

**Threshold resummation for top-pair hadroproduction to next-to-next-to-leading log**

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We derive the threshold-resummed total cross section for heavy quark production in hadronic collisions accurate to next-to-next-to-leading logarithm, employing recent advances on soft anomalous dimension matrices for massive pair production in the relevant kinematic limit. We also derive the relation between heavy quark threshold resummations for fixed pair kinematics and the inclusive cross section. As a check of our results, we have verified that they reproduce all poles of the color-averaged  $q\bar{q} \rightarrow t\bar{t}$  amplitudes at two loops, noting that the latter are insensitive to the color-antisymmetric terms of the soft anomalous dimension.

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**I. INTRODUCTION**

Heavy quark production has a long and continuing history of phenomenological interest. Top-pair production is among the most important standard model processes in the context of searches for new physics. It is also among the most challenging in computation. Indeed over 20 years passed between the landmark first next-to-leading order (NLO) calculations of heavy quark production [1] and the derivation [2] of analytic expressions for the inclusive cross section.

As in many hard hadronic processes, higher order perturbative calculations contain logarithmic enhancements, associated with the approach to partonic threshold, that is, configurations where the initial-state partons have just enough energy to produce the observed final state. Threshold resummation [3] organizes such logarithms, in a manner we review below. The current state of the art for heavy quark production is next-to-leading log (NLL) resummation matched onto exact NLO results. In this paper, we study the extension of this formalism to next-to-next-to-leading log (NNLL) resummation and beyond in the production of heavy quark-antiquark pairs at hadron colliders. In this context, we derive the NNLL inclusive cross section, generalizing the NLL results of [4], starting from the resummation formalism at fixed parton kinematics described in [5]. The numerical impact of our present work will be detailed elsewhere.

While our considerations are reasonably general and can be applied to a larger class of processes, we choose to present our results and their derivation for heavy quark production because recent advances [6–8] make it possible for us to determine the essentially two-loop inputs necessary for explicit NNLL resummation in this case. These inputs are the so-called soft anomalous dimension matrices for heavy quark pair production [5] which we exhibit

below in the relevant kinematic configuration for the total cross section. Drawing from the formalism of Ref. [5], we will perform a single one-loop calculation, corresponding to a boundary condition in the evolution of soft gluon emission, which is necessary for the complete NNLL result. As noted at the level of NLL, for the inclusive cross section, resummation can be carried out separately for pair production in the  $s$ -channel color singlet and octet states, without color mixing. We will find the same structure at NNLL, and present our final results in a form that follows the NLL formalism of Ref. [4].

We begin with a review of threshold resummation for semi-inclusive cross sections at fixed kinematics for the partonic scattering process, in the formalism developed in Ref. [5], and applicable in principle to any logarithmic approximation. This formalism relies on the factorization of color-diagonal “jet” functions associated with the external energetic and/or massive partons that take part in the scattering at short distances and a “soft function” describing the exchange of low-energy quanta between these particles. We identify, in particular, a scheme to resolve the ambiguity between the jet and soft functions, based on the singularities of form factors in dimensional regularization. We go on in Section III to show how an expression for the threshold-resummed inclusive cross section may be derived from the resummation at fixed kinematics. With this result in hand, we determine two-loop soft anomalous dimension matrices in Sec. IV, which we need to determine the soft functions at NNLL. We describe a very nontrivial check of these results, which fully reproduce the two-loop pole structure of heavy quark pair production in light quark annihilation. In Sec. V, we assemble the remaining ingredients in the NNLL resummation, including the one-loop boundary condition mentioned above. We conclude with a summary and a few comments on prospects for future work.

## II. THRESHOLD RESUMMATION AT FIXED KINEMATICS

In this section, we review the threshold resummation formalism of Ref. [5], which is adapted to semi-inclusive reactions characterized by fixed partonic scattering kinematics, as in, for example,

$$f_1(p_1) + f_2(p_2) \rightarrow f_a(p_a) + f_b(p_b), \quad (1)$$

where  $f_i(p_i)$  denotes a parton of flavor  $f_i$  and momentum  $p_i$ . We have shown a  $2 \rightarrow 2$  process, but final states with more than two particles are also possible, so long as all invariants  $p_i \cdot p_j$  are large. The formalism we sketch in this section applies to processes involving light quarks and gluons, and also to the production of heavy quarks. In the latter case, we can also study the inclusive cross section, for which threshold resummation has been developed from a related point of view [4]. In Sec. III we will derive resummed inclusive cross sections for heavy quark production from their semi-inclusive forms.

### A. Factorization near partonic threshold

Our starting point for the resummation of observables involving initial and/or final-state hadrons is the formalism of Ref. [5]. To be specific, we restrict our discussion to the  $2 \rightarrow 2$  processes of Eq. (1), although many of our considerations can be directly generalized. For the production of a pair of particles with mass  $m$ , the kinematics can be described by the invariant mass  $M$  and rapidity  $y$  of the partonic final state and the pair center-of-mass rapidity difference  $\hat{\eta}$ . Assuming that  $m \gg \Lambda_{\text{QCD}}$ , this cross section can be written in standard factorized form as

$$\begin{aligned} M^4 \frac{d\sigma_{h_1 h_2 \rightarrow Q\bar{Q}}}{dM^2 dy d\hat{\eta}} &= \sum_f \int_{\tau}^1 dz \int \frac{dx_a}{x_a} \frac{dx_b}{x_b} \phi_{f/h_1}(x_a, \mu^2) \\ &\times \phi_{\bar{f}/h_2}(x_b, \mu^2) \delta\left(z - \frac{\tau}{x_a x_b}\right) \\ &\times \delta\left(y - \frac{1}{2} \ln \frac{x_a}{x_b}\right) \omega_{f\bar{f} \rightarrow Q\bar{Q}}\left(z, \hat{\eta}, \frac{M^2}{\mu^2}, \right. \\ &\left. \frac{m^2}{\mu^2}, \alpha_s(\mu^2)\right), \end{aligned} \quad (2)$$

where we have normalized the cross section so that all quantities are dimensionless. The purpose of threshold resummation is to organize plus distributions in the variable

$$z = \frac{\tau}{x_a x_b} = \frac{M^2}{x_a x_b S}, \quad (3)$$

with  $x_a$  and  $x_b$  the usual fractional momenta. Partonic threshold is defined as the limit  $z \rightarrow 1$ , at which the incoming partons provide just enough energy to produce the

observed final state. The mismatch between real gluon emission and virtual corrections gives rise to singular distributions at  $z = 1$ . These distributions appear in the  $n$ th order expansion of the perturbative function  $\omega_{f\bar{f} \rightarrow Q\bar{Q}}$  up to the level of  $\alpha_s^n [\ln^{2n-1}(1-z)/(1-z)]_+$ .

In Ref. [5], it was observed that as  $z \rightarrow 1$ , partonic cross sections can be factorized into a set of universal factors associated with the incoming and outgoing partons of the underlying process, along with process-dependent factors that describe the coherent interactions of those partons, at short and long distances. The resummed dependence in  $1-z$  is conveniently generated by taking Mellin moments with respect to  $z$ , schematically,

$$\begin{aligned} \sigma(N) &= \int_0^1 dz z^{N-1} \sigma(z) \\ &= \int_0^1 dz e^{-(N-1)(1-z)} \sigma(z) + \mathcal{O}(1/N). \end{aligned} \quad (4)$$

For example, in the inclusive Drell-Yan process, the corresponding kinematical variable is  $z = Q^2/s$ , where  $s$  is the partonic c.m. energy [3]. For resummation of the total inclusive cross section of heavy quark pair production at hadron colliders the corresponding variable is  $z = 4m^2/s$  where  $m$  is the mass of the top quark. Another example relevant for this paper is the invariant mass  $M_{i\bar{i}}^2 = (p_i + p_{\bar{i}})^2$  distribution of a top quark-antiquark pair; the relevant partonic variable is  $z = M_{i\bar{i}}^2/s$ . In any case we assume that the partonic variable is defined such that threshold kinematics is attained in the limit  $z \rightarrow 1$ . In moment space this corresponds to the limit  $N \rightarrow \infty$ . The analysis of Ref. [5] exploits factorization near threshold, according to which the cross section can be written as a convolution in an appropriate momentum component of the soft radiation associated with a set of functions [9]. In threshold resummation for hadronic collisions, this component is the energy,  $E_i^*$ , of each final-state particle in the center-of-mass frame of the hard collision. That is, for any threshold resummation at hadronic collisions, we can identify

$$1 - z = \sum_{\text{particles } i} \frac{2E_i^*}{\sqrt{s}}, \quad (5)$$

where the partonic variable  $s \equiv x_a x_b S$  equals  $M^2$  at threshold, with  $M$  the invariant mass of the observed pair of heavy particles. The cross section then factorizes into simple products in the corresponding moment space. Dependence on the moment variable enters only through the transform, and is therefore always in the form  $N/M$ , up to corrections that decrease as powers of  $N$ .

As a result of this analysis, the partonic cross section takes a factorized form in moment space, which we can represent as

$$\omega_P\left(N, \hat{\eta}, \frac{M^2}{\mu^2}, \frac{m^2}{\mu^2}, \alpha_s(\mu^2)\right) = J_1(N, \alpha_s(\mu^2)) \dots J_k(N, M/\mu, m/\mu, \alpha_s(\mu^2)) \text{Tr}\left[\mathbf{H}^P\left(\frac{M^2}{\mu^2}, \frac{m^2}{\mu^2}, \hat{\eta}, \alpha_s(\mu^2)\right)\right] \\ \times \mathbf{S}^P\left(\frac{N^2\mu^2}{M^2}, \frac{M^2}{m^2}, \hat{\eta}, \alpha_s(\mu^2)\right) + \mathcal{O}(1/N), \quad (6)$$

where the label  $P$  refers to a particular partonic process, for example  $q\bar{q} \rightarrow t\bar{t}$ , with  $q$  a light flavor. The Mellin moment  $N$  is conjugate to the kinematical variable  $z$ . As shown, the various functions appearing in Eq. (6) depend on other kinematical variables and masses as well as the factorization and renormalization scales. These functions depend on the specific process. Below, we will give them more explicitly in the specific examples considered here. We will refer to the factors  $J_i$  appearing in Eq. (6) as the *jet functions* for the underlying process. They are color diagonal functions that describe the factorized dynamics of initial and/or final state hard partons, whether massive or massless, and as such are independent of the details of the hard subprocess. Jet functions for initial-state partons absorb the collinear subtractions necessary to define the hard scattering function  $\omega$  in Eq. (6), so that they are infrared safe. Jet functions for final-state partons are automatically infrared safe for the differential and inclusive cross sections that we discuss here. The formalism can be extended as well to a variety of jet observables and to single-hadron cross sections. The number  $k$  of such functions in Eq. (6) corresponds to the number of hard colored partons in the process being considered.

