragmentation contributions.

Instead of using fitted functions for f_a we will take the perturbative result for the fragmentation functions $D_{a\to\gamma}$. They are known in next-to-leading order [25] but we will restrict ourselves on the leading order for consistency with the investigation of the annihilation subprocess. The scale dependence of $D_{g\to\gamma}$ and $D_{q\to\gamma}$ is given by the leading order DGLAP equations [26,27]

$$\mu^2\frac{\partial}{\partial\mu^2}D_{q\to\gamma}(\xi,\mu^2)=\frac{e_q^2\alpha_{\rm em}(\mu^2)}{2\pi}P_{q\to\gamma}(\xi), \tag{10a}$$

$$\mu^2\frac{\partial}{\partial\mu^2}D_{g\to\gamma}(\xi,\mu^2)=\frac{\alpha_s(\mu^2)}{2\pi}\int_\xi^1\frac{d\eta}{\eta}P_{g\to q}(\eta)\times D_{q\to\gamma}(\xi/\eta,\mu^2) \tag{10b}$$

where e_q is the charge of the light quark measured in units of the elementary charge. The Altarelli-Parisi splitting functions are [27]

$$P_{q\to\gamma}(\xi)=\frac{1+(1-\xi)^2}{\xi},\quad P_{g\to q}(\xi)=\frac{1}{2}[\xi^2+(1-\xi)^2]. \tag{11}$$

Integrating Eq. (10a) one obtains the quark fragmentation function

$$D_{q\to\gamma}(\xi,\mu^2)=\frac{e_q^2\alpha_{\rm em}(\mu^2)}{2\pi}P_{q\to\gamma}(\xi)\ln\left(\frac{\mu^2}{\mu_0^2(1-\xi)^2}\right)+D_{q\to\gamma}(\xi,\mu_0^2). \tag{12}$$

The ξ dependence of the starting value $D_{q\to\gamma}(\xi,\mu_0^2)$ for the evolution in the factorization scale μ is mainly determined by a logarithm $\ln(1/(1-\xi)^2)$ originating from the phase space integration [28]. It is already separated in Eq. (12). The remaining rest term cannot be calculated perturbatively. Therefore it has to be modeled, e.g., with a vector dominance model, or fitted to data. The latter was done by the ALEPH Collaboration in a measurement of the $\gamma+(1\text{ jet})$ rates for $\xi>0.7$ [29]. They get the best fit for a constant rest term $C=-1-\ln\{M_Z^2/(2\mu_0^2)\}$ in

$$D_{q\to\gamma}(\xi,\mu^2)=\frac{e_q^2\alpha_{\rm em}(\mu^2)}{2\pi}\left[P_{q\to\gamma}(\xi)\ln\left(\frac{\mu^2}{\mu_0(1-\xi)^2}\right)+C\right]. \tag{13}$$

The non-perturbative scale μ_0 extracted from data is then

$$\mu_0=0.14^{+0.43}_{-0.12}\text{ GeV}\Rightarrow C=-13.26^{+2.81}_{-3.89}. \tag{14}$$

The non-perturbative piece of the gluon fragmentation function $D_{g\to\gamma}$ cannot be determined experimentally. For the sake of simplicity we will set $D_{g\to\gamma}(\xi,\mu_0)=0$. The leading quadratic logarithmic term reads

$$D_{g\to\gamma}(\xi,\mu^2)=\frac{\alpha_s(\mu^2)}{2\pi}\int_\xi^1\frac{d\eta}{\eta}P_{g\to q}(\eta)\times D_{q\to\gamma}(\xi/\eta,\mu^2)\frac{1}{2}\ln\left(\frac{\mu^2}{\mu_0^2}\right). \tag{15}$$

Since the experimental investigation of the photon spectrum in radiative quarkonia decays is limited to $z>0.4$ due to large uncertainties for soft photons caused by π^0 decays we need the fragmentation functions for $\xi>0.4$ only. In this region the contribution of the gluon fragmentation function is negligible. However, the quark fragmentation into a photon is significant for $\xi\sim0.4$. Furthermore possibly large contributions in the end point region we are especially interested in are caused by the logarithmic divergence $\ln(1/(1-\xi)^2)$.

