Soft-gluon resummation for boosted top-quark production at hadron colliders

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We investigate the production of highly energetic top-quark pairs at hadron colliders, focusing on the case where the invariant mass of the pair is much larger than the mass of the top quark. In particular, we set up a factorization formalism appropriate for describing the differential partonic cross section in the double soft and small-mass limit, and explain how to resum simultaneously logarithmic corrections arising from soft gluon emission and from the ratio of the pair-invariant mass to that of the top quark to next-to-next-to-leading logarithmic accuracy. We explore the implications of our results on approximate next-to-next-to-leading order formulas for the differential cross section in the soft limit, pointing out that they offer a simplified calculational procedure for determining the currently unknown delta-function terms in the limit of high invariant mass.

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I. INTRODUCTION

Top-quark pair production plays an important role in the physics programs of hadron colliders such as the Tevatron and the LHC. While much information about the top quark is already available, its high production rate at the LHC will eventually bring studies of its properties into the realm of precision physics. An especially useful observable is the differential cross section at large values of the top-pair invariant mass M. Many models of physics beyond the Standard Model predict the existence of new particles which decay into energetic top quarks and whose characteristic signal would be either resonant bumps or more subtle distortions in the high invariant-mass region of the differential distribution. In fact, Tevatron measurements of the forward-backward asymmetry at high values of the pair invariant mass may already hint at the existence of such particles [1,2]. Therefore, precision calculations of the pair invariant-mass distribution within the Standard Model are well motivated.

The starting point for any study of two-particle inclusive differential cross sections such as the pair invariant-mass distribution is the next-to-leading order (NLO) calculations carried out roughly two decades ago [3]. Recently, these have been supplemented with soft-gluon resummation at next-to-next-to-leading logarithmic (NNLL) accuracy in [4,5], building on the next-to-leading logarithmic (NLL) results of [6,7]. While such resummed calculations contain what are argued to be the dominant perturbative corrections at next-to-next-to-leading order (NNLO) and beyond, they suffer from two potential shortcomings. First, while they fully determine the coefficients of a subset of logarithmic plus-distribution corrections which become large in the soft limit $z = M^2/\hat{s} \to 1$, with $\sqrt{\hat{s}}$ the partonic center-of-mass energy, they do not fully determine the delta-function corrections in this limit at NNLO. The numerical contribution of these unknown coefficients as well as less singular terms in the soft limit are typically estimated through the method of scale variations, but this is by no means a fail-safe technique and additional information about the structure of these terms is valuable. Second, while [5] uses the parametric counting $M \sim m_t$, when the top quarks are truly very boosted this counting breaks down. One must assume instead that $M \gg m_t$, and recognize that resummed perturbation theory should also take into account powers of mass logarithms of the ratio m_t/M.

The primary aim of this work is to develop the theoretical framework needed to describe the invariant-mass distribution in the double soft and small-mass limit, and to explore some of its implications for perturbative predictions for the large-M distribution. The basic idea behind our approach is to weave together current understanding of factorization in either the small-mass or the soft limit into a unified description encompassing both. The first component is the factorization of partonic cross sections for highly boosted heavy-quark production worked out in [8]. In the case at hand, where $m_t \ll M$, the results of that work imply that the partonic cross section can be factorized into a convolution of two functions: the cross section for *massless* quark production, and a convolution of perturbative fragmentation functions for each of the heavy quarks. Given this form of the cross section for the small-mass limit, it is then an easy matter to perform the additional layer of factorization for the soft limit on the component parts. On the one hand, the massless partonic cross section in this limit can be factorized into a product of soft and hard functions using the techniques from [6], and on the other hand, the fragmentation function can be factorized into a product of collinear and soft-collinear functions using the results of [9–13]. A fully resummed cross section appropriate for both limits is then obtained by deriving and solving the renormalization-group (RG) evolution equations for the different functions separately. The anomalous dimensions appearing in the RG equations are known to the level sufficient for resummation of both mass and soft logarithms to NNLL accuracy. As simple and obvious as this approach is, it has yet to be fully worked out for any particular observable in top-quark pair production at hadron collider experiments.

This formalism for the simultaneous resummation of soft and mass logarithms in the invariant-mass distribution is interesting in its own right. Moreover, with use of a proper matching procedure, it provides supplemental information to the current state-of-the-art predictions based on soft-gluon resummation with the counting $m_t \sim M$ [5]. Particularly important in this regard is its use as a tool to calculate, up to easily quantifiable power corrections in m_t/M, the full NNLO corrections to the massive hard and soft functions. Together, these pieces determine the coefficient of the delta-function coefficient in the fixed-order expansion at NNLO, a missing piece in currently available "approximate NNLO" formulas for generic values of the top-quark mass. Using our factorization formula for the double soft and small-mass limit, we can calculate the pieces of the NNLO delta-function correction enhanced by logarithms of the ratio m_t/M. Furthermore, using the explicit NNLO results for the heavy-quark fragmentation function [14] and the virtual corrections to massless $q\bar{q} \to q'\bar{q}'$ [15] and $gg \to q\bar{q}$ [16] scattering, we can very nearly determine the piece of the delta-function coefficients which is constant in the limit $m_t/M \to 0$. The missing piece is the NNLO soft function for massless partons, related to double real emission for $gg \to q\bar{q}$ and $q\bar{q} \to q\bar{q}$ scattering in the soft limit. We do not calculate this function here, but plan to return to it in future work. While these delta-function pieces of the NNLO partonic cross section are of N^{3}LL in the counting of soft-gluon resummation, including them can only make the predictions more precise and potentially strengthen the arguments in favor of the logarithmic counting underlying approximate NNLO formulas. This is currently an open point in soft-gluon resummation for the invariant-mass distribution, where the assumed dominance of logarithmic corrections is justified mainly through numerical studies at NLO and arguments based on dynamical threshold enhancement [17].

The remainder of the paper is organized as follows. First, in Sec. II, we derive a factorization formula for the partonic cross section valid in the double small-mass and soft limit. This fixed-order expression contains large logarithms for any choice of the factorization scale. We deal with this in Sec. III by deriving and solving the RG equations for the component functions of the factorization formula, presenting in addition explicit perturbative results for their fixed-order expansions. In Sec. IV we combine those results into an expression for the resummed partonic cross section at NNLL in perturbation theory, and discuss different matching procedures needed to take into account power-suppressed terms away from the double small-mass and soft limit. In that section we also discuss approximate NNLO implementations of the NNLL formula. Finally, in Sec. V, we make preliminary explorations into phenomenological consequences of our results. We conclude in Sec. VI.