The functions  $\mathbf{H}$  and  $\mathbf{S}$  appearing in Eq. (6) are known as *hard* and *soft* functions, respectively. They are both matrices in the space of tensors that describe the exchange of color at short distances [5]. Examples for quark-antiquark scattering are color singlet or octet in the  $s$ - or  $t$ -channel. We will denote these tensors in boldface, and their product

is traced over the combinations of color tensors in the amplitude and its complex conjugate. In the limit  $N \rightarrow \infty$  the hard function  $\mathbf{H}$  is free of logarithmic dependence on  $N$ ; it is obtained from a dedicated, process-specific calculation.

## B. Moment-dependence and the soft anomalous dimension matrix

The soft function  $\mathbf{S}$  contains terms due to wide-angle soft emissions and thus contributes a single power of  $\ln(N)$  per loop. It is also process dependent, and in the general case is dependent on the four-velocities  $\{\beta_i\}$  of the partons that take part in the hard scattering. For processes involving four or more colored hard partons it is a matrix in the space of color tensors. Assuming fixed-angle scattering, the soft function depends on the scalar products of these velocities, in addition to a single overall scale, which we will take to be  $M$ , the invariant mass of the pair for the case of heavy quark production. For a massive quark of velocity  $\beta_q$ , we shall set  $\beta_q^2 = m_q^2/M^2$ , and for most of this discussion, treat this ratio as a number of order unity.

As noted above, all  $N$ -dependence is of the form  $N/M$ . As a result, in the dimensionless soft function,  $N$ -dependence appears only in the combination  $M/(N\mu)$ . In Ref. [5], it was shown that the  $N$ -dependence of the soft function  $\mathbf{S}(N, \dots)$  entering the cross section Eq. (6) can be made explicit in terms of a ‘‘soft anomalous dimension matrix,’’  $\Gamma_S$ . Making the natural choice,  $\mu = M$ , we have

$$\mathbf{S}\left(\frac{N^2\mu^2}{M^2}, \beta_i \cdot \beta_j, \alpha_s(\mu^2)\right)\Big|_{\mu=M} = \bar{\mathcal{P}} \exp\left[-\int_{M/\bar{N}}^M \frac{d\mu'}{\mu'} \Gamma_S^\dagger(\beta_i \cdot \beta_j, \alpha_s(\mu'^2))\right] \mathbf{S}(1, \beta_i \cdot \beta_j, \alpha_s(M^2/\bar{N}^2)) \\ \times \mathcal{P} \exp\left[-\int_{M/\bar{N}}^M \frac{d\mu'}{\mu'} \Gamma_S(\beta_i \cdot \beta_j, \alpha_s(\mu'^2))\right] \\ = \bar{\mathcal{P}} \exp\left[\int_0^1 dx \frac{x^{N-1} - 1}{1-x} \Gamma_S^\dagger(\beta_i \cdot \beta_j, \alpha_s((1-x)^2 M^2))\right] \mathbf{S}(1, \beta_i \cdot \beta_j, \alpha_s(M^2/N^2)) \\ \times \mathcal{P} \exp\left[\int_0^1 dx \frac{x^{N-1} - 1}{1-x} \Gamma_S(\beta_i \cdot \beta_j, \alpha_s((1-x)^2 M^2))\right], \quad (7)$$

where the second expression is accurate to next-to-next-to-leading logarithms (i.e. terms  $\sim \alpha_s^n \ln^{n-1} N$  in the cross section) for  $\bar{N} = Ne^{\gamma_E}$ , with  $\gamma_E$  the Euler constant. Throughout this paper  $\alpha_s = \alpha_s(\mu^2)$  is the standard  $\overline{\text{MS}}$  coupling evolving with  $N_L$  light flavors. Decoupling of the heavy flavor will simplify our results significantly. The relation between the bare  $\alpha_s^b$  and renormalized couplings

reads

$$\alpha_s^b S_\epsilon = \alpha_s(\mu^2) \left[ 1 - \frac{\beta_0}{4\epsilon} \frac{\alpha_s(\mu^2)}{\pi} + \mathcal{O}(\alpha_s^2) \right], \quad (8)$$

where  $S_\epsilon = (4\pi)^\epsilon \exp(-\epsilon\gamma_E)$  and  $\beta_0 = (11/3)C_A - (4/3)T_F N_L$ . The color factors in an  $\text{SU}(N)$ -gauge theory are  $C_A = N$ ,  $C_F = (N^2 - 1)/(2N)$  and  $T_F = 1/2$ .

The structure of Eq. (7) follows from the renormalization group equation satisfied by the soft function  $\mathbf{S}(N^2 \mu^2/M^2, \dots)$ , where  $\Gamma_S$  plays the role of a matrix of anomalous dimensions [5]. The function  $\mathbf{S}(1, \dots)$  plays the role of a boundary condition, which is chosen to be the soft function at unit  $N$ , that is, with unit weight. In general, this factor contributes a single  $\ln(N)$  starting from two loops, which is due, however, entirely to the presence of  $N$  in the scale of the running coupling in its one-loop expression. To determine this contribution one need only calculate the soft function in Eq. (6) through one loop.

At  $N = 1$ , the computation of the soft function is given by a total eikonal cross section, subtracted for eikonal jet functions to eliminate collinear enhancements [5]. In the formalism of Ref. [5], virtual corrections are pure counterterms, because the corresponding eikonal diagrams are scaleless and vanish in dimensional regularization. In the full soft function, however, the hard scale sets a maximum total energy for the soft function at  $N = 1$ , and the corresponding integrals are not scaleless. Their infrared poles are cancelled by the virtual diagrams, but finite corrections may remain.

In summary, the soft function  $\mathbf{S}$  at  $N = 1$  takes the form

$$\begin{aligned} & \mathbf{S}(1, \beta_i \cdot \beta_j, \alpha_s(M^2/N^2)) \\ &= \mathbf{S}^{(0)} + \frac{\alpha_s(M^2/N^2)}{\pi} \mathbf{S}^{(1)}(1, \beta_i \cdot \beta_j) + \dots, \end{aligned} \quad (9)$$

where  $\mathbf{S}^{(0)}$  is a constant diagonal matrix independent of the coupling and  $\mathbf{S}^{(1)}(1, \beta_i \cdot \beta_j)$  is free of dependence on  $N$ , but can depend on the eikonal velocities that define the soft function. Explicit expressions for  $\mathbf{S}^{(0)}$  relevant to heavy quark production can be found in [10]. We will give the one-loop correction below, after specifying a scheme that defines the soft function unambiguously. At this stage, we note that to compute the soft function fully at next-to-next-to-leading logarithm it is necessary to compute the two-loop anomalous dimension matrix and the one-loop soft function.

### C. The form factor scheme

The soft function is not unique, but is ambiguous at the level of single logarithmic contributions that can be absorbed into the jet functions. These ambiguities, must be proportional to the unit matrix in the color exchange space (since the jet functions are diagonal in color). To resolve this ambiguity one has to specify a prescription for the definition of the anomalous dimension matrix  $\Gamma_S$ , which we discuss next.

A fundamental observation of Ref. [5] is that the matrix  $\Gamma_S$  appearing in Eq. (7) can be extracted from the corresponding (virtual) amplitude for the process under consideration. To review how this can be done, we first observe that any on-shell, renormalized scattering amplitude at fixed angles can be factorized as follows [11]:

$$M_I(\epsilon, \dots) = j_1(\epsilon, \dots) \dots j_s(\epsilon, \dots) \cdot h_J(\dots) \cdot s_{IJ}(\epsilon, \dots). \quad (10)$$

Here  $I, J$  are indices that label color exchange tensors; in particular, they indicate that the amplitude  $M$  can be thought of as a vector in the space of color representations [12]. In order to emphasize the similarity between the objects appearing in Eqs. (6) and (10) we have used the same letters to denote jet, soft and hard functions. It should be stressed, however, that these are not the same objects. In particular, the moment  $N$  does not appear in an amplitude. To distinguish clearly between the objects appearing in the cross section and in the amplitude we use lower case letters, and explicitly show the dependence on the infrared regulator  $\epsilon$  where  $d = 4 - 2\epsilon$ .

For both massive and massless external partons the amplitude soft function  $s_{IJ}(\epsilon, \dots)$  appearing in Eq. (10) is fully determined by its (matrix) anomalous dimension  $\Gamma_{IJ}$ . It can be computed order by order in perturbation theory, as a series in the coupling  $\alpha_s(\mu^2)$ . The properties of  $\Gamma_{IJ}$  have been studied extensively in the massless [13–16] and in the massive [6–8] cases. To unambiguously fix the soft function in the massless case, a natural and convenient scheme was proposed in Ref. [17]. There, the jet functions for each external parton were identified with the square root of the massless on-shell spacelike form factor for the corresponding parton. We will assume this prescription, which we call *the form factor scheme* by default from now on. In this scheme, the jet functions for massless particles are series in the coupling  $\alpha_s(\mu^2)$  with coefficients that are  $\epsilon$ -dependent numbers. A natural extension [18] in the massive case is to identify the jet function with the small-mass limit of the corresponding massive spacelike QCD form factor. Therefore, in the massive case the jet function contains also powers of  $\ln(\mu^2/m^2)$ , where  $m$  is the pole mass of the heavy quark.