At this stage one comment is in order. Since our approximation for the fragmentation functions and in particular relation (8) holds the better the larger the scale μ is, i.e., the larger the heavy quark mass m_Q is, the leading log approximation is inaccurate or even not reliable for $m_Q=m_c$. Therefore we will concentrate our numerical investigation on the Υ decay as long as we do not restrict ourselves on large values for z.

Finally we need the perturbative results for the coefficient $\mathcal{C}_a^{\rm dir}[n]$ in Eq. (6). Again we distinguish between color singlet and color octet contributions. The calculation of the color singlet mode [Fig. 2(a) without the fragmentation subprocess] is, except for color factors, the same as the decay rate of ortho-positronium [30]. Similarly the coefficient $\mathcal{C}_a^{\rm dir}[^3S_1^{(1)}]$ can be extracted from the photon energy spectrum (4). The relative factor

$$B_F=\frac{\sum_{abc}\left(\frac{T_F}{2}d^{abc}\right)\left(\frac{T_F}{2}d^{abc}\right)}{\sum_{ab}\left(\frac{1}{2}\delta^{ab}\right)\left(\frac{1}{2}\delta^{ab}\right)}=\frac{N_c^2-4}{4N_c}\overset{(N_c=3)}{=}\frac{5}{12} \tag{16}$$

gives the ratio of the corresponding color traces. Inclusive of the coupling constants the triple gluon energy spectrum in the decay $Q\overline{Q}[^3S_1^{(1)}]\to ggg$ results in

$$\mathcal{C}_g^{\rm dir}[^3S_1^{(1)}](\hat{x})=B_F\frac{\alpha_s(m_Q)}{e_Q^2\alpha_{\rm em}(m_Q)}\mathcal{C}_\gamma^{\rm dir}[^3S_1^{(1)}](\hat{x}). \tag{17}$$

This formula contains a combinatorial factor $1/3=1/3!:1/2!$ which compensates the aforementioned factor of three coming from the fact that all three final state gluons can fragment into a photon.

The color octet coefficients $\mathcal{C}_a^{\rm dir}[^{2S+1}L_J^{(8)}]$ are determined by the hard subprocesses in diagrams like Fig. 2(b) and Fig. 2(c). In both cases the kinematics are trivial. Thus we get for $\mathcal{C}_g^{\rm dir}[n]$ with $n\in\{^1S_0^{(8)},{}^3P_0^{(8)},{}^3P_2^{(8)}\}$ from diagram 2(b):

$$\mathcal{C}_g^{\rm dir}[n](\hat{x})=2\frac{1}{2(2m_Q)}\frac{1}{8\pi}H[Q\overline{Q}[n]\to gg](2m_Q)\,\delta(1-\hat{x}). \tag{18}$$

Up to a factor of two which again is caused by the possibility for both gluons to fragment into a photon $\mathcal{C}_g^{\rm dir}[n](\hat{x})$ matches the corresponding differential decay modes $d\hat{\Gamma}_n/d\hat{x}$ without the NRQCD matrix element. The spin and color averaged square of the amplitudes are [9]

$$H[Q\bar{Q}[^1S_0^{(8)}]\to gg](2m_Q)=B_F\frac{128\pi^2\alpha_s^2(m_Q)}{2m_Q}, \tag{19a}$$

$$H[Q\bar{Q}[^3P_0^{(8)}]\to gg](2m_Q)=B_F\frac{384\pi^2\alpha_s^2(m_Q)}{2m_Q}, \tag{19b}$$

$$H[Q\bar{Q}[^3P_2^{(8)}]\to gg](2m_Q)=B_F\frac{512\pi^2\alpha_s^2(m_Q)}{5(2m_Q)}. \tag{19c}$$