II. FACTORIZATION IN THE SOFT AND SMALL-MASS LIMITS

We study the top-quark pair production process

$$N_1(P_1) + N_2(P_2) \to t(p_3) + \bar{t}(p_4) + X(p_X), \qquad (1)$$

where N_1 and N_2 are the colliding protons (or proton-antiproton pair), X is an inclusive hadronic state, and the top quarks are treated as on-shell particles. Two partonic channels contribute at lowest order in perturbation theory: the quark annihilation channel

$$q(p_1) + \bar{q}(p_2) \to t(p_3) + \bar{t}(p_4), \qquad (2)$$

and the gluon fusion channel

$$g(p_1) + g(p_2) \to t(p_3) + \bar{t}(p_4). \qquad (3)$$

The momenta of the incoming partons are related to the hadron momenta by the relation $p_i = x_i P_i$ $(i = 1, 2)$. The relevant Mandelstam invariants are defined as

$$\begin{aligned} s &= (P_1 + P_2)^2, \qquad \hat{s} = (p_1 + p_2)^2, \\ M^2 &= (p_3 + p_4)^2, \qquad t_1 = (p_1 - p_3)^2 - m_t^2, \\ u_1 &= (p_2 - p_3)^2 - m_t^2. \end{aligned} \qquad (4)$$

In order to describe the invariant-mass distribution near the partonic threshold, it is convenient to introduce the following variables:

$$\begin{aligned} z &= \frac{M^2}{\hat{s}}, \qquad \tau = \frac{M^2}{s}, \\ \beta_t &= \sqrt{1 - \frac{4m_t^2}{M^2}}, \qquad \beta = \sqrt{1 - \frac{4m_t^2}{\hat{s}}}. \end{aligned} \qquad (5)$$

The quantity β_t is the 3-velocity of the top quarks in the $t\bar{t}$ rest frame. In the soft limit $z \to 1$, one has $\beta \to \beta_t$. Moreover, in that limit the scattering angle θ is related to the Mandelstam variables according to

$$t_1 = -\frac{M^2}{2}(1 - \beta_t \cos\theta), \qquad u_1 = -\frac{M^2}{2}(1 + \beta_t \cos\theta), \qquad (6)$$

and $M^2 + t_1 + u_1 = 0$ can be used to eliminate u_1 as an independent variable.

We will be interested in the double differential cross section with respect to the invariant mass of the top-quark pair and the scattering angle θ in the parton center-of-mass frame. According to factorization in QCD, the double differential cross section can be written as a convolution of a partonic cross section with parton distribution functions (PDFs). We write this as

$$\frac{d^2\sigma}{dM\,d\cos\theta} = \frac{8\pi\beta_t}{3sM}\sum_{i,j}\int_\tau^1 \frac{dz}{z} ff_{ij}(\tau/z,\mu_f) \times C_{ij}(z,M,m_t,\cos\theta,\mu_f), \tag{7}$$

where μ_f is the factorization scale. The parton luminosity functions ff_{ij} are defined as a convolution of PDFs:

$$ff_{ij}(y,\mu_f) = f_{i/N_1}(y,\mu_f)\otimes f_{j/N_2}(y,\mu_f). \tag{8}$$

Here and throughout the paper the symbol $\otimes$ denotes the following convolution between two functions

$$f(z)\otimes g(z) = \int_z^1 \frac{dx}{x} f(x) g(z/x). \tag{9}$$

When there are several arguments in the functions f and g, the convolution is always over the first argument. As described in more detail below, we choose to define the PDFs with $n_l = 5$ active light flavors, so that all physics associated with the scale of the top-quark is absorbed into the perturbative coefficient functions C_{ij}. These coefficient functions are proportional to differential partonic cross sections. Our aim is to study the factorization properties of these partonic cross sections in the double soft and small-mass limit, where $(1-z)\ll 1$ and $m_t \ll M$. (More precisely, we work in the limit where the Mandelstam variables $\hat{s}$, t_1, $u_1 \gg m_t^2$.) Our strategy is to first discuss the soft and small-mass limits separately, and then combine them into a single formula which is true for both limits simultaneously.

Factorization of differential partonic cross sections in the soft limit has been studied in [5,6,18–26]. In the soft limit $z\to 1$, the partonic cross section can be factorized into a hard function and a soft function according to

$$C_{ij}(z,M,m_t,\cos\theta,\mu_f) = \mathrm{Tr}[\boldsymbol{H}^m_{ij}(M,m_t,t_1,\mu_f)\boldsymbol{S}^m_{ij}(\sqrt{\hat{s}}(1-z),m_t,t_1,\mu_f)] + \mathcal{O}(1-z), \tag{10}$$

where we have used that in the soft limit dependence on the scattering angle can be expressed in terms of t_1, see (6). The superscript m on the hard function $\boldsymbol{H}^m_{ij}$ and the soft function $\boldsymbol{S}^m_{ij}$ indicates that they are computed with finite top-quark mass, as opposed to the massless hard and soft functions introduced below. Both of these functions are matrices in the space of color-singlet operators for Born-level production. The hard function is related to virtual corrections to the two-to-two scattering processes $q\bar{q}(gg)\to t\bar{t}$. The soft function is related to real emissions in the soft limit, or more precisely to the vacuum expectation value of a Wilson-loop operator built from time and light-like Wilson lines associated with soft emissions from the heavy and light quarks. Note that in this limit, we only need to consider $ij = q\bar{q}$, gg, since the qg channel is suppressed by powers of $(1-z)$.

Factorization of differential partonic cross sections for heavy-quark production in the small-mass limit was considered in [8].[1] It was shown that partonic cross sections in this limit can be factorized into a product of massless cross sections with perturbatively calculable heavy-quark fragmentation functions. Generically, for a cross section differential in the energy fraction $z = E/E_{\max}$ of the top quark, this factorization is written as (see, for instance, [14])

$$\frac{d\sigma_t}{dz}(z,m_t,\mu) = \sum_a \int_z^1 \frac{dx}{x}\frac{d\tilde{\sigma}_a}{dx}(x,m_t,\mu) D^{(n_l+n_h)}_{a/t}\left(\frac{z}{x},m_t,\mu\right), \tag{11}$$

where $d\tilde{\sigma}_a/dx$ is the $\overline{\mathrm{MS}}$-renormalized differential cross section for the production of a massless parton a, and $D^{(n_f)}_{a/t}$ is the heavy-quark fragmentation function defined using an α_s with n_f active flavors. The sum over the massless partons labeled by a includes the case $a = t$, and the heavy quark is considered massless in the calculation of $d\tilde{\sigma}_t$. Much as the PDFs describe radiation collinear to initial-state partons, the heavy-quark fragmentation functions describe radiation collinear to the energetic final-state heavy quarks. The heavy-quark fragmentation functions are however perturbatively calculable, since the mass of the top quark serves as a collinear regulator.