In the form factor scheme, we can derive an explicit expression for  $\mathbf{s}(\epsilon, \dots)$  in terms of the matrix soft anomalous dimension,

$$\mathbf{s}(\epsilon, \dots) = \mathcal{P} \exp \left\{ - \int_0^1 \frac{dx}{1-x} \Gamma_S(\bar{\alpha}_s[(1-x)^2 Q^2]) \right\}, \quad (11)$$

where  $\Gamma_S = (a/\pi) \Gamma_S^{(1)} + (a/\pi)^2 \Gamma_S^{(2)} + \mathcal{O}(\alpha_s^3)$ , and  $a$  stands for either  $\alpha_s(\mu^2)$  or  $\bar{\alpha}_s$ . The coupling  $\bar{\alpha}_s(k^2)$  is the  $d$ -dimensional strong coupling constant [19,20], known through NNLO [21]. It is a function of the usual four dimensional coupling  $\alpha_s(\mu^2)$  and the dimensional regulator  $\epsilon$  (the explicit relation we use here can be found in Refs. [18,22]). The result of Eq. (11) depends on the vanishing of the running coupling  $\alpha_s(\mu^2)$  at  $\mu = 0$  for  $\epsilon < 0$ , that is, in more than four dimensions.

Note the similarity between Eq. (11) and (7): the amplitude term can be directly obtained from one of the exponents in Eq. (7) by simply ignoring the term with  $x^{N-1}$  and

replacing the four dimensional coupling with the  $d$ -dimensional one. Such *duality* is not accidental; physically both exponents can be thought of as two different regularizations of the soft limit with regulators, respectively,  $\epsilon$  and  $\ln(N)$ . This relation has been explored and detailed, for example, in Ref. [18].

Without affecting the value of the soft anomalous dimension matrix, one has the freedom to add finite  $\epsilon$ -terms in the soft function which amounts to a redefinition of the hard function  $\mathbf{h}$ . In Eq. (11) we choose a minimal,  $\overline{\text{MS}}$ -inspired scheme, where only  $\epsilon$  poles are kept in the soft function. With this scheme defining the separation between the soft and hard functions, the explicit relation between the soft function and the anomalous dimension matrix through two loops reads:

$$\ln \mathbf{s}(\epsilon, \dots) = \frac{\alpha_s(\mu^2)}{\pi} \frac{\mathbf{\Gamma}_S^{(1)}}{2\epsilon} + \left( \frac{\alpha_s(\mu^2)}{\pi} \right)^2 \left( -\frac{\beta_0 \mathbf{\Gamma}_S^{(1)}}{16\epsilon^2} + \frac{\mathbf{\Gamma}_S^{(2)}}{4\epsilon} \right). \quad (12)$$

To summarize our discussion up to here, we have shown that the soft function in Eq. (6) can be fully specified by (7) and (9) in terms of the anomalous dimension matrix  $\mathbf{\Gamma}_S$  which in turn is derived solely from the knowledge of the purely virtual corrections to the same process. Ambiguities in  $\mathbf{\Gamma}_S$  are fixed by choosing a prescription at the level of the amplitude and we work with the form factor prescription for both massless and massive partons. Once the soft function in Eq. (6) has been fixed, in order to perform NNLL resummation in observables, one has to determine the number and the form of the various jet functions related to that observable in a manner consistent with the prescription implicit in the definition of the soft function. We turn to this next.

In the spirit of the form factor scheme that we employ here, we will associate a jet function in (10) for each of the hard partons, *both massless and massive*. The number of hard partons in the same underlying process determines also the number of jet functions in the decomposition of an observable (6). To derive the expressions for various jet functions in the following we use their process independence to either calculate them directly or to extract them from known results.

#### D. Jet functions for incoming partons

We start with the jet function  $J_{\text{in}}$  for an initial state hard parton (quark or gluon) which is basic for all hadron collider processes. To this end, we can use the well-known results from Drell-Yan vector boson or Higgs boson production. In these reactions, Eq. (6) takes the form

$$\sigma^P(N, Q) = [J_{\text{in}}^P(N, Q)]^2 H(Q) S(N, Q) + \mathcal{O}(1/N), \quad (13)$$

for  $P \in (q \leftrightarrow \text{DY}, g \leftrightarrow \text{Higgs})$ . In the two processes, the hard scale  $Q$  is simply the virtuality of the outgoing color singlet vector boson in DY or the mass of the Higgs boson.

Since in these two reactions exactly two hard colored partons are involved, the hard and soft functions are just  $1 \times 1$  matrices, i.e. the color structure is trivial. Upon setting  $\ln(\mu^2/s) = 0$  in the results of Ref. [13], it follows that the soft-anomalous dimension matrix vanishes through two-loops (and possibly to all orders [13–16]). Therefore, in Drell-Yan and Higgs boson production we have simply  $S(N, Q) = 1$ . Thus, the jet function  $J_{\text{in}}$  is simply the square root of the corresponding Sudakov factors, see, for example, Refs. [23,24]:

$$\ln J_{\text{in}}^P(N, Q) = \frac{1}{2} \int_0^1 dx \frac{x^{N-1} - 1}{1-x} \left\{ \int_{\mu_F^2}^{(1-x)^2 Q^2} \frac{dq^2}{q^2} 2A_P(\alpha_s[q^2]) + D_P(\alpha_s[(1-x)^2 Q^2]) \right\}. \quad (14)$$

The functions  $A_P$ ,  $P = (q, g)$  and  $D_P$ ,  $P = (q, g)$  are currently known through three loops ([23,25–28], respectively). The factorization scale  $\mu_F$  appearing in Eq. (14) is related to the factorization of the nonperturbative parton distributions, assumed to be defined in the  $\overline{\text{MS}}$  scheme. Utilizing a perturbative distribution function [29–31] one can also extend that result to processes initiated by massive partons [18].

The derivation of the jet functions for final state hard partons is more involved since these depend on the definition of the observable. Similarly to Drell-Yan/Higgs, one can use the vanishing of the soft anomalous dimension matrix (and thus the absence of nontrivial soft-gluon correlations) in any process involving two hard colored partons in order to extract various jet factors. For example, jet functions for “observed” outgoing hard partons (fragmentation) can be derived from semi-inclusive  $e^+e^-$  annihilation to hadrons [32–35]. Extension to the massive case can be done in a fashion similar to the case of Drell-Yan discussed above.

Of particular interest to us in this work are observables with inclusive final states; a very well known example is inclusive DIS [3,24] which can be treated similarly to Drell-Yan and  $e^+e^-$ , as discussed above. We are furthermore interested in processes with nontrivial color correlations, like the resummation of soft gluons at NNLL in  $t\bar{t}$  hadro-production. In order to calculate all jet factors that enter that observable we need to first specify the soft anomalous dimension matrix in this process which is done in Sec. IV. The calculation of the final-state jet factors and the final result for the cross section are relegated to Sec. V.

Finally we would like to comment on the process independence of the various jet factors discussed above. In principle, the presence of a process-dependent hard scale  $Q$  indicates process dependence of the whole result. What is process independent is the functional form of the corresponding jet functions, while the dependence of the hard scale should be thought of as a sort of functional argument related to the phase-space for soft-gluon radiation available

in the given process. Therefore in different processes the ‘‘argument’’ of the jet functions will in general be different but their functional form stays the same.

### III. FROM DIFFERENTIAL TO INCLUSIVE CROSS SECTIONS

The resummed partonic hard scattering function  $\omega_P(z)$  at fixed invariant mass is found from its moments with respect to  $z = M^2/s$ , with  $M$  the pair invariant mass and  $s$  the partonic center-of-mass energy squared. The fully inclusive hard scattering cross section is then found by integrating over  $M$ , or equivalently, over  $z$ , and the result is a function of

$$\rho \equiv \frac{4m^2}{s} \quad (15)$$

only. We must also integrate over the center-of-mass scattering angle (equivalently,  $\hat{\eta}$  above), but as we shall see, this does not affect our reasoning, and we suppress this integral for simplicity of notation. In expressing our results, we will find it useful to note that the ratio of pair and particle masses obeys the relation

$$\frac{4m^2}{M^2} = \frac{\rho}{z}. \quad (16)$$

We denote the inclusive cross section at parton level as  $\sigma_P(\rho, s)$ . It is related to the differential cross section in  $z$  at fixed  $s$  by simply integrating over  $z$ , with lower limit  $\rho$ ,

$$\sigma_P(\rho, s) = \int_{\rho}^1 dz \omega_P(z, M, m). \quad (17)$$

We have observed that the singular dependence of  $\omega_P$  on  $z$  can be found in turn by an inverse transform,

$$\omega_P(z, M, m) = \int \frac{dN}{2\pi i} z^{-N} \omega_P^{\text{res}}(N, M, m). \quad (18)$$

The  $z$ -resummed cross section is taken at fixed pair invariant mass  $M$ , and therefore fixed velocity in the hard-scattering c.m.,

$$\beta_M^2 \equiv 1 - \frac{4m^2}{M^2} = 1 - \frac{\rho}{z}. \quad (19)$$

Our goal is to relate the expression for  $\omega^{\text{res}}(N, M, m)$  at fixed  $M$  to the inclusive resummed cross section  $\sigma_P(\rho, s)$  with respect to  $\rho$ , as an inverse transform from moment space in terms of that variable.