Final states with $J=1$ are forbidden by the Landau-Yang theorem [31], i.e., $n={}^3P_1^{(8)}$ and $n={}^3S_1^{(8)}$ do not contribute to $Q\bar{Q}[n]\to gg$. Instead the latter configuration can decay into a light quark-antiquark pair [cf. Fig. 2(c)]. The corresponding coefficient is

$$\mathcal{C}_a^{\rm dir}[^3S_1^{(8)}](\hat{x})=\frac{1}{2(2m_Q)}\frac{1}{8\pi}H[Q\bar{Q}[^3S_1^{(8)}]\to q\bar{q}](2m_Q)\times\delta(1-\hat{x}) \tag{20}$$

where $a\in\{q,\bar{q}\}$ and

$$H[Q\bar{Q}[^3S_1^{(8)}]\to q\bar{q}](2m_Q)=\frac{64\pi^2\alpha_s^2(m_Q)}{3(2m_Q)}. \tag{21}$$

Hence we have collected all the results for the partonic decay of a $Q\bar{Q}$ pair that are needed for the photon energy distribution in radiative decays of heavy quarkonia. Henceforth we will construct a model for shape functions in quarkonia decays and embed the partonic results into it.

III. THE SHAPE FUNCTION MODEL

In the following both direct and fragmentation contributions are improved by the application of the shape functions. We model these functions with the following physical picture in mind. According to the factorization assumption of NRQCD quarkonium decays are divided into two subprocesses as illustrated in Fig. 3. In the first stage the quarkonium H radiates off a cluster of gluons with a momentum $k=\Sigma_i k_i\sim\mathcal{O}(m_Q v^2)$. The final state of this non-perturbative subprocess is a $Q\bar{Q}$ pair in the quantum state n that annihilates perturbatively in the second stage. Its momentum is given by $p_{Q\bar{Q}}=P-l$ with $P^2=(2m_Q)^2$, i.e., the non-perturbative momentum $l\sim\mathcal{O}(\Lambda_{\rm QCD})$ measures the off-shellness of the quark-antiquark pair.

It is important to be careful with neglecting non-perturbative momenta in the hard subprocess because the light cone component l_+ of the $Q\bar{Q}$ off-shellness is responsible for the shift of the partonic end point m_Q to the physically correct hadronic value $E_\gamma^{\rm max}=M_H/2$ [20]. Therefore we will keep the kinematics exact here.

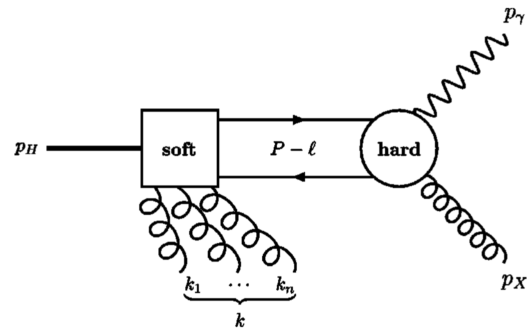

FIG. 3. Schematic representation of direct color octet contributions to the radiative quarkonium decay.

Nevertheless we have to model the radiation of the gluons from the initial state. This is done by our shape function [22]

$$f_n^H(l)=\int\frac{dk^2}{2\pi}\frac{d^3\boldsymbol{k}}{(2\pi)^3 2k^0}(2\pi)^4\times\delta^4(p_H+k-P+l)\Phi_n(k;p_H,P) \tag{22}$$

where Φ_n is a radiator function parametrizing the emission of a soft gluon cluster with total momentum k. In our ansatz

$$\Phi_n(k;p_H,P)=a_n\cdot|\boldsymbol{k}|^{b_n}\exp\{-k_0^2/\Lambda_n^2\}\cdot k^2\exp\{-k^2/\Lambda_n^2\} \tag{23}$$