In the case of the invariant-mass distribution in top-quark pair production at hadron colliders, we need to modify the generic formula (11) in several ways. First, since this observable contains information about both the top and the anti-top quark, we need a fragmentation function for each of them. Second, we must introduce heavy-flavor coefficients related to matching six-flavor PDFs onto five-flavor ones, which induces an additional source of m_t-dependence into the formula. Finally, although not strictly necessary, we will follow [13] and also perform such a matching for the fragmentation functions. The matching relations between the PDFs and fragmentation functions in the $n_l + n_h$- and n_l-flavor theories are

$$D^{(n_l+n_h)}_{a/t}(z,m_t,\mu_f) = C_{a/t}(z,m_t,\mu_f)\otimes D^{(n_l)}_{t/t}(z,m_t,\mu_f), \tag{12}$$

$$ff^{(n_l+n_h)}_{ij}(z,m_t,\mu_f) = C^{ij}_{ff}(z,m_t,\mu_f)\otimes ff^{(n_l)}_{ij}(z,\mu_f). \tag{13}$$

[1] We note that for the *total* cross section, potentially large corrections in the limit $\hat{s}\gg m_t^2$ limit have been considered in, e.g. [27,28], and that NNLO corrections within this framework were recently calculated in [29]. These results for the total cross section are however not applicable to the differential cross section in the pair invariant mass considered here.

The heavy-flavor matching coefficients $C_{a/t}$ and C_{ff}^{ij} on the right-hand side of the above equation are proportional to powers of $n_h = 1$. They are obtained by comparing partonic matrix elements with and without the top quark as an active flavor, and are known to NNLO in fixed-order for both the fragmentation functions [13] and the parton luminosity functions [30]. We will encounter them again in Sec. IV, when we discuss the RG running of massless coefficient functions to scales below the flavor threshold at $\mu_t \sim m_t$.

Taking these points into account, the factorization formula for the coefficient function (7) in the small-mass limit reads[2]

$$\begin{aligned} C_{ij}(z, M, m_t, \cos\theta, \mu_f) = \sum_{a,b} & C_{ij}^{ab}(z, M, t_1, \mu_f) \\ & \otimes \mathbb{D}_{ab}^{(n_l)}(z, m_t, \mu_f) \\ & \otimes C_{a/t}(z, m_t, \mu_f) \\ & \otimes C_{b/\bar{t}}(z, m_t, \mu_f) \\ & \otimes C_{ff}(z, m_t, \mu_f) + \mathcal{O}\left(\frac{m_t}{M}\right), \end{aligned} \quad (14)$$

where the sum is over all parton species $a,\ b \in \{t, \bar{t}, q, \bar{q}, g\}$. The functions C_{ij}^{ab} are the partonic cross sections obtained from the massless scattering process $ij \to ab + \hat{X}$, where $\hat{X}$ indicates additional final-state partons. The objects $\mathbb{D}_{ab}^{(n_l)}$ are defined as the following convolution of heavy-quark fragmentation functions:

$$\mathbb{D}_{ab}^{(n_l)}(z, m_t, \mu_f) = D_{a/t}^{(n_l)}(z, m_t, \mu_f) \otimes D_{b/\bar{t}}^{(n_l)}(z, m_t, \mu_f). \quad (15)$$

This convolution of heavy-quark fragmentation functions is completely analogous to that defining the parton luminosities in (8). It arises after generalizing (11) to a two-fold convolution and performing a change of variables.

We are now ready to discuss the joint limit $z \to 1$ and $m_t/M \to 0$, which is the main theme of this paper. The key point is that these two limits are independent and commutative, so that we can take them one-by-one in any order and obtain the same result. We choose to start from the factorization formula (14) for the small-mass limit, and then study the behavior of its component parts in the limit $z \to 1$. We thus discuss the factorization of the massless coefficient functions and the fragmentation function in the soft limit. The alternate method of starting from the factorization formula (10) for the soft limit and then studying the factorization of its component parts in the small-mass limit is discussed in Appendix A.

We first deal with the massless coefficient function C_{ij}^{ab}. To factorize it in the soft limit, we observe that nothing in the derivation of factorization for the massive coefficient function (10) makes reference to the mass of the top-quark. Therefore, the form of factorization for the massless coefficient function is exactly the same. The result is thus

$$\begin{aligned} C_{ij}^{t\bar{t}}(z, M, t_1, \mu_f) = \mathrm{Tr}[&\boldsymbol{H}_{ij}(M, t_1, \mu_f)\boldsymbol{S}_{ij}(\sqrt{\hat{s}}(1-z), t_1, \mu_f)] \\ &+ \mathcal{O}(1-z). \end{aligned} \quad (16)$$

We have used that only $a = t$ contributes to (12) at leading power in $(1-z)$. The hard function $\boldsymbol{H}_{ij}$ is obtained from virtual corrections to two-to-two scattering with massless top quarks, and the soft function $\boldsymbol{S}_{ij}$ involves only light-like Wilson lines related to real emission from massless partons. The top quark is treated as massless in both the external states and in internal fermion loops, so both the hard and soft function are defined in a theory with six active massless flavors.

The factorization of the fragmentation functions in the $z \to 1$ limit was explained in [9–12], and also within an effective field-theory framework in [13]. The main result of those works is that after the matching onto the n_l-flavor theory as in (12), the fragmentation function factorizes into a product of two functions: one depending on the collinear scale m_t, and the other on the soft-collinear scale $m_t(1-z)$. We write this factorization as

$$D_{t/t}^{(n_l)}(z, m_t, \mu_f) = C_D(m_t, \mu_f) S_D(m_t(1-z), \mu_f) + \mathcal{O}(1-z). \quad (17)$$

The fragmentation of $\bar{t}$ to $\bar{t}$ follows the same factorization with the same coefficient functions. The soft function S_D is related to soft-collinear emission and is equivalent to the partonic shape-function appearing in B-meson decays [12,13]. The matching coefficient C_D is independent of z and is a simple function related to virtual corrections.