The resummed expression for  $\omega(N)$  is given in Eq. (6). For the following analysis, we make a slight change in notation, and recognize that the hard-scattering function  $\mathbf{H}$ , which describes the short-distance part of the cross section, vanishes linearly in the center-of-mass velocity at absolute threshold, and lowest order in  $\alpha_s$ . Since  $\beta_M$  depends only on the ratio  $m/M$ , this quantity is fixed for Mellin moments with respect to  $z$ . It will, however, be important for  $\sigma_P$ . To make this trivial but important factor

explicit, we change the notation slightly, and write

$$\mathbf{H}^P\left(\frac{M^2}{\mu^2}, \frac{m^2}{\mu^2}, \alpha_s(\mu^2)\right) \rightarrow \beta_M \mathbf{H}^P\left(\frac{\rho}{z}, \frac{M^2}{\mu^2}, \alpha_s(\mu^2)\right), \quad (20)$$

so that Eq. (6) becomes

$$\omega_P^{\text{res}}(N, M, m) = \beta_M \prod_i J_i(N) \text{Tr} \left[ \mathbf{H}^P\left(\frac{\rho}{z}, \frac{M^2}{\mu^2}, \alpha_s(\mu^2)\right) \times \mathbf{S}^P\left(\frac{N^2 \mu^2}{M^2}, \frac{M^2}{m^2}, \alpha_s(\mu^2)\right) \right], \quad (21)$$

where we have represented the jet functions schematically. We emphasize that moments in  $z$  at fixed  $M$  are equivalent to integrals over  $s$ . They thus leave  $\beta_M$ , but not  $\rho$ , fixed. Dependence on  $\rho$  enters only after the integral over  $M^2$ , or equivalently  $z$ , as in Eq. (17).

We now relate the inclusive cross section, which depends on  $\rho$ , to the fixed- $M^2$   $z$  moments of  $\omega$  by

$$\begin{aligned} \sigma_P(\rho, s) &= \int_{\rho}^1 dz \int \frac{dN}{2\pi i} z^{-N} \omega_P^{\text{res}}(N, M^2, m^2) \\ &= \int \frac{dN}{2\pi i} \int_{\rho}^{\infty} dz z^{-N} \sqrt{1 - \frac{\rho}{z}} \prod_i J_i(N) \\ &\quad \times \text{Tr} \left[ \mathbf{H}^P\left(\frac{\rho}{z}, \frac{M^2}{\mu^2}, \alpha_s(\mu^2)\right) \right. \\ &\quad \left. \times \mathbf{S}^P\left(\frac{N^2 \mu^2}{M^2}, \frac{z}{\rho}, \alpha_s(\mu^2)\right) \right], \end{aligned} \quad (22)$$

where in the second form we have observed that  $\omega_P(z)$  vanishes for  $z > 1$ , and have exchanged the  $N$  and  $z$  integrals. We note that when we choose  $\mu = \text{cm}$ , with  $c$  some constant of order unity, the full right-hand side of Eq. (22) depends on  $M$  only through logarithms of the ratio  $4m^2/M^2 = \rho/z$ , see Eq. (16). Making such a choice of renormalization scale and changing variable from  $z$  to

$$\xi \equiv \frac{z}{\rho} = \frac{1}{1 - \beta_M^2}, \quad (23)$$

we derive the desired form of an inverse transform,

$$\sigma_P(\rho, s) = \int \frac{dN}{2\pi i} \rho^{-N+1} \sigma_P(N, m), \quad (24)$$

with

$$\begin{aligned} \sigma_P(N, m) &\equiv \int_1^{\infty} d\xi \xi^{-N} \sqrt{1 - \xi^{-1}} \prod_i J_i(N, \xi, \alpha_s) \\ &\quad \times \text{Tr}[\mathbf{H}^P(\xi, \alpha_s(\mu^2)) \mathbf{S}^P(N^2 \xi, \xi, \alpha_s)]. \end{aligned} \quad (25)$$

Here we have simplified the notation for the arguments of the jet, hard and soft functions somewhat to emphasize their  $\xi$ -dependence. The scale of the running coupling is, as indicated above, of order of the quark mass,  $m$ . The relationship between the  $N$ -dependence of the resummed cross section at fixed  $M$  in  $\omega_P^{\text{res}}(N)$  and in  $\sigma_P(N, m)$  can be

found readily in the large- $N$  limit, by noting that the integral over  $\xi$  in (25) is dominated by the factor

$$\xi^{-N} \sim e^{N \ln(1 - \beta_M^2)}, \quad (26)$$

which forces  $M^2$  towards  $4m^2$ . Center-of-mass velocities  $\beta_M \gg 1/\sqrt{N}$  are thus exponentially suppressed. Correspondingly, the scale of energy evolution in the soft cross section, Eq. (7) is over an interval from  $m$  to  $m/N \geq m\beta_M^2$ . For this range of energies, the evolution variable  $\mu'$  in (7) is larger than the kinetic energy of the pair in their center of mass. We shall assume below that, as suggested in Ref. [36], radiation in this energy range decouples from the pair, whose interactions give rise to Coulomb enhancements that appear as inverse powers of  $\beta_M$ . In the soft anomalous dimension matrix appropriate to this range of energies, the pair of heavy quark eikonals is effectively replaced by a singlet or octet eikonal line, with a separate term that describes the evolution of the pair. This approximation results in a smooth limit at absolute threshold  $\beta_M = 0$  [37].

Corrections due to the logarithmic  $\xi$ -dependence in the jet and soft factors are suppressed by inverse powers of  $N$ . Up to such corrections, the result is the Born cross section for heavy quark production in process  $P$  times the remaining jet, hard and soft functions, which we write as

$$\begin{aligned} \sigma_P(N, m) &= \sigma_{\text{Born}}^P(N) \prod_i J_i(N, 1, \alpha_s) \text{Tr}[\hat{\mathbf{H}}^P(1, \alpha_s(\mu^2))] \\ &\times \mathbf{S}^P(N, 1, \alpha_s) \left[ 1 + \mathcal{O}\left(\frac{1}{N}\right) \right], \end{aligned} \quad (27)$$

where the hat on the hard matrix indicates that have factored out the  $N$ -dependence of the Born cross section, which behaves at leading power in  $N$  as

$$\begin{aligned} \sigma_{\text{Born}}^P(N) &\sim \int_1^\infty d\xi \xi^{-N+1/2} \sqrt{\xi-1} \\ &= \frac{\sqrt{\pi}}{2} \frac{1}{N^{3/2}} \left( 1 + \mathcal{O}\left(\frac{1}{N}\right) \right). \end{aligned} \quad (28)$$

Equation (27) is the form that we will use below. As suggested above, we will evaluate the soft function  $\mathbf{S}^P(N, 1, \alpha_s)$  using Eq. (7) computed with a soft anomalous dimension appropriate to the range energy range  $m > \mu' > \beta_M^2 m$ .

#### IV. THE TWO-LOOP ANOMALOUS DIMENSION MATRIX AT ABSOLUTE THRESHOLD

In this section we derive the relevant result for the two-loop anomalous dimension matrix  $\Gamma_S$ . We also show that these results are enough to predict the full pole structure of the two-loop color-averaged amplitudes for  $q\bar{q} \rightarrow t\bar{t}$ .

The one-loop massive anomalous dimension matrix for an amplitude with  $n$  colored partons,  $\mathcal{N}_m$  of which are massive and with equal mass  $m$  has been known for some time [5,40]:

$$\begin{aligned} \Gamma_S^{(1)} &= \frac{1}{2} \sum_{(i \neq j)=1}^n T_i \cdot T_j \ln\left(-\frac{\mu^2}{\sigma_{ij}}\right) + \frac{1}{2} \sum_{(i \neq j) \in \mathcal{N}_m} T_i \cdot T_j \\ &\times \left[ \ln(1 + x_{ij}^2) + \frac{2x_{ij}^2}{1 - x_{ij}^2} \ln(x_{ij}) \right], \end{aligned} \quad (29)$$

where  $s_{ij} = (p_i + p_j)^2$  and  $\sigma_{ij} = 2p_i \cdot p_j = s_{ij} - m_i^2 - m_j^2$  (with  $m_{i,j} = \{0, m\}$ ). The spacelike variables  $x_{ij}$  read [41]:

$$\frac{m^2}{s_{ij}} = -\frac{x_{ij}}{(1 - x_{ij})^2}, \quad x_{ij} = \frac{\sqrt{1 - \frac{4m^2}{s_{ij}} - 1}}{\sqrt{1 - \frac{4m^2}{s_{ij}} + 1}}, \quad (30)$$

when, in the unphysical spacelike kinematics, all invariants  $s_{ij} < 0$ . In specific applications some of them have to be continued to timelike kinematics. This can be done with the help of the replacement  $x_{ij} = -y_{ij} + i\epsilon$ , where  $s_{ij}$  is now in the physical region  $s_{ij} \geq 4m^2$  and the ‘‘timelike’’ variable is  $0 < y_{ij} \leq 1$ . The color generators  $T_i$  are defined such that they satisfy  $\sum_k^n T_k = 0$ , and can be either in the fundamental or adjoint representation of the color group for quarks or gluons. The index  $i$  labels the leg where the generator is inserted; see also the appendix for more details.

In parallel to the two-loop massless case [13], the two-loop massive anomalous dimension matrix  $\Gamma_S^{(2)}$  is built up from 2- and 3-eikonal (3E) contributions, i.e. configurations where soft gluons are exchanged between two (resp. three) external hard partons.

$$\begin{aligned} \Gamma_S^{(2)} &= \frac{1}{2} \sum_{(i \neq j)=1}^n T_i \cdot T_j \frac{K}{2} \ln\left(-\frac{\mu^2}{\sigma_{ij}}\right) \\ &+ \frac{1}{2} \sum_{(i \neq j) \in \mathcal{N}_m} T_i \cdot T_j P_{ij}^{(2)} + 3E \text{ terms}, \end{aligned} \quad (31)$$

where, as for the massless case,  $K = (67/18 - \pi^2/6)C_A - (5/9)N_L$ . Even before treating the 3E terms, we see that at two loops exchanges involving two eikonals take on the same color structure as in the one-loop anomalous dimension, Eq. (29).

Even without using explicit forms for the 3E contributions [38], we have adequate information to study the behavior of the soft anomalous dimension in the range  $\mu > \beta^2 m$ , subject to our assumption of factorization, as discussed above. In [6] it was observed, for example, that 3E contributions to the reactions  $q\bar{q} \rightarrow Q\bar{Q}$  and  $gg \rightarrow Q\bar{Q}$  vanish, either identically (when two eikonal lines are massless) or at  $u = t$  (for two massive eikonals). Given our assumption of the decoupling of soft radiation from the dynamics of the pair in the range  $\mu' > \beta^2 m$ , we may extend the anomalous dimension, appropriate for this range of energies to absolute threshold,  $\beta = \sqrt{1 - 4m^2/s} \rightarrow 0$ . To the order at which we work, power singularities in  $\beta$  associated with independent evolution of the pair of heavy

eikonal lines cancel in the soft function  $S$  of Eq. (7). It is this simplification that enables us to present a full expression for the threshold-resummed inclusive cross section at NNLL. To derive this result, we need only the  $2E$  diagrams.