the cutoff parameter $\Lambda_n\sim\mathcal{O}(m_Q v^2)$ reflects the expectation that the main contribution comes from the ultrasoft region where the energy k_0 and the invariant mass k^2 of the gluon cluster are of order $m_Q v^2$ and $(m_Q v^2)^2$ respectively. The choice

$$b[^1S_0^{(8)}]=2,\quad b[^3P_0^{(8)}]=b[^3S_1^{(8)}]=0, \tag{24a}$$

$$\Lambda[^1S_0^{(8)}]=\Lambda[^3P_0^{(8)}]\equiv\Lambda,\quad \Lambda[^3S_1^{(8)}]=c\Lambda \tag{24b}$$

for the constants in Eq. (23) is motivated by the fact that the gluon coupling for a M1 magnetic dipole transition from the quarkonium H to $Q\bar{Q}[^1S_0^{(8)}]$ is proportional to the gluon momentum while an E1 or a double E1 electric dipole transition to $Q\bar{Q}[^3P_{0,2}^{(8)}]$ or $Q\bar{Q}[^3S_1^{(8)}]$ respectively does not have any k dependence. Furthermore the necessity of at least two transitions for $n={}^3S_1^{(8)}$ suggests the introduction of a factor $c=1.5$ to enlarge the average radiated energy and invariant mass in this case. Finally we fix a_n by the normalization condition

$$\int\frac{d^4l}{(2\pi)^4}f_n^H(l)=\frac{1}{(2\pi)^3}\int_0^\infty dk^2\int_{\sqrt{k^2}}^\infty dk_0\sqrt{k_0^2-k^2}\times\Phi_n(k;p_H,P)=\langle H|\mathcal{O}_n|H\rangle. \tag{25}$$

A. Direct contributions

After we have determined our model ansatz for the shape functions we proceed with the implementation of the hard subprocess. First we deal with the direct contributions. As mentioned above in leading order only the color octet modes are interesting in the shape function formalism. Thus we start with the expression

$$d\Gamma_8^{\rm dir}=\sum_n \int \frac{d^4l}{(2\pi)^4}\frac{1}{2M_H}\int \widetilde{dp}_\gamma \widetilde{dp}_X(2\pi)^4 \times\delta^4(P-l-p_\gamma-p_X) \times H[Q\bar{Q}[n]\to\gamma g](P,l,p_\gamma,p_X) \times\int\frac{dk^2}{2\pi}\frac{d^3\boldsymbol{k}}{(2\pi)^3 2k_0}(2\pi)^4 \times\delta^4(p_H-k-P+l)\Phi_n(k;p_H,P) \tag{26}$$

where one can easily recognize the shape function in the second line of the equation. In Eq. (26) M_H denotes the quarkonium mass, $\widetilde{dp}_\gamma$ and $\widetilde{dp}_X$ the invariant phase space measures of the photon and the hard gluon respectively and finally the spin and color averaged square H_n of the hard subprocess amplitude is given by Eq. (5).

Manipulating Eq. (26) we start with integration out the four momenta k and p_X with $p_X^2=0$ which determines the light cone components $l_\perp^2$ and l_+ by the delta functions to

$$l_\perp^2=(M_H-2m_Q)(M_H-2m_Q+2l_0)+l_+(2l_0-l_+)-k^2, \tag{27a}$$

$$l_+=\frac{1}{2E_\gamma}[4m_Q(M_H-E_\gamma)-M_H^2-2(M_H-2E_\gamma)l_0+k^2]. \tag{27b}$$