Combining all of the information above, the factorization formula for the partonic cross sections in the joint soft and small-mass limit is

$$\begin{aligned} &C_{ij}(z, M, m_t, \cos\theta, \mu_f) \\ &\quad = C_D^2(m_t, \mu_f)\mathrm{Tr}[\boldsymbol{H}_{ij}(M, t_1, \mu_f)\boldsymbol{S}_{ij}(\sqrt{\hat{s}}(1-z), t_1, \mu_f)] \\ &\qquad \otimes C_{ff}^{ij}(z, m_t, \mu_f) \otimes C_{t/t}(z, m_t, \mu_f) \otimes C_{t/t}(z, m_t, \mu_f) \\ &\qquad \otimes S_D(m_t(1-z), \mu_f) \otimes S_D(m_t(1-z), \mu_f) \\ &\qquad + \mathcal{O}(1-z) + \mathcal{O}\left(\frac{m_t}{M}\right). \end{aligned} \quad (18)$$

The factorization formula (18) is the central result of this section. In the limit in which it is derived, any choice of μ_f

[2]We have used a slight abuse of notation and expressed the dependence on the scattering angle in terms of t_1, which is in general only possible in the soft limit. In converting to the scattering angle, we keep the exact mass dependence in t_1 according to (6), otherwise a t-channel singularity emerges upon integration over θ.

generates large logarithms in the soft or small-mass limits. We deal with this problem in the next section using RG techniques. In deriving and solving the RG equations it will be useful to introduce the Laplace-transformed functions

$$\begin{aligned}
\tilde{c}_{ij}\left(N,M,m_t,\cos\theta,\mu_f\right) &= \int_0^\infty d\xi e^{-\xi N} C_{ij}(z,M,m_t,\cos\theta,\mu_f),\\
\tilde{\boldsymbol{s}}_{ij}\left(\ln\frac{M^2}{\bar{N}^2\mu_f^2},t_1,\mu_f\right) &= \int_0^\infty d\xi e^{-\xi N} \boldsymbol{S}_{ij}(\sqrt{\hat{s}}(1-z),t_1,\mu_f),\\
\tilde{c}_t^{ij}\left(\ln\frac{1}{\bar{N}^2},m_t,\mu_f\right) &= \int_0^\infty d\xi e^{-\xi N} C_{ff}^{ij}(z,m_t,\mu_f)\\
&\quad \otimes C_{t/t}(z,m_t,\mu_f)\otimes C_{t/t}(z,m_t,\mu_f),\\
\tilde{s}_D\left(\ln\frac{m_t}{\bar{N}\mu_f},\mu_f\right) &= \int_0^\infty d\xi e^{-\xi N} S_D(m_t(1-z),\mu_f),
\end{aligned} \tag{19}$$

where $\xi = (1-z)/\sqrt{z}$ and $\bar{N} = Ne^{\gamma_E}$. In Laplace space, the factorization formula becomes a simple product of the different functions and reads

$$\begin{aligned}
&\tilde{c}_{ij}(N, M, m_t, \cos\theta, \mu_f)\\
&\quad = C_D^2(m_t, \mu_f)\mathrm{Tr}\left[\boldsymbol{H}_{ij}(M, t_1, \mu_f)\tilde{\boldsymbol{s}}_{ij}\left(\ln\frac{M^2}{\bar{N}^2\mu_f^2}, t_1, \mu_f\right)\right]\\
&\qquad \times \tilde{c}_t^{ij}\left(\ln\frac{1}{\bar{N}^2}, m_t, \mu_f\right)\tilde{s}_D^2\left(\ln\frac{m_t}{\bar{N}\mu_f}, \mu_f\right)\\
&\qquad + \mathcal{O}\left(\frac{1}{N}\right) + \mathcal{O}\left(\frac{m_t}{M}\right).
\end{aligned} \tag{20}$$

III. THE MATCHING FUNCTIONS: FIXED-ORDER EXPANSIONS AND RG EVOLUTION

The component parts of the factorization formula (18) can be viewed as matching functions in effective theory. In this section we explain the one-scale calculations needed to extract the fixed-order expansions of these matching functions, present their RG equations and the solutions thereof, and give the ingredients needed to evaluate these RG-improved matching coefficients at NNLL. While such NNLL calculations require only the NLO perturbative expansion of the matching coefficients, we also collect all current knowledge at NNLO, part of which we will use in our numerical analysis later on.

A. Hard function

The hard function is related to virtual corrections to the two-to-two scattering processes underlying Born-level production. The method for calculating the hard-function matrix for the counting $M \sim m_t$ in fixed-order perturbation theory was described in detail in [5], where results valid to NLO were given. This boiled down to calculating color-decomposed UV-renormalized on-shell scattering amplitudes and subtracting poles in the $4 - d = 2\epsilon \to 0$ limit using an IR renormalization factor.

There are in fact two ways to calculate the hard function in the massless case. The first is to set $m_t = 0$ at the start of the calculation and follow the same procedure as for the massive case. Then the UV-renormalized scattering amplitudes and the IR renormalization factors change compared to the massive case, but the method for extracting the hard function is exactly the same. The second way is to Taylor-expand the massive result [5] in the limit $m_t \to 0$ and then convert the result to the massless case using the relation between massive and massless amplitudes in the small-mass limit derived in [31]. We have calculated the NLO hard function using both methods and confirmed that they agree. This NLO result for massless scattering is not new: it is actually a special case of the more general results for four-parton scattering given in [32], using the one-loop calculations of [33]. We have checked that we reproduce those results using the procedure described below.

As opposed to the massive case, where only a limited set of NNLO virtual corrections have been calculated [34–41], both the one-loop times one-loop and two-loop times Born interference terms are known for the case of massless two-to-two scattering [15,42–44]. These results are implicitly summed over colors and cannot be used to extract the hard matrix directly, on the other hand they *can* be used to extract the contribution of the NNLO hard function to the approximate NNLO formulas covered below. Although we do not go through this straightforward but tedious exercise here, it is an important point that all of the diagrammatic calculations are in place.