The  $2E$ , dipole-type contributions, can be readily derived in complete generality. Here we note first that Eq. (31) reproduces the known massless result for a massless dipole. Second, it reflects the fact that, similarly to the one loop case, the mixed corrections between massive and massless legs do not produce any power corrections in  $m^2/s_{ij}$ . To verify that one-mass dipoles do not involve additional power corrections, we have repeated for this case the arguments given below for the derivation of the function  $P_{ij}^{(2)}$ . In that check we have used the recent two-loop calculation of the heavy-to-light form factor in QCD [42,43]; see also [44–46]. For partial checks we have made use of the packages HPL [47] and FIESTA [48]. Note also that the absence of power corrections in the mass in the one-mass dipoles is related to the choice of the variable  $\sigma_{ij} = 2p_i \cdot p_j$  instead of  $s_{ij} = (p_i + p_j)^2$  in the first term of Eqs. (29) and (31).

Finally, we explain how the functions  $P_{ij}^{(2)}$  can be determined. The dependence on the indices  $(i, j)$  of the function  $P_{ij}^{(2)}$  in Eq. (31) is only through the corresponding kinematical invariant  $s_{ij}$ , i.e.  $P_{ij}^{(2)} = P^{(2)}(s_{ij})$ , and the dependence on  $s_{ij}$  enters through the variable  $x_{ij}$  defined in Eq. (30). That implies its functional form is universal and therefore can be extracted from the simplest two-loop amplitude with  $n = 2$ : the two-loop massive vector form factor  $F_1(\gamma^* \rightarrow Q\bar{Q})$  [41,49]. In this case Eq. (31) simplifies to

$$\Gamma_S^{(2)}(n = 2) = -C_F \left[ \frac{K}{2} \ln\left(-\frac{\mu^2}{\sigma}\right) + P^{(2)}(s) \right], \quad (32)$$

where  $\sigma = s - 2m^2$  and  $s = (p_1 + p_2)^2 < 0$ . Of course, there are no  $3E$  contributions for  $n = 2$ .

As we remarked above, the soft anomalous dimension matrix is defined only up to a term proportional to the unit matrix. In this context, we can use that ambiguity in the definition of the soft function to define it through the condition  $H = 1$  in the factorization of the form factor  $F_1 = J \cdot S \cdot H$  following from Eq. (10). From the known results for the form factor  $F_1$  and the jet function  $J$  [18] and taking into account Eq. (12) we derive:

$$P^{(2)} = \frac{K}{2} P^{(1)} + P^{(2),m}, \quad (33)$$

where, similarly to the definition of  $P^{(2)}$  in Eq. (31), the function  $P^{(1)}$  equals the term in the square brackets in Eq. (29). The presence of the term  $P^{(2),m}$  in the above equation indicates that the property of the two-loop massless amplitudes  $\Gamma^{(2)} = K/2\Gamma^{(1)}$  [13] is broken in the massive case by power corrections of the mass. The function

$P^{(2),m}$  is given by

$$\begin{aligned} P^{(2),m}(x) = & \frac{C_A}{(1-x^2)^2} \left\{ -\frac{(1+x^2)^2}{2} \text{Li}_3(x^2) \right. \\ & + \left( \frac{(1+x^2)^2}{2} \ln(x) - \frac{1-x^4}{2} \right) \text{Li}_2(x^2) \\ & + \frac{x^2(1+x^2)}{3} \ln^3(x) + x^2(1-x^2) \ln^2(x) \\ & + (-1-x^4) \ln(1-x^2) + x^2(1+x^2) \zeta_2 \ln(x) \\ & \left. + x^2(1-x^2) \zeta_2 + 2x^2 \zeta_3 \right\}, \quad (34) \end{aligned}$$

where  $\zeta_n$  is the Riemann zeta function:  $\zeta_2 = \pi^2/6$ ,  $\zeta_3 = 1.202057\dots$

The function  $P^{(2),m}$  (and, in particular, its real part) does not vanish at threshold; for example, for a timelike argument  $x = -(1-\beta)/(1+\beta) + i\varepsilon$  with  $\beta = \sqrt{1-4m^2/s}$  and  $0 \leq \beta \leq 1$ , this limit is

$$\begin{aligned} P^{(2),m}(x \sim -1 + i\varepsilon) = & \frac{1-\zeta_3}{2} C_A + \left( \frac{\pi^2}{24} - \frac{1}{2} \right) \frac{i\pi}{\beta} C_A \\ & + \mathcal{O}(\beta). \quad (35) \end{aligned}$$

This result contains, as usual, a Coulomb enhancement in its imaginary part, which reflects the pair's internal evolution.

Combining the results above, the two-loop soft anomalous dimension matrix for the two-to-two quark- and gluon-initiated reactions [see Eqs. (A1) and (A2)] takes the following form close to absolute threshold  $\beta \rightarrow 0$ ,

$$\Gamma_S^{(2)} = \frac{K}{2} \Gamma_S^{(1)} + T_3 \cdot T_4 P_{34}^{(2),m}, \quad (\text{for } \beta \rightarrow 0), \quad (36)$$

with  $P_{34}^{(2),m}$  given by Eq. (35). The explicit results for the matrices  $\Gamma_S^{(1)}$  and  $T_3 \cdot T_4$  can be found in the appendix.

The mass-dependent soft anomalous dimension of Eq. (32) for processes with the color structure of the form factor was derived in Ref. [7], using a slightly different scheme for the soft function. Equation (31) for soft matrices of arbitrary  $n$ -point amplitudes involving massive colored particles was presented in Ref. [8]. To determine the analogue of the function  $P^{(2),m}$ , the authors of that reference have utilized the results of Refs. [7,50]. We find agreement between our  $P^{(2),m}$  and ( $-1$  times) the function appearing in Eq. (15) of version 2 of the arXiv preprint of Ref. [8]. The fact that the results of Ref. [8] reproduce the IR poles of the massive form factor (which we have used to extract the function  $P^{(2),m}$ ) implies a nontrivial consistency between our results and the results of Refs. [7,8].

Moreover we have performed for the first time a truly nontrivial check of Eq. (31) as a whole, by predicting the IR poles of the squared two-loop  $q\bar{q} \rightarrow Q\bar{Q}$  amplitude and comparing them to the numerical calculation of Ref. [51].



We have found a complete agreement between the predictions of our formalism and the color-averaged squared amplitude at two loops.

In order to be able to make this prediction, we have noticed that in squaring the amplitude and summing/averaging over colors, any  $3E$ -type contributions in Eq. (31) with color structure  $f^{abc}T^aT^bT^c$  would vanish simply by color projection, and would not contribute to the squared amplitude at this level. Thus the calculation in question does not test for the presence of such terms at the amplitude level.

The setup of our prediction is as follows: the amplitude  $M$ , multiplied by the Born amplitude and summed over spin/color, can be expanded in the coupling  $a_s = \alpha_s(\mu^2)/(2\pi)$  as

$$M = M^{(0)}(\epsilon) + a_s M^{(1)}(\epsilon) + a_s^2 M^{(2)}(\epsilon) + \mathcal{O}(a_s^3). \quad (37)$$

The factorization properties of on-shell amplitudes detailed in Sec. II C give the following prediction for the poles of the amplitude  $M$  through two loops

$$\begin{aligned} M^{(1)}(\epsilon) &= \left\{ \frac{1}{\epsilon} \Gamma_1 + J^{(1)} \right\} M^{(0)} + \mathcal{O}(\epsilon^0), \\ M^{(2)}(\epsilon) &= \left\{ J^{(2)} - (J^{(1)})^2 + \frac{1}{\epsilon} (-J^{(1)} \Gamma_1 + \Gamma_2) \right. \\ &\quad \left. + \frac{1}{\epsilon^2} \left( -\frac{1}{2} (\Gamma_1)^2 - \frac{\beta_0}{4} \Gamma_1 \right) \right\} M^{(0)} \\ &\quad + \left\{ \frac{1}{\epsilon} \Gamma_1 + J^{(1)} \right\} M^{(1)} + \mathcal{O}(\epsilon^0). \end{aligned} \quad (38)$$

The function  $J(\epsilon)$  represents the product of the four  $\epsilon$ -dependent jet functions corresponding to the two incoming massless and two outgoing massive fermions (see Refs. [52] for more details) and has an expansion in  $a_s$  analogous to Eq. (37). Similarly,  $\Gamma_1$  and  $\Gamma_2$  are the expansion in terms of the coupling  $a_s$  of the anomalous dimension matrix  $\Gamma_S$  given through Eqs. (29) and (31).

Predicting all two-loop poles in the squared amplitude requires also the one-loop amplitude for the same process evaluated to sufficiently high order in  $\epsilon$ . We have calculated them separately. Our results will provide a nontrivial check on future extension of the results of Refs. [53] to the analytic calculation of the nonplanar contributions in this process.