To make use of these relations we also decompose d^4l into its light cone components

$$\int d^4l=\int_0^{2\pi}d\phi\int dl_0 dl_+\frac{dl_\perp^2}{2}\Theta(l_\perp^2) \tag{28}$$

and rewrite the l_0 integration into a k_0 integration by $l_0=k_0-(M_H-2m_Q)$. Then the integration over the azimuthal angular can be performed trivially because the partonic process is ϕ independent. Analogously the angular dependence in $\widetilde{dp}_\gamma$ is integrated out trivially and one gets $\widetilde{dp}_\gamma=E_\gamma dE_\gamma\Theta(E_\gamma)/(4\pi^2)$. Finally we evaluate Eqs. (27a), (27b). In simultaneous consideration of the theta function in Eq. (28) there arise integration bounds for k_0 where the physical ones are

$$\frac{(M_H-2E_\gamma)^2+k^2}{2(M_H-2E_\gamma)}\leqslant k_0\leqslant\frac{M_H^2+k^2}{2M_H}. \tag{29}$$

From this we can read off an upper bound for the k^2 integration

$$k^2\leqslant M_H(M_H-2E_\gamma) \tag{30}$$

while the lower one is determined by $k^2\geqslant 0$. Introducing the abbreviations

$$\alpha=(p_H-p_\gamma)_+=M_H-2E_\gamma,\quad \beta=(p_H-p_\gamma)_-=M_H \tag{31}$$

we finally end up with

$$\frac{d\Gamma_8^{\rm dir}}{dE_\gamma}=\sum_n\int_0^{\alpha\beta}\frac{dk^2}{2\pi}\int_{(\alpha^2+k^2)/(2\alpha)}^{(\beta^2+k^2)/(2\beta)}dk_0\frac{1}{2M_H}\frac{1}{8\pi} \times H[Q\bar{Q}[n]\to\gamma g](M_{Q\bar{Q}}(k)) \times\frac{1}{4\pi^2}\Phi_n(k;p_H). \tag{32}$$

This is our master equation for the direct color octet contributions to the photon energy spectrum that take into account shape functions effects within our model framework. Note that according to our model the partonic rate depends on

$$M_{Q\bar{Q}}(k)=\sqrt{M_H^2-2M_Hk_0+k^2} \tag{33}$$

rather than on $2m_Q$, i.e., the quark mass in the partonic subprocess is effectively larger than m_Q. The color singlet contributions are obtained by multiplying Eq. (3) with the color singlet NRQCD matrix element $\langle H|\mathcal{O}_1(^3S_1)|H\rangle$. Here the heavy quark mass is set equal to $M_H/2$.

B. Fragmentation contribution

The treatment of the fragmentation contributions is done in the following way: First we apply our shape function model on the color octet contribution $d\hat{\Gamma}/d\hat{E}_a(Q\bar{Q}[n]\to a\overset{(-)}{a})$ to extend the reliability of the partonic NRQCD calculation up to higher values of the parton energy $\hat{E}_a$ in the $Q\bar{Q}$ rest frame. Afterwards we fold the received spectrum $d\Gamma/dE_a$ with the corresponding fragmentation function $D_{a\to\gamma}$:

$$\frac{d\Gamma_8^{\rm frag}}{dE_\gamma}=\sum_{a=g,q,\bar{q}}\int_{E_\gamma}^{M_H/2}\frac{dE_a}{E_a}\frac{d\Gamma_8^{\rm dir}}{dE_a}D_{a\to\gamma}(E_\gamma/E_a). \tag{34}$$

Note that the upper bound for the parton energy E_a in the quarkonium rest frame is given by the hadronic value $M_H/2$ rather than by the heavy quark mass $\hat{E}_a^{\rm max}=m_Q$ which defines the end point in the partonic calculation.