In order to give explicit results valid to NLO we define expansion coefficients of the hard function $\boldsymbol{H}$ as

$$\boldsymbol{H} = \alpha_s^2\frac{3}{8d_R}\left[\boldsymbol{H}^{(0)} + \frac{\alpha_s}{4\pi}\boldsymbol{H}^{(1)} + \left(\frac{\alpha_s}{4\pi}\right)^2\boldsymbol{H}^{(2)} + \cdots\right], \tag{21}$$

where $d_R = N_c$ in the quark annihilation channel and $d_R = N_c^2 - 1$ in the gluon fusion channel, with $N_c = 3$ colors in QCD. The LO result $\boldsymbol{H}^{(0)}$ is trivially obtained from the formulas in [5], which is regular in the limit $m_t \to 0$. For the $q\bar{q}$ channel we have

$$\boldsymbol{H}_{q\bar{q}}^{(0)} = \begin{pmatrix} 0 & 0 \\ 0 & 2 \end{pmatrix}\frac{t_1^2 + u_1^2}{M^2}, \tag{22}$$

and the result for the gg channel is

$$\boldsymbol{H}_{gg}^{(0)} = \begin{pmatrix} \frac{1}{N_c^2} & \frac{1}{N_c}\frac{t_1-u_1}{M^2} & \frac{1}{N_c} \\ \frac{1}{N_c}\frac{t_1-u_1}{M^2} & \frac{(t_1-u_1)^2}{M^4} & \frac{t_1-u_1}{M^2} \\ \frac{1}{N_c} & \frac{t_1-u_1}{M^2} & 1 \end{pmatrix}\frac{t_1^2 + u_1^2}{2t_1u_1}. \tag{23}$$

We do not list the explicit result for the NLO hard function $\boldsymbol{H}^{(1)}$, since it has essentially been given in [32]. For what concerns the quark annihilation channel, we convert those results to our case by extracting the elements of the hard matrix from Eq. (39) of [32]. Subsequently, one needs to consider crossing symmetry and to permute the arguments of the various matrix elements according to $H_{ij}(s,t,u)\to H_{ij}(u,s,t)$, as explained in Table 1 of [32]. Finally, one should exchange the element indices $1\leftrightarrow 2$ to match the notation employed here, and compensate for an overall factor, so that

$$\boldsymbol{H}^{(0)}_{q\bar{q}}+\frac{\alpha}{4\pi}\boldsymbol{H}^{(1)}_{q\bar{q}}=-\frac{1}{64\pi^2\alpha_s^2}\begin{pmatrix}H_{22}(u,s,t) & H_{21}(u,s,t)\\ H_{12}(u,s,t) & H_{11}(u,s,t)\end{pmatrix}, \tag{24}$$

where all of the elements of the matrix on the right-hand side are taken from Eq. (39) of [32]. The gluon fusion case is slightly more complicated because the authors of [32] use a different color basis. In that case, the NLO correction can obtained from Eqs. (56) in [32] through the rotation

$$\boldsymbol{H}^{(1)}_{gg}=4O^T\begin{pmatrix}H^{\rm NLO}_{11} & H^{\rm NLO}_{12} & H^{\rm NLO}_{13}\\ H^{\rm NLO}_{12} & H^{\rm NLO}_{22} & H^{\rm NLO}_{23}\\ H^{\rm NLO}_{13} & H^{\rm NLO}_{23} & H^{\rm NLO}_{33}\end{pmatrix}O, \tag{25}$$

where the matrix elements on the right-hand side are from [32], and

$$O=\begin{pmatrix}\frac{1}{2N_c} & \frac{1}{2} & \frac{1}{2}\\ \frac{1}{2N_c} & -\frac{1}{2} & \frac{1}{2}\\ 1 & 0 & 0\end{pmatrix}. \tag{26}$$

In the resummed formulas below we will need an expression for the hard function evaluated at an arbitrary scale μ_f, given its value at an initial scale $\mu_h\sim M$ where it contains no large logarithms and the fixed-order expansions above can be applied. This is obtained by deriving and solving the RG equation. As with the matching coefficient itself, we can derive the RG equation either by setting $m_t=0$ from the start and using the exact same methods as the massive case [5], or we can start from the massive result and take the limit $m_t\to 0$ using the relations between massive and massless amplitudes mentioned above. We have checked that the two methods agree. In any case, the RG equation for the massless hard function is completely analogous to the massive case studied in [5] and is given by (here and below we suppress dependence on the channels $q\bar{q}$ and gg when there is no potential for confusion)

$$\frac{d}{d\ln\mu}\boldsymbol{H}(M,t_1,\mu)=\boldsymbol{\Gamma}_H(M,t_1,\mu)\boldsymbol{H}(M,t_1,\mu)+\boldsymbol{H}(M,t_1,\mu)\boldsymbol{\Gamma}^\dagger_H(M,t_1,\mu). \tag{27}$$

The explicit result for the anomalous dimension matrix to two-loop order in the color basis of [5] is easily derived by making use of the general result [45,46] for massless scattering amplitudes, and reads

$$\begin{aligned}\boldsymbol{\Gamma}_{q\bar{q}}&=\left[2C_F\gamma_{\rm cusp}(\alpha_s)\left(\ln\frac{M^2}{\mu^2}-i\pi\right)+4\gamma^q(\alpha_s)\right]\boldsymbol{1}\\&\quad+N_c\gamma_{\rm cusp}(\alpha_s)\left(\ln\frac{-t_1}{M^2}+i\pi\right)\begin{pmatrix}0&0\\0&1\end{pmatrix}\\&\quad+\gamma_{\rm cusp}(\alpha_s)\ln\frac{t_1^2}{u_1^2}\begin{pmatrix}0&\frac{C_F}{2N_c}\\1&-\frac{1}{N_c}\end{pmatrix},\end{aligned} \tag{28}$$

and

$$\begin{aligned}\boldsymbol{\Gamma}_{gg}&=\left[(N_c+C_F)\gamma_{\rm cusp}(\alpha_s)\left(\ln\frac{M^2}{\mu^2}-i\pi\right)+2\gamma^g(\alpha_s)\right.\\&\quad\left.+2\gamma^q(\alpha_s)\right]\boldsymbol{1}+N_c\gamma_{\rm cusp}(\alpha_s)\left(\ln\frac{-t_1}{M^2}+i\pi\right)\begin{pmatrix}0&0&0\\0&1&0\\0&0&1\end{pmatrix}\\&\quad+\gamma_{\rm cusp}(\alpha_s)\ln\frac{t_1^2}{u_1^2}\begin{pmatrix}0&\frac{1}{2}&0\\1&-\frac{N_c}{4}&\frac{N_c^2-4}{4N_c}\\0&\frac{N_c}{4}&-\frac{N_c}{4}\end{pmatrix}.\end{aligned} \tag{29}$$

For convenience, we have collected results for the various scalar anomalous dimension functions in Appendix C.