## V. NNLL RESUMMATION FOR TOTAL $t\bar{t}$ HADRO-PRODUCTION CROSS SECTION

We can summarize the results of Secs. II and III for the resummed partonic total-inclusive cross section for  $t\bar{t}$  pair production at hadron colliders in moment space by

$$\begin{aligned} \sigma^P(N, m^2, \mu^2) &= \sigma_{\text{Born}}^P(N) [J_{\text{in}}^P(N, m^2, \mu^2)]^2 \\ &\quad \times [J_{\text{incl}}(N, m^2, \mu^2)]^2 \text{Tr}[\hat{\mathbf{H}}^P(m^2, \mu^2)] \\ &\quad \times \mathbf{S}^P(N, m^2, \mu^2)] + \mathcal{O}(1/N). \end{aligned} \quad (39)$$

The index  $P = (q, g)$  labels the jet functions as well as the two reactions  $q\bar{q} \rightarrow t\bar{t}$  and  $gg \rightarrow t\bar{t}$ . The factorization/re-normalization scales are denoted by  $\mu$ . The jet factors  $J_{\text{in}}^P$  are given in Eq. (14) with  $Q^2 = 4m^2$ , where  $m$  is the pole mass of the top quark. The only factors remaining to compute in (39) are functions  $J_{\text{incl}}$  for the final-state jets and the one-loop correction to the soft function at  $N = 1$  in Eq. (7), which serves as a boundary condition for the evolved soft function. We turn first to the outgoing jets.

The outgoing jet functions are specified by our choice of the form factor scheme, as described in Sec. II C. Their virtual contributions precisely cancel the terms subtracted from the soft anomalous dimension matrix  $\Gamma_S$  in Eq. (29), and hence in the soft function  $\mathbf{S}$  appearing in Eq. (39). Specifically, we have subtracted those soft singularities corresponding to the low-mass limit of the outgoing legs. For a completely inclusive observable, like the total inclusive cross section, such factorization is not strictly necessary. The resulting expression, however, Eq. (39), provides a unified threshold resummation for the total inclusive cross section and for the cross section at measured pair invariant mass  $s \geq 4m^2$ , including the limit  $s \gg m^2$ , where logarithms of the heavy quark mass can be important.

As described above, the outgoing jet function can be constructed directly from the exponentiation of its infrared singularities in the low-mass limit, and therefore is of the form,

$$\begin{aligned} J_{\text{incl}}(N, m^2, \mu^2) &= \exp \left\{ \frac{1}{2} \int_0^1 dx \frac{x^{N-1} - 1}{1-x} \right. \\ &\quad \left. \times \Gamma_{\text{incl}}(\alpha_s [4m^2(1-x)^2]) \right\}. \end{aligned} \quad (40)$$

The jet anomalous dimension  $\Gamma_{\text{incl}}$  is proportional to the unit matrix in color space. Specifically, it is given by the single poles of the logarithm of the massive quark form factor in the small mass limit, which defines the jet factor of a massive line in an amplitude [18], and which we have adapted here for the form factor scheme. The explicit expression for  $\Gamma_{\text{incl}}$  through two loops is

$$\begin{aligned} \Gamma_{\text{incl}} &= \frac{\alpha_s(\mu^2)}{\pi} C_F \left[ -1 - \ln\left(\frac{m^2}{\mu^2}\right) \right] + \left( \frac{\alpha_s(\mu^2)}{\pi} \right)^2 \\ &\quad \times \left[ \frac{K}{2} C_F \left( -1 - \ln\left(\frac{m^2}{\mu^2}\right) \right) - \frac{\zeta_3 - 1}{2} C_F C_A \right]. \end{aligned} \quad (41)$$

The nonlogarithmic part of  $\Gamma_{\text{incl}}$  can be naturally expressed in terms of the anomalous dimensions  $G, K$  needed for the exponentiation of the massive form factor to NNLL [18],

$$\begin{aligned} \Gamma_{\text{incl}}(\text{non-log term}) &= \frac{\alpha_s(\mu^2)}{\pi} \frac{1}{4} [G_1^{(0)} + K_1] + \left( \frac{\alpha_s(\mu^2)}{\pi} \right)^2 \\ &\quad \times \frac{1}{4^2} [G_2^{(0)} + K_2 - \beta_0 G_1^{(1)}]. \end{aligned} \quad (42)$$

The functions  $G$  and  $K$  are defined in [18] as expansions of  $\alpha_s/(4\pi)$ , hence the additional powers of  $1/4$  in the equa-

tion above, and with  $N_L$  active flavors. The function  $G$  is  $\epsilon$ -dependent:  $G_n = \sum_{i=0} G_n^{(i)} \epsilon^i$ , and it equals (minus) the function  $G$  in the massless form factor [19–21]. The origin of the term  $\beta_0 G_1^{(1)}$  can be understood along the lines of Ref. [54].

The last step remaining is the derivation of the boundary condition  $\mathbf{S}^{(1)}(1, \beta_i \cdot \beta_j)$  for the soft function  $\mathbf{S}$ , see section II B. We recall that the boundary condition is uniquely defined once the form factor scheme has been adopted. To extract it, we need to calculate the total inclusive cross section in the eikonal approximation. After the appropriate eikonal jet functions have been factored out (see Ref. [5]) we are left with the desired boundary condition.

The required one-loop calculation is in fact quite straightforward. To that end one can use the factorization in the soft limit of the squared one-gluon real emission amplitude into the square  $\mathcal{S}_{ij}$  of the eikonal current and the Born amplitude with appropriate insertions of the color operators  $T_i \cdot T_j$  summed over all pairs of legs ( $i, j$ ); see, for example, Ref. [55] for details. Combining matrix element factorization with the factorization of phase space in the soft limit, we arrive at  $\sigma_{\text{eikonal}}^{(1),\text{real}} = \sum_{i,j=1}^4 \text{Born}^{ij} \times I_{ij}$ . We label the legs according to the momenta of the hard partons; see Eq. (A2). The functions  $I_{ij}$  are simply the integrals of the eikonal current squared over the phase space of the emitted gluon. While the integrand is scaleless by construction, the integrals do not vanish because we integrate up to the maximal energy  $E_{\text{max}}$  available to the emitted gluon in the partonic c.m. system. Their expressions read:

$$I_{ij} = \frac{\alpha_s(\mu^2)}{\pi} \left( \frac{\mu^2}{4E_{\text{max}}^2} \right)^\epsilon J_{ij},$$

where:  $J_{ij} = -\frac{e^{\epsilon\gamma_E}}{2^{2-2\epsilon}\pi^{1-\epsilon}} \int_0^1 E_g^{1-2\epsilon} dE_g$

$$\times \int d\Omega_{d-1} \frac{(p_i \cdot p_j)}{(p_i \cdot g)(p_j \cdot g)}. \quad (43)$$

Working out the color algebra we get the following result for the one-loop real-emission contribution for the reaction  $gg \rightarrow Q\bar{Q}$  (which covers the general case),

$$\sigma_{\text{eikonal}}^{(1),\text{real}} = \sigma_{\text{Born}} \frac{\alpha_s(\mu^2)}{\pi} \left( \frac{\mu^2}{4E_{\text{max}}^2} \right)^\epsilon \left[ -2(C_F(J_{34} - J_{33})) \right.$$

$$+ C_A J_{12} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + C_A (J_{12} + J_{34}$$

$$- 2J_{13}) \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \left. \right], \quad (44)$$

where  $\sigma^{\text{Born}}$  above is a diagonal matrix; we work in the singlet-octet basis given in the appendix.

Equation (44) is derived in the back-to-back scattering configuration where  $u = t$  and holds for any  $\beta = \sqrt{1 - 4m^2/s}$ . Nicely, the result is diagonal and the two octets are degenerate. To complete this result one has to add the corresponding virtual corrections. Since they are all scaleless and thus vanish in dimensional regularization, the only contributions comes from their counterterms.

The result simplifies significantly if one takes the limit  $\beta \rightarrow 0$  which is relevant for the resummation of the total cross section. In that limit (i.e. working up to powers of  $\beta$ ) we can set  $\beta = 0$  everywhere in the integrals  $J_{ij}$ . In this limit we have  $J_{13} = J_{12}/2$  and  $J_{33} = J_{34}$  as well as  $4E_{\text{max}}^2 = s\beta^4$ . The two independent integrals read:

$$J_{12} = \frac{e^{\epsilon\gamma_E}}{\Gamma(1-\epsilon)} \frac{1}{2\epsilon} \frac{\Gamma(-\epsilon)\Gamma(1-\epsilon)}{\Gamma(1-2\epsilon)}$$

$$= -\frac{1}{2\epsilon^2} + \frac{\pi^2}{8} + \mathcal{O}(\epsilon), \quad (45)$$

$$J_{34} = \frac{e^{\epsilon\gamma_E}}{\Gamma(1-\epsilon)} \frac{1}{4\epsilon} \frac{2^{2\epsilon}\sqrt{\pi}\Gamma(1-\epsilon)}{\Gamma(3/2-\epsilon)} = \frac{1}{2\epsilon} + 1 + \mathcal{O}(\epsilon). \quad (46)$$

After subtracting the eikonal jets in such a way that the singlet eigenvalue vanishes (i.e., to reproduce the well known result from Drell-Yan-type processes) we finally get,

$$\sigma_{\text{eikonal}}^{(1)} = \sigma_{\text{Born}} \frac{\alpha_s(\mu^2)}{\pi} C_A \left[ 1 + \frac{1}{2} \ln \left( \frac{\mu^2}{4E_{\text{max}}^2} \right) \right]$$

$$\times \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (47)$$

The constant coefficient above follows from the constant term in Eq. (46). We have verified that Eq. (47) correctly reproduces the  $\ln\beta$  terms in the color-singlet color-octet difference of the total inclusive cross section (see Eqs. (8–10) in Ref. [56]).

Following the discussion in Sec. III we set the ratio  $\mu^2/4E_{\text{max}}^2$  to unity, so that the logarithmic term in Eq. (47) vanishes. This way we get the following result for the boundary condition of the soft function in Eq. (7) relevant for the resummation of the total heavy-pair cross section,

$$\begin{aligned}
& \mathbf{S}(1, \alpha_s(Q^2/N^2)) \\
&= \mathbf{S}^{(0)} \left[ 1 + \frac{\alpha_s(Q^2/N^2)}{\pi} C_A \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \dots \right] \\
&= \mathbf{S}^{(0)} \left[ 1 + C_A \frac{\alpha_s(\mu^2)}{\pi} \left\{ 1 + \frac{\alpha_s(\mu^2)}{\pi} \frac{\beta_0}{4} \ln\left(\frac{N^2 \mu^2}{Q^2}\right) \right\} \right. \\
&\quad \left. \times \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \dots \right], \tag{48}
\end{aligned}$$

which as shown results in a term  $\beta_0(C_A/2) \ln N$  in the NNLL result. The  $\mathcal{O}(\alpha_s)$  correction appears only when the pair is produced in an octet configuration at short distances. The result for  $q\bar{q} \rightarrow Q\bar{Q}$  follows from Eq. (A16).