In Eq. (34) the folding of the gluon and the (anti)quark energy spectrum $d\Gamma_8^{\rm dir}/dE_a$ is calculated completely analogous to Eq. (32):

$$\frac{d\Gamma_8^{\rm dir}}{dE_a}=\sum_n\int_0^{\bar{\alpha}\bar{\beta}}\frac{dk^2}{2\pi}\int_{(\bar{\alpha}^2+k^2)/(2\bar{\alpha})}^{(\bar{\beta}^2+k^2)/(2\bar{\beta})}dk_0\frac{1}{2M_H}\frac{1}{8\pi} \times H[Q\bar{Q}[n]\to a\overset{(-)}{a}](M_{Q\bar{Q}}(k))\frac{1}{4\pi^2}\Phi_n(k;p_H)$$

where the sum again runs only over the color octet modes. $\bar{\alpha}$ and $\bar{\beta}$ are obtained from Eq. (31) by the substitution $E_\gamma\to E_a$. As described in Sec. II B the partonic subprocess $Q\bar{Q}[n]\to gg$ contributes only for $n={}^1S_0^{(8)}$, $n={}^3P_0^{(8)}$, and $n={}^3P_2^{(8)}$ while $n={}^3S_1^{(8)}$ needs a light quark-antiquark pair in

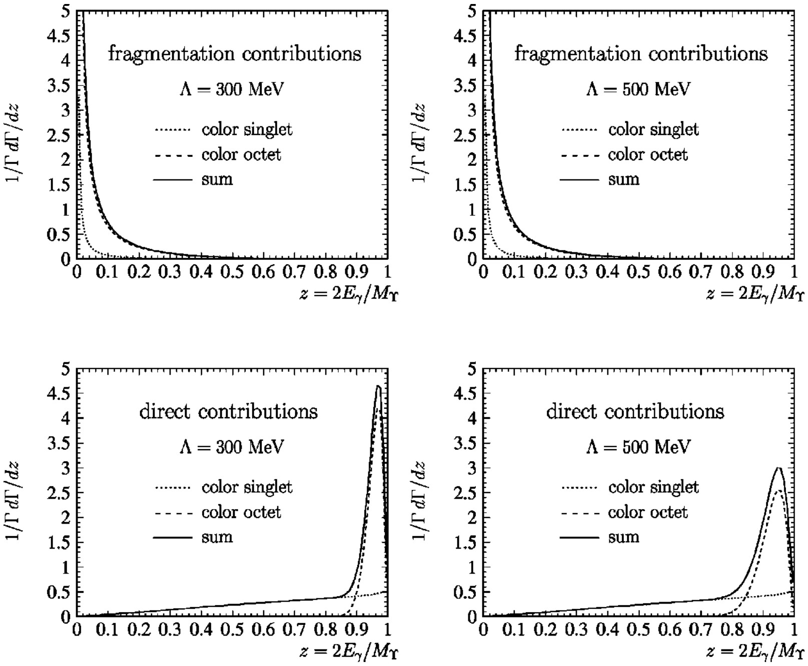

FIG. 4. Leading order fragmentation (upper panel) and direct (lower panel) contribution to the photon energy spectrum in the radiative decay $\Upsilon(1S)\rightarrow\gamma+$ *light hadrons* for two different values of the shape function model parameter: $\Lambda=300$ MeV (left) and $\Lambda=500$ MeV (right).

the final state. The sum in Eq. (34) runs not only over the gluon but also over different (anti)quark flavors $q=\{u,d,s(,c)\}$ where we additionally assume $D_{q\rightarrow\gamma}(\xi)=D_{\bar{q}\rightarrow\gamma}(\xi)$.