Since the evolution equation has the same structure as in the massive case, it can be solved using the same methods. In presenting the solution it is convenient to decompose the anomalous dimension into a logarithmic piece multiplying the unit matrix and a nonlogarithmic part containing the nontrivial matrix structure:

$$\boldsymbol{\Gamma}_H(M,t_1,\mu)=A(\alpha_s)\left(\ln\frac{M^2}{\mu^2}-i\pi\right)\boldsymbol{1}+\boldsymbol{\gamma}^h(M,t_1,\alpha_s), \tag{30}$$

where $A=2C_F\gamma_{\rm cusp}\equiv 2\Gamma^q_{\rm cusp}$ in the $q\bar{q}$ channel and $A=(N_c+C_F)\gamma_{\rm cusp}\equiv\Gamma^g_{\rm cusp}+\Gamma^q_{\rm cusp}$ in the gg channel. The solution to the RG equation can then be written as

$$\boldsymbol{H}(M,t_1,\mu)=\boldsymbol{U}(M,t_1,\mu_h,\mu)\boldsymbol{H}(M,t_1,\mu_h)\boldsymbol{U}^\dagger(M,t_1,\mu_h,\mu), \tag{31}$$

with

$$\begin{aligned}\boldsymbol{U}(M,t_1,\mu_h,\mu)&=\exp\left[2S_A(\mu_h,\mu)-a_A(\mu_h,\mu)\left(\ln\frac{M^2}{\mu_h^2}-i\pi\right)\right]\\&\quad\times\boldsymbol{u}(M,t_1,\mu_h,\mu).\end{aligned} \tag{32}$$

The RG exponents are given by

$$\begin{aligned}S_A(\mu_h,\mu)&=-\int_{\alpha_s(\mu_h)}^{\alpha_s(\mu)}d\alpha\frac{A(\alpha)}{\beta(\alpha)}\int_{\alpha_s(\mu_h)}^{\alpha}\frac{d\alpha'}{\beta(\alpha')},\\a_A(\mu_h,\mu)&=-\int_{\alpha_s(\mu_h)}^{\alpha_s(\mu)}d\alpha\frac{A(\alpha)}{\beta(\alpha)},\end{aligned} \tag{33}$$

where $\beta(\alpha_s) = d\alpha_s/d\ln\mu$ is the QCD β-function (whose expansion coefficients are given in Appendix C). The matrix-valued contribution to the evolution function reads

$$\boldsymbol{u}(M, t_1, \mu_h, \mu) = \mathcal{P}\exp\int_{\alpha_s(\mu_h)}^{\alpha_s(\mu)} \frac{d\alpha}{\beta(\alpha)}\boldsymbol{\gamma}^h(M, t_1, \alpha). \qquad (34)$$

The exact solution to the RG equation is evaluated as a series in RG-improved perturbation theory as in [5], where explicit expressions valid to NNLL order were presented. Such an NNLL calculation requires the NLO corrections to both the hard matching function (a one-loop calculation) and the anomalous dimension (a two-loop calculation).

B. Soft function

The soft function is related to real emission corrections to massless $q\bar{q}$, $gg \to t\bar{t}$ scattering in the soft limit. A more formal definition in terms of the vacuum expectation value of a Wilson-loop operator was given for the massive case in [5]. The position-space result for this object can be directly converted into the Laplace-transformed function (19). We can adapt that definition to the massless case simply by changing time-like Wilson lines representing emissions from massive particles to light-like Wilson lines representing emissions from massless ones. We will present results for the Laplace-transformed soft function directly. We define the perturbative expansion of this function as

$$\tilde{\boldsymbol{s}} = \tilde{\boldsymbol{s}}^{(0)} + \frac{\alpha_s}{4\pi}\tilde{\boldsymbol{s}}^{(1)} + \left(\frac{\alpha_s}{4\pi}\right)^2\tilde{\boldsymbol{s}}^{(2)} + \cdots. \qquad (35)$$

At lowest order, the result depends on whether the initial-state partons are quarks or gluons, but not on the mass. The result is

$$\tilde{\boldsymbol{s}}^{(0)}_{q\bar{q}} = \begin{pmatrix} N_c & 0 \\ 0 & \frac{C_F}{2} \end{pmatrix} \qquad (36)$$

in the quark annihilation channel, and

$$\tilde{\boldsymbol{s}}^{(0)}_{gg} = \begin{pmatrix} N_c & 0 & 0 \\ 0 & \frac{N_c}{2} & 0 \\ 0 & 0 & \frac{N_c^2-4}{2N_c} \end{pmatrix} \qquad (37)$$

in the gluon fusion channel.

To obtain the Laplace-transformed soft function at NLO we evaluate the following position-space integrals [5]

$$\mathcal{I}_{ij}(\epsilon, x_0, \mu) = -\frac{(4\pi\mu^2)^\epsilon}{\pi^{2-\epsilon}} v_i \cdot v_j \int d^dk \frac{e^{-ik^0x_0}}{v_i\cdot k v_j\cdot k}(2\pi)\delta(k^2)\theta(k^0), \qquad (38)$$

where v_i are the light-like four-velocities of the partons from the Born-level scattering process. When $i = j$ these integrals vanish since $v_i^2 = 0$, while for $i \neq j$ they are equal to

$$\mathcal{I}_{ij} = -(4\pi)^\epsilon e^{-\epsilon\gamma}\Big[\frac{2}{\epsilon^2} + \frac{2}{\epsilon}\Big(L_0 - \ln\frac{v_1\cdot v_2}{2}\Big) + \Big(L_0 - \ln\frac{v_1\cdot v_2}{2}\Big)^2 + \frac{\pi^2}{6} + 2\mathrm{Li}_2\Big(1 - \frac{v_1\cdot v_2}{2}\Big)\Big], \qquad (39)$$

where

$$L_0 = \ln\Big(-\frac{\mu^2x_0^2e^{2\gamma_E}}{4}\Big). \qquad (40)$$

We make use of this result by expressing the scalar products $v_i\cdot v_j$ in terms of the Mandelstam variables, by subtracting the IR poles in $\overline{\mathrm{MS}}$, and by Laplace-transforming the integrals through the replacement $L_0 \to -L$. This leads to

$$\begin{aligned}
\tilde{\mathcal{I}}_{12} &= -\Big(L^2 + \frac{\pi^2}{6}\Big),\\
\tilde{\mathcal{I}}_{13} &= \tilde{\mathcal{I}}_{24} = -(L + \ln(r))^2 - \frac{\pi^2}{6} - 2\mathrm{Li}_2(1-r),\\
\tilde{\mathcal{I}}_{14} &= \tilde{\mathcal{I}}_{23} = -(L + \ln(1-r))^2 - \frac{\pi^2}{6} - 2\mathrm{Li}_2(r),\\
\tilde{\mathcal{I}}_{11} &= \tilde{\mathcal{I}}_{22} = \tilde{\mathcal{I}}_{33} = \tilde{\mathcal{I}}_{44} = 0,
\end{aligned} \qquad (41)$$

where $r = -t_1/M^2$. One obtains the matrix-valued soft function in Laplace space by evaluating

$$\tilde{\boldsymbol{s}}^{(1)} = \sum_{(i,j)} \boldsymbol{w}_{ij}\tilde{\mathcal{I}}_{ij}(L, r), \qquad (42)$$

where the $\boldsymbol{w}_{ij}$ are the color matrices from [5], which are different for the $q\bar{q}$ and gg channels, but make no reference to the parton mass.