We are now ready to combine our previous findings and present our result for the resummed heavy quark cross section in moment space up to NNLL. Working in the singlet/octet basis for the soft anomalous dimension  $\Gamma_S$ , where it is diagonal [6], the result for the resummed cross section for heavy-pair hadroproduction reads

$$\begin{aligned}
\frac{\sigma^P(N, m^2, \mu^2)}{\sigma_{\text{Born}}^P(N)} &= \text{Tr} \left[ \hat{\mathbf{H}}^P(m^2, \mu^2) \mathbf{S}_P^{(0)} \left[ 1 \right. \right. \\
&\quad \left. \left. + \frac{\alpha_s(Q^2/N^2)}{\pi} C_A \mathbf{\Pi}_8 \right] \right. \\
&\quad \times \exp \left[ \int_0^1 dx \frac{x^{N-1} - 1}{1-x} \right. \\
&\quad \times \left( \int_{\mu_f^2}^{4m^2(1-x)^2} \frac{dq^2}{q^2} 2A_P(\alpha_s[q^2]) \mathbf{1} \right. \\
&\quad \left. \left. + \hat{D}_{Q\bar{Q}}^P(\alpha_s[4m^2(1-x)^2]) \right) \right] \\
&\quad \left. + \mathcal{O}(1/N, N^3 LL), \tag{49}
\end{aligned}$$

where  $\mathbf{\Pi}_8$  projects onto the color octet states [see Eq. (A16)], and where  $\hat{D}_{Q\bar{Q}}^P$  contains single-logarithmic anomalous dimensions from both the jet and soft functions, in a color-diagonal form (see below). This expression is our central result. It may be cast in a more familiar form, by combining the constant piece of the soft function into the hard function, and generating the  $\ln N$  dependence in the soft function from a slightly modified version of the function  $\hat{D}_{Q\bar{Q}}^P$ , which we denote as simply  $D_{Q\bar{Q}}^P$ , and which includes a new term proportional to  $\alpha_s^2 \beta_0$ ,

$$\begin{aligned}
\frac{\sigma^P(N, m^2, \mu^2)}{\sigma_{\text{Born}}^P(N)} &= \text{Tr} \left[ \mathbf{H}^P(m^2, \mu^2) \exp \left\{ \int_0^1 dx \frac{x^{N-1} - 1}{1-x} \right. \right. \\
&\quad \times \left( \int_{\mu_f^2}^{4m^2(1-x)^2} \frac{dq^2}{q^2} 2A_P(\alpha_s[q^2]) \mathbf{1} \right. \\
&\quad \left. \left. + D_{Q\bar{Q}}^P(\alpha_s[4m^2(1-x)^2]) \right) \right] \\
&\quad \left. + \mathcal{O}(1/N, N^3 LL), \tag{50}
\end{aligned}$$

where

$$\begin{aligned}
D_{Q\bar{Q}}^P &= D_P \mathbf{1} + 2 \text{Re} \Gamma_P + 2 \Gamma_{\text{incl}} \mathbf{1} \\
&\quad - \frac{1}{2} \left( \frac{\alpha_s}{\pi} \right)^2 C_A \beta_0 \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \tag{51}
\end{aligned}$$

The explicit form for  $D_{Q\bar{Q}}^P$  uses the results for  $\Gamma_P$  in Sec. IV and the appendix. In the reactions  $q\bar{q} \rightarrow Q\bar{Q}$  and  $gg \rightarrow Q\bar{Q}$ , which we label, respectively, by  $P \in (q\bar{q}, gg)$ , it reads through two loops:

$$\begin{aligned}
D_{Q\bar{Q}}^P &= \frac{\alpha_s(\mu^2)}{\pi} (-C_A) \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} + \left( \frac{\alpha_s(\mu^2)}{\pi} \right)^2 \left\{ D_P^{(2)} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right. \\
&\quad \left. + \left( -C_A \frac{K}{2} - \frac{\zeta_3 - 1}{2} C_A^2 - C_A \frac{\beta_0}{2} \right) \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \right\}, \tag{52}
\end{aligned}$$

where  $D_{q\bar{q}} = D_{\text{DY}}$  and  $D_{gg} = D_{\text{Higgs}}$  [24]. Corrections to Eq. (50) begin, as indicated, at next-to-next-to-next-to leading logarithm, and are determined by the three-loop soft anomalous dimension matrix and the inclusive soft function at two loops.

The hard function  $\mathbf{H}(m^2, \mu^2)$  in Eq. (50) is known exactly through one loop [56] (see also Ref. [57]). Interestingly, the total cross section is the only  $t\bar{t}$  observable for which at present the hard function is known beyond the leading order with full color dependence. We have used the degeneracy of the eigenvalues of the matrix  $\Gamma_S$  in the gluon fusion reaction (see also the appendix) to explicitly perform the trace over the degenerate octet eigenvalue in Eq. (50). Therefore the hard function  $\mathbf{H}$  in this reaction is also a two-by-two matrix as computed in Ref. [56].

The interplay of the jet anomalous dimension  $\Gamma_{\text{incl}}$  with the soft matrix is quite interesting. As can be seen from the results in the appendix, through two loops  $\Gamma_{\text{incl}}$  equals minus the singlet component of the anomalous dimension matrix  $\Gamma_S$ . Indeed, it is natural to expect that the anomalous dimension for producing a color singlet is the same as the one in Drell-Yan or Higgs production, a fact that has been anticipated already in Ref. [4]. Reproducing this property, without imposing it by hand, represents a very strong check on the consistency of our setup and results.

The vanishing of the sum of the color singlet anomalous dimension and  $\Gamma_{\text{incl}}$  is even more striking given the fact that they refer to very different kinematics: the former is related to the ‘‘very heavy mass’’ limit close to partonic threshold

where the mass is comparable in value to the hard scale, while the former is extracted from the small mass limit where the mass is negligible compared to the hard scale. This result is quite intriguing, and it is clear that it is not accidental, as implied by the argument that the singlet anomalous dimension should not receive corrections beyond Drell-Yan/Higgs. Clearly, one can explore this property to relate the anomalous dimension in heavy flavor hadroproduction to the small-mass limit of the form factor beyond two loops assuming, of course, the findings of Ref. [6] extend to three loops. Combining the results in [18,49] one can cast the three-loop result in terms of only one unknown constant  $K_3$  (note that the function  $G_3$  is known from the massless form factor [21,58]).

The explicit form given in Eq. (52) is among the main results of this work. These anomalous dimensions provide explicit corrections to the form proposed in Ref. [59], which was based on generalizing the proportionality between the one- and two-loop massive anomalous dimension matrices of the massless case [13]. The results of the present work as well as of Refs. [6–8] provide the necessary corrections, which arise even for the special kinematics close to absolute threshold.

## VI. DISCUSSION AND OUTLOOK

In the present paper we have extended the formalism for the resummation of soft gluon logarithms in cross sections with massive partons to the NNLL level. A central role in our construction is played by the massive two-loop soft anomalous dimension matrix for processes with  $n \geq 4$  colored hard partons. In this paper we have presented the most general form of the so-called  $2E$  (dipole) contributions. Combined with the results of Ref. [6] this allows resummation in observables with special kinematics, like the total inclusive cross section for hadroproduction of a pair of heavy flavors.

In our discussion we have detailed the relation between the soft function in an observable and the soft function in the corresponding factorized (virtual) amplitude. Following [5], we have shown how the two are closely related for generic processes, and that the infrared poles of the amplitudes can be used to specify properties of the cross sections near partonic threshold, particularly in the form factor scheme defined and applied here.

We have also explained how to construct the various jet factors needed for the completion of our threshold resummation, and have used their process independence to derive initial-state partonic jets from the Drell-Yan vector production process. We have also used heuristic arguments to identify and construct natural jet factors needed for inclusive observables, like the total cross section for heavy pair production. Factorized jet functions, although not strictly necessary, provide a form that can be extended to cross sections at measured pair mass, even far above absolute threshold.

The most phenomenologically relevant application of our work is the total cross section for heavy pair production at hadron colliders. In this paper we have shown how to derive this quantity from resummed cross sections at fixed scattering kinematics. We have also given the exact result for the two-loop anomalous dimensions controlling the exponentiation of the NNLL terms in the cross section, and we have verified that even above threshold the part of the two-loop soft anomalous dimension constructed here is adequate to determine exactly the pole structure of the two-loop color-averaged amplitudes for top production through light quark annihilation.

Our result provides not only the result for the resummed logs to NNLL but also a framework for studying the higher order effects in this observable and the associated theoretical uncertainties. We will provide a detailed numerical analysis in a dedicated publication.

The formalism we have presented here can also be applied to more differential observables in heavy flavor production at hadron colliders, including cross sections at fixed rapidity and pair mass. To complete such studies one will, however, require explicit results, whether analytic or numerical, for the  $3E$ -type contributions to the anomalous dimension matrix involving two massive partons.

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## APPENDIX: COLOR BASES

In this appendix we present calculations of the one-loop anomalous dimension in singlet-octet basis, and the evaluation of the two-loop expression of Eq. (36).

### 1. One-loop results in singlet-octet basis

We work out the general result for the one-loop soft anomalous dimension matrices in the form factor scheme for the two reactions:

$$q(p_1)\bar{q}(p_2) \rightarrow Q(p_3)\bar{Q}(p_4) \quad (\text{A1})$$

$$g(p_1)g(p_2) \rightarrow Q(p_3)\bar{Q}(p_4) \quad (\text{A2})$$

where  $p_1^2 = p_2^2 = 0$ ;  $p_3^2 = p_4^2 = m^2$ . We define the invariants  $s = (p_1 + p_2)^2$ ,  $t_1 = (p_1 - p_3)^2 - m^2 = (p_2 - p_4)^2 - m^2$ ,  $u_1 = (p_1 - p_4)^2 - m^2 = (p_2 - p_3)^2 - m^2$ . In the massive case  $\sigma_{34} = 2p_3 \cdot p_4 = s - 2m^2 \neq s$ .