IV. RESULTS

As mentioned above we restrict our numerical analysis on the bottomonium system since the fragmentation contributions in the charmonium sector are not very trustworthy within our approach. For the photon spectrum in the radiative decay of a $\Upsilon(1S)$ we choose the following set of parameters: $M_\Upsilon=9.46$ GeV, $\alpha_s(\mu^2)=0.190$, $\alpha_{\rm em}(\mu^2)=1/132$ where the factorization scale μ is fixed at the b quark mass $m_b=4.8$ GeV. Unfortunately the values of the NRQCD matrix elements are unknown. While the production matrix elements of the bottomonium sector have been fitted in a recent analysis by Braaten, Fleming, and Leibovich [6] we have to make do with the NRQCD scaling rules

$$\langle\Upsilon|\mathcal{O}_8(^1S_0)|\Upsilon\rangle\sim\frac{\langle\Upsilon|\mathcal{O}_8(^3P_0)|\Upsilon\rangle}{m_b^2}\sim\langle\Upsilon|\mathcal{O}_8(^3S_1)|\Upsilon\rangle$$
$$\sim v^4\langle\Upsilon|\mathcal{O}_1(^3S_1)|\Upsilon\rangle \qquad (35)$$

to estimate at least the order of magnitude of the decay matrix elements needed for the normalization, i.e., for the relative weights, of the different contributing channels. For our numerical evaluation we take for each color octet matrix element 2.20×10^{-2} GeV^2 and $\langle\Upsilon|\mathcal{O}_1(^3S_1)|\Upsilon\rangle=3.43$ GeV^2, i.e., we set $v^2=0.08$ for bottomonia. Finally we normalize the total rate to one. In case of a comparison with data this could be changed easily.

The result for two different values of our shape function model parameter $\Lambda\sim m_b v^2$ is shown in Fig. 4. One recognizes that fragmentation contributions (upper panel) are non-negligible for small photon energies only. Therefore they are not influenced by the shape function and show no Λ dependence. In the region $0.1\lesssim z\lesssim0.4$ the fragmentation is mainly dominated by the color octet channels. The main contribution stems from the $^3S_1^{(8)}$ mode that is connected with the fragmentation function $D_{q\rightarrow\gamma}(\xi)$. Though this function diverges for $\xi\rightarrow1$ the numerical contribution of $d\Gamma/dz[^3S_1^{(8)}]$ to the spectrum for large values of z is negligible. This matches to our expectation that fragmentation processes prefer to transfer small energy fractions from the gluon (quark) to the photon.

The upper end point region $z\gtrsim0.8$ is dominated by direct color octet contributions (at least in leading order α_s). While the partonic result is proportional to $\delta(1-\hat{z})$ the soft gluon radiation in the initial state smears out the delta peak and also shifts its maximum to $z_{Q\bar{Q}}=M_{Q\bar{Q}}^{\rm eff}/M_\Upsilon<1$. The higher the model parameter Λ is the smaller is $z_{Q\bar{Q}}$ and therewith the effective heavy quark mass and the broader is the width of the peak. Comparing the integrated rates of the direct color singlet mode $^3S_1^{(1)}$ and the direct color octet ones we realize that their contributions are almost equal. This can be explained by the fact that the suppression factor $v^4=6.4\times10^{-3}$ of the color octet modes is canceled by an additional factor $\alpha_s(m_b)/(4\pi)=1.5\times10^{-2}$ in the color singlet mode [cf. Eq. (1)]. Furthermore one has to consider that there are contributions from many color octet modes ($^{2S+1}L_J^{(C)}={}^1S_0^{(8)}$, $^3S_1^{(8)}$, $^3P_0^{(8)}$, and $^3P_2^{(8)}$) but only from one color singlet mode ($^3S_1^{(1)}$).

Let us finally concentrate on the region of middle high photon energies. From the theoretical point of view the part between $0.4\lesssim z\lesssim0.75$ is the cleanest one of the spectrum. Here the color singlet contribution which is assumed to be dominating over the whole photon energy range in the color singlet model can be extracted within shape function improved NRQCD without any pollution from other channels. This is still true after including the next-to-leading order con-