To obtain the NNLO correction to the soft function requires a new calculation which is beyond the scope of this paper. However, as a compromise, we can use the RG equation below to derive all of the coefficients proportional to powers of logarithms in the Laplace-transformed NNLO correction, whose form is

$$\tilde{\boldsymbol{s}}^{(2)}(L, M, t_1) = \sum_{n=0}^{4} \boldsymbol{s}_n(M, t_1)L^n. \qquad (43)$$

The results for the coefficients are fairly lengthy and since we use them in this paper only for the factorization check described in Sec. IV B we do not list them here.

The Laplace-transformed functions are the central objects used in solving the RG equations below. One can also convert them to the momentum-space functions using a set of replacement rules. In the case where the first argument of the soft function is expressed in terms of $\sqrt{\hat{s}}(1-z) = M(1-z)/\sqrt{z}$, the resulting distributions are

$$P'_n(z) = \left[\frac{1}{1-z}\ln^n\left(\frac{M^2(1-z)^2}{\mu^2 z}\right)\right]_+. \tag{44}$$

As shown in [5], the momentum-space soft function is derived from the Laplace-space function by making the replacements

$$\begin{aligned}
&1 \to \delta(1-z), \qquad L \to 2P'_0(z) + \delta(1-z)\ln\left(\frac{M^2}{\mu^2}\right),\\
&L^2 \to 4P'_1(z) + \delta(1-z)\ln^2\left(\frac{M^2}{\mu^2}\right),\\
&L^3 \to 6P'_2(z) - 4\pi^2 P'_0(z) + \delta(1-z)\left[\ln^3\left(\frac{M^2}{\mu^2}\right) + 4\zeta_3\right],\\
&L^4 \to 8P'_3(z) - 16\pi^2 P'_1(z) + 128\zeta_3 P'_0(z)\\
&\qquad + \delta(1-z)\left[\ln^4\left(\frac{M^2}{\mu^2}\right) + 16\zeta_3\ln\left(\frac{M^2}{\mu^2}\right)\right].
\end{aligned} \tag{45}$$

In order to translate the P'_n into the conventional P_n distributions,

$$P_n(z) = \left[\frac{1}{1-z}\ln^n(1-z)\right]_+, \tag{46}$$

we employ the general relation

$$\begin{aligned}
P'_n(z) = &\sum_{k=0}^{n}\binom{n}{k}\ln^{n-k}\left(\frac{M^2}{\mu^2}\right)\left[2^k P_k(z) + \sum_{j=0}^{k-1}\binom{k}{j}2^j(-1)^{k-j}\right.\\
&\times\left(\frac{\ln^j(1-z)\ln^{k-j}z}{1-z} - \delta(1-z)\right.\\
&\left.\left.\times\int_0^1 dx\frac{\ln^j(1-x)\ln^{k-j}x}{1-x}\right)\right].
\end{aligned} \tag{47}$$

The numerical affects of keeping the power-suppressed terms proportional to $\ln^m z/(1-z)$ was discussed in detail in [5,26].

The soft function obeys a nonlocal RG equation which is solved using the Laplace transform technique [47]. The RG invariance of the total cross section implies that the Laplace-transformed soft function satisfies

$$\begin{aligned}
&\frac{d}{d\ln\mu}\tilde{\mathbf{s}}\left(\ln\frac{M^2}{\mu^2}, M, t_1, \mu\right)\\
&\quad = -\left[A(\alpha_s)\ln\frac{M^2}{\mu^2} + \boldsymbol{\gamma}^{s\dagger}(M, t_1, \alpha_s)\right]\tilde{\mathbf{s}}\left(\ln\frac{M^2}{\mu^2}, M, t_1, \mu\right)\\
&\qquad - \tilde{\mathbf{s}}\left(\ln\frac{M^2}{\mu^2}, M, t_1, \mu\right)\left[A(\alpha_s)\ln\frac{M^2}{\mu^2} + \boldsymbol{\gamma}^{s}(M, t_1, \alpha_s)\right].
\end{aligned} \tag{48}$$

We have defined

$$\boldsymbol{\gamma}^s(M, t_1, \alpha_s) = \boldsymbol{\gamma}^h(M, t_1, \alpha_s) + [2\gamma^\phi(\alpha_s) + 2\gamma^{\phi_q}(\alpha_s)]\mathbf{1}. \tag{49}$$

Note that while the form of the anomalous dimension is analogous to that in the massive case, it picks up an extra term $2\gamma^{\phi_q}$, which is needed to cancel the μ-dependence from the fragmentation function as determined by the RG equation (57) below.

The solution for the momentum-space soft function reads

$$\begin{aligned}
\mathbf{S}(\omega, M, t_1, \mu_f) = &\sqrt{\hat{s}}\exp[-4S_A(\mu_s, \mu_f) + 4a_{\gamma^\phi}(\mu_s, \mu_f)\\
&+ 4a_{\gamma^{\phi_q}}(\mu_s, \mu_f)]\mathbf{u}^\dagger(M, t_1, \mu_f, \mu_s)\\
&\times\tilde{\mathbf{s}}(\partial_{\eta_A}, M, t_1, \mu_s)\mathbf{u}(M, t_1, \mu_f, \mu_s)\\
&\times\frac{1}{\omega}\left(\frac{\omega}{\mu_s}\right)^{2\eta_A}\frac{e^{-2\gamma_E\eta_A}}{\Gamma(2\eta_A)},
\end{aligned} \tag{50}$$

where one is to set $\eta_A = 2a_A(\mu_s, \mu_f)$ after performing the derivatives. For values of $2\eta_A < 0$, the ω-dependence must be interpreted in the sense of distributions.

As always in RG-improved perturbation theory, the aim of a formula such as (50) is to allow one to evaluate the soft function at an arbitrary scale μ_f given its result at a scale μ_s where it is free of large logarithms. However, the question of what exactly this μ_s should be is currently a source of debate in the literature. We will discuss this issue in more detail when presenting results for the RG-improved partonic cross section in Sec. IV.