We first consider the reaction (A1). To evaluate the color matrices  $T_i \cdot T_j$  a color basis needs to be specified. The simplest one is:

$$c_1 = \delta_{12}\delta_{34}, \quad c_2 = \delta_{13}\delta_{24}, \quad (\text{A3})$$

There are six combinations of the indices  $(i, j)$  that need to be considered. Only three of them are different. Denoting these three color matrices by  $\hat{\Gamma}_S$ ,  $\hat{\Gamma}_T$  and  $\hat{\Gamma}_U$  defined through  $\hat{\Gamma}_S = T_1 \cdot T_2$ , etc., we get:

$$\begin{aligned} \Gamma_S^{(1)} &= 2T\hat{\Gamma}_T + 2U\hat{\Gamma}_U + (S_0 + S_m + P)\hat{\Gamma}_S \\ &= \begin{pmatrix} \Gamma_{11}^{(1)} & \Gamma_{12}^{(1)} \\ \Gamma_{21}^{(1)} & \Gamma_{22}^{(1)} \end{pmatrix}, \end{aligned}$$

where:

$$\begin{aligned} \Gamma_{11}^{(1)} &= (2U - 2T - S_0 - S_m - P)C_F + (T - U)C_A, \\ \Gamma_{12}^{(1)} &= \frac{1}{2}(2U - S_0 - S_m - P), \quad \Gamma_{21}^{(1)} = U - T, \\ \Gamma_{22}^{(1)} &= (2U - 2T - S_0 - S_m - P)C_F \\ &\quad - (2U - S_0 - S_m - P)\frac{C_A}{2}. \end{aligned} \quad (\text{A4})$$

The individual matrices  $\hat{\Gamma}_S$ ,  $\hat{\Gamma}_T$  and  $\hat{\Gamma}_U$  can be easily read off from the above equations. We have also included an overall minus sign in  $\hat{\Gamma}_S$ ,  $\hat{\Gamma}_T$  as follows from the sign conventions for the color generators of Ref. [13,60]: a generator  $T_i$  is multiplied by  $-1$  if it is inserted in a line that represents incoming quark or gluon or outgoing antiquark.

The expressions for the velocity factors  $U$ ,  $T$ ,  $S_0$ ,  $S_m$ , and  $P$  follow directly from Eq. (29):

$$\begin{aligned} U &= \ln\left(-\frac{\mu^2}{u_1}\right), \quad T = \ln\left(-\frac{\mu^2}{t_1}\right), \\ S_0 &= \ln\left(\frac{\mu^2}{s}\right) + i\pi, \quad S_m = \ln\left(\frac{\mu^2}{s - 2m^2}\right) + i\pi, \quad (\text{A5}) \\ P &= P_{ij}^{(1)}\left(x_{ij} = -\frac{1 - \beta}{1 + \beta} + i\varepsilon, s \geq 4m^2\right). \end{aligned}$$

We have labeled these functions according to their respective channel  $(s, t, u)$ , and as to whether they refer to a massless or massive dipole. The function  $P$  collects all power corrections in the mass, i.e. in the massless case  $S_m = S_0$ ,  $P = 0$ .

For physical applications to heavy flavor hadroproduction one chooses the  $s$ -channel singlet-octet color basis:

$$v_1 = c_1, \quad v_8 = -\frac{1}{2N}c_1 + \frac{1}{2}c_2. \quad (\text{A6})$$

The change of basis for the anomalous dimension matrix in Eq. (A4) (or for any one of  $\hat{\Gamma}_S$ ,  $\hat{\Gamma}_T$ ,  $\hat{\Gamma}_U$ ) is:

$$\Gamma_S^{(1),\text{S.O.}} = \mathbf{R}^{-1} \cdot \Gamma_S^{(1)} \cdot \mathbf{R}, \quad (\text{A7})$$

where the transformation matrix  $\mathbf{R}$  reads:

$$\mathbf{R} = \begin{pmatrix} 1 & -\frac{1}{2N} \\ 0 & \frac{1}{2} \end{pmatrix}, \quad \mathbf{R}^{-1} = \begin{pmatrix} 1 & \frac{1}{N} \\ 0 & 2 \end{pmatrix}. \quad (\text{A8})$$

The matrix elements of the matrix  $\Gamma_S^{(1),\text{S.O.}}$  read:

$$\begin{aligned} \Gamma_{11}^{(1),\text{S.O.}} &= -(S_0 + S_m + P)C_F, \\ \Gamma_{12}^{(1),\text{S.O.}} &= (U - T)\frac{C_F}{C_A}, \quad \Gamma_{21}^{(1),\text{S.O.}} = 2(U - T), \\ \Gamma_{22}^{(1),\text{S.O.}} &= (4U - 4T - S_0 - S_m - P)C_F \\ &\quad - (4U - 2T - S_0 - S_m - P)\frac{C_A}{2}. \end{aligned} \quad (\text{A9})$$

Rearranging the above expressions we arrive at the following expression for the anomalous dimension matrix  $\Gamma_S^{(1),\text{S.O.}}$  in the singlet-octet color basis:

$$\begin{aligned} \Gamma_{11}^{(1),\text{S.O.}} &= \left[ 2\ln\left(\frac{m^2}{\mu^2}\right) - \ln\left(\frac{m^2}{s}\right) - L_\beta - i\pi \right] C_F, \\ \Gamma_{12}^{(1),\text{S.O.}} &= \ln\left(\frac{t_1}{u_1}\right)\frac{C_F}{C_A}, \quad \Gamma_{21}^{(1),\text{S.O.}} = 2\ln\left(\frac{t_1}{u_1}\right), \\ \Gamma_{22}^{(1),\text{S.O.}} &= \left[ 4\ln\left(\frac{t_1}{u_1}\right) + 2\ln\left(\frac{m^2}{\mu^2}\right) - \ln\left(\frac{m^2}{s}\right) - L_\beta - i\pi \right] C_F \\ &\quad - \left[ 2\ln\left(\frac{t_1}{u_1}\right) - 2\ln\left(-\frac{u_1}{s}\right) + \ln\left(\frac{m^2}{s}\right) \right. \\ &\quad \left. - L_\beta - i\pi \right] \frac{C_A}{2}. \end{aligned} \quad (\text{A10})$$

We have kept the traditional notations and defined:

$$L_\beta = \frac{1 + \beta^2}{2\beta} \left( \ln\left(\frac{1 - \beta}{1 + \beta}\right) + i\pi \right). \quad (\text{A11})$$

The result for the anomalous dimension matrix in  $\Gamma_S^{(1),\text{S.O.}}$  in Eq. (A10) agrees with the one derived first in Ref. [5] provided we add to the above result (A10) the term  $(-\ln(m^2/\mu^2) - 1)C_F\mathbf{1}$  and set  $\mu^2 = s$ . The addition of this (color diagonal) term corresponds to working in a scheme where the two jet factors for the heavy quark and antiquark are absorbed into the soft function (see the discussion in Sec. V).

Finally, we give the expression for the real part of the anomalous dimension matrix  $\Gamma_S^{(1),\text{S.O.}}$  at absolute threshold.

To that end we set  $u_1 = t_1 = -s/2$  as well as  $\ln(\mu^2/s) = 0$ . Up to corrections  $\sim \mathcal{O}(\beta)$  the result reads:

$$\begin{aligned} \text{Re}\Gamma_S^{(1),\text{S.O.}} &= C_F \left[ \ln\left(\frac{m^2}{\mu^2}\right) + 1 \right] \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \frac{C_A}{2} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \\ &= -\Gamma_{\text{incl}}^{(1)} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \frac{C_A}{2} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \end{aligned} \quad (\text{A12})$$

## 2. Evaluation of Eq. (36)

The threshold limit of the two-loop matrix  $\Gamma_S^{(2)}$  in the basis (A6) can be easily derived from Eq. (36) by using that

$$T_3 \cdot T_4 = \hat{\Gamma}_S^{\text{S.O.}} = \begin{pmatrix} -C_F & 0 \\ 0 & -C_F + \frac{C_A}{2} \end{pmatrix}. \quad (\text{A13})$$

Up to corrections  $\sim \mathcal{O}(\beta)$ , the result for  $\Gamma_S^{(2)}$  reads:

$$\begin{aligned} \text{Re}\Gamma_S^{(2),\text{S.O.}} &= -\Gamma_{\text{incl}}^{(2)} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \left( \frac{C_A K}{4} + \frac{\zeta_3 - 1}{4} C_A^2 \right) \\ &\quad \times \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \end{aligned} \quad (\text{A14})$$

where  $\Gamma_{\text{incl}}^{(1)}$  and  $\Gamma_{\text{incl}}^{(2)}$  are given in Eq. (41).

The calculation of the gluon fusion reaction Eq. (A2) can be done in the same way as in the quark-antiquark annihilation one described above. The appropriate  $s$ -channel singlet-octet color basis is:

$$v_1 = \delta_{12}\delta_{34}, \quad v_8^s = d^{12c}T_{34}^c, \quad v_8^a = if^{12c}T_{34}^c. \quad (\text{A15})$$

A direct calculation shows that in the limit  $\beta \rightarrow 0$  the matrices  $T_3 \cdot T_4$ ,  $\text{Re}\Gamma_S^{(1),\text{S.O.}}$  and  $\text{Re}\Gamma_S^{(2),\text{S.O.}}$  for the gluon fusion reaction can be obtained from the corresponding matrices in the quark-antiquark initiated one Eqs. (A13), (A12), and (A14) with the help of the simple replacements:

$$\mathbf{1}_{2 \times 2} \rightarrow \mathbf{1}_{3 \times 3} \quad \text{and} \quad \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \rightarrow \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (\text{A16})$$

The results of Ref. [61] can be used to simplify the calculations.

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