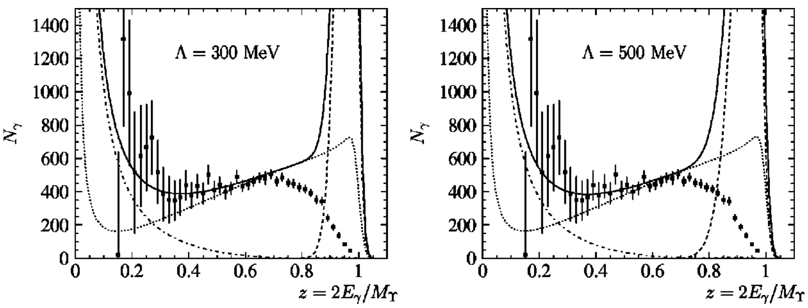

FIG. 5. Comparison of the theoretical spectrum (solid line) for $\Lambda=300$ MeV (left) and $\Lambda=500$ MeV (right) with data of CLEO. The dashed line shows the direct, the dash-dotted line the fragmentation contribution from the color octet modes. The spectrum predicted by the color singlet model (direct+fragmentation, without any hadronization model) is indicated by the dotted curvature.

tributions: While the color singlet corrections steepen the slope [8] the color octet terms are negligible for $0.4 \lesssim z \lesssim 0.75$ [9].

Since the extraction of $\alpha_s(m_b)$ needs an extrapolation of the measured spectrum towards $z=0$, a complete theoretical understanding of the part of the spectrum the fit is based on is indispensable to reach an accurate value for the strong coupling constant. In our opinion this is not possible for high photon energies. To illustrate the problems in the upper end point region we smear out our theoretical result with the energy resolution of the CLEO detector

$$\frac{\sigma_E}{E}(\%) = \frac{0.35}{E^{0.75}} + 1.9 - 0.1E \tag{36}$$

and fit it to their most recent data [17] for $0.4 \leqslant z \leqslant 0.7$. The result is shown in Fig. 5. While the spectrum is described satisfactorily within the fragmentation uncertainties for small and middle high values of z the discrepancy between theory and experiment is overwhelming for $z \gtrsim 0.75$. As shown by the CLEO Collaboration [17] the CSM result combined with the color singlet fragmentation contributions according to [12] can be brought into agreement with data using a hadronization model by Field [13] even though the consequential value of $\alpha_s(m_b)$ is slightly to small compared to the one measured on the Z_0 resonance.

Although the (direct) color octet contributions in Fig. 5 have not been suppressed by a hadronization model yet, they seem to be in strong contradiction to the experimental observation.[2] The simplest explanation for this deviation would be an extreme smallness of the color octet NRQCD decay matrix elements even smaller than the v^4 suppression still acknowledged by the power counting rules. Some hints for such small color octet decay matrix elements also come from the estimation of the α_s corrections [9]. Furthermore a recent analysis of the corresponding production matrix elements [6] yielded smaller values than predicted by velocity scaling rules, too. Although the crossing symmetry between these production matrix elements and the ones of the decay holds only in leading order perturbation theory this could also be interpreted as indication for somehow suppressed (or even negative?) values of the NRQCD matrix elements.

Nevertheless the understanding of the upper end point region in the radiative decay of the $\Upsilon(1S)$ is not good enough to conclude convincingly that the color octet matrix elements are extremely small. Without having investigated the Sudakov corrections on the color octet contributions and without a better understanding of the hadronization process it seems impossible to give a stringent theoretical prediction for $z \gtrsim 0.75$. Furthermore the experimental investigation of this spectrum suffers from large systematic problems in this kinematical regime, too.

In summary an extraction of a precise value for the strong coupling constant from the radiative Υ decay seems to be impossible as long the upper end point region is included in the fit. Unless both theoretical and experimental progress concerning the physics in the upper end point region is achieved $\alpha_s(m_b)$ should be fitted from the data between $0.4 \leqslant z \leqslant 0.7$ only.

[2]The inclusion of color octet fragmentation contributions seems to be favored by the data. However, considering that the analysis is only leading order at a (for fragmentation processes) relatively low factorization scale m_b we should not deduce anything conclusive from this observation.

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