C. Fragmentation function

The perturbative fragmentation function was calculated at NNLO for generic values of z in [14]. In this section we focus on the parts of that result required for the resummed analysis, namely the leading terms in the soft limit of the function with n_l active flavors defined in (12). In particular, we list results for the functions S_D and C_D appearing in the factorized form (17), determined previously in [13].

The function S_D is related to the partonic shape-function in B-meson decays and can be derived from the two-loop calculations in [48]. We define its perturbative expansion in Laplace space as

$$\tilde{s}_D = 1 + \frac{\alpha_s}{4\pi}\tilde{s}_D^{(1)} + \left(\frac{\alpha_s}{4\pi}\right)^2\tilde{s}_D^{(2)} + \cdots. \tag{51}$$

The expansion coefficients with $N_c = 3$ colors are

$$\tilde{s}_D^{(1)}(L/2) = -\frac{4}{3}L^2 - \frac{8}{3}L - \frac{10\pi^2}{9}, \tag{52}$$

$$\tilde{s}_D^{(2)}(L/2) = \frac{8}{9}L^4 + \left(\frac{76}{9} - \frac{8}{27}n_l\right)L^3 + \left(-\frac{104}{9} + \frac{76\pi^2}{27} + \frac{16}{27}n_l\right)L^2 + \left(\frac{440}{27} + \frac{416\pi^2}{27} - 72\zeta_3 + \frac{16}{81}n_l - \frac{16\pi^2}{27}n_l\right)L - \frac{1304}{81} - \frac{233\pi^2}{9} + \frac{1213\pi^4}{405} - \frac{1132\zeta_3}{9} + \left(-\frac{16}{243} + \frac{14\pi^2}{27} + \frac{88\zeta_3}{27}\right)n_l. \tag{53}$$

It is a nontrivial check on the factorization formula (17) that the plus-distributions in the fragmentation function are all related to the momentum-space representation of this function, obtained by the set of replacement rules analogous to (45), but with the substitution $M(1-z)/\sqrt{z} \to m_t(1-z)$.

The coefficient C_D is related to virtual corrections to the fragmentation function and is a simple function independent of z. Since the NNLO correction to the fragmentation function obtained in [14] was not split into real and virtual corrections, it is not possible to obtain the coefficient directly from that work. Instead, it must be determined by using the result for the shape-function given above along with the factorization formula (17) for the fragmentation function. Defining expansion coefficients in analogy to (51), we have (with $N_c = 3$ colors)

$$C_D^{(1)}(m_t, \mu) = \frac{4}{3}\left(L_m^2 + L_m + 4 + \frac{\pi^2}{6}\right), \tag{54}$$

$$C_D^{(2)}(m_t, \mu) = \frac{8}{9}L_m^4 + \left(\frac{20}{3} - \frac{8}{27}n_l\right)L_m^3 + \left(\frac{406}{9} - \frac{28\pi^2}{27} - \frac{52}{27}n_l\right)L_m^2 + \left(\frac{2594}{27} + \frac{248\pi^2}{27} - \frac{232\zeta_3}{3} - \frac{308}{81}n_l - \frac{16\pi^2}{27}n_l\right)L_m + \frac{21553}{162} + \frac{107\pi^2}{3} - \frac{749\pi^4}{405} + \frac{260\zeta_3}{9} + \frac{16\pi^2}{9}\ln 2 - \left(\frac{1541}{243} + \frac{74\pi^2}{81} + \frac{104\zeta_3}{27}\right)n_l, \tag{55}$$

with $L_m = \ln(\mu^2/m_t^2)$. We discuss a possible cross-check of this result in Appendix A.

In the factorization formula for the invariant-mass distribution we need the convolution of two fragmentation functions, which up to NNLO has the form

$$\mathbb{D}(z, m_t, \mu) = \delta(1-z) + 2\left(\frac{\alpha_s}{4\pi}\right)D^{(1)}(z, m_t, \mu) + \left(\frac{\alpha_s}{4\pi}\right)^2[2D^{(2)}(z, m_t, \mu) + D^{(1)}(z, m_t, \mu) \otimes D^{(1)}(z, m_t, \mu)]. \tag{56}$$

The convolutions between the different plus-distributions in the last term can be evaluated by employing the methods illustrated in [49]. For the reader's convenience we collect the relevant convolutions in Appendix B.

The RG equation for the fragmentation function is a nonlocal one. It is given by

$$\frac{d}{d\ln\mu}D_{t/H}^{(n_l)}(z, m_t, \mu) = P_{qq}(z, \mu) \otimes D_{t/H}^{(n_l)}(z, m_t, \mu), \tag{57}$$

where P_{qq} is a time-like Altarelli-Parisi splitting function whose structural form in the soft limit is

$$P_{qq}(z, \mu) = \frac{2\Gamma_{\rm cusp}^q(\alpha_s)}{(1-z)_+} + 2\gamma^{\phi_q}(\alpha_s)\delta(1-z). \tag{58}$$

From this equation, and the fact the S_D is equivalent to the perturbative shape-function from B-meson decays [12,13], the RG equations for the function C_D can be derived. The RG equation for C_D is local, while that for S_D is nonlocal and solved using the Laplace transform technique. The result for the RG-improved fragmentation function reads

$$D(z, m_t, \mu_f) = \exp[2S_{\Gamma_{\rm cusp}^q}(\mu_{ds}, \mu_{dh}) + 2a_{\gamma^S}(\mu_{ds}, \mu_{dh}) + 2a_{\gamma^{\phi_q}}(\mu_f, \mu_{dh})]\left(\frac{m_t}{\mu_{ds}}\right)^{-2a_{\Gamma_{\rm cusp}^q}(\mu_f, \mu_{dh})} \times C_D(m_t, \mu_{dh})\tilde{s}_D(\partial_{\eta_d}, \mu_{ds})\frac{e^{-\gamma_E\eta_d}}{\Gamma(\eta_d)}\left(\frac{m_t}{\mu_{ds}}\right)^{\eta_d}\frac{1}{(1-z)^{1-\eta_d}}, \tag{59}$$

with $\eta_d = 2a_{\Gamma_{\rm cusp}^q}(\mu_f, \mu_{ds})$. The explicit results for the anomalous dimension γ^S can be found in [13] as well as in Appendix C of this paper. While it is obvious that the scale choice $\mu_{dh} \sim m_t$ eliminates large logarithms in the coefficient function C_D, the choice of the scale μ_{ds} is again a debatable point which we come back to later on.

D. The heavy-flavor coefficients

The definition of the heavy-flavor coefficients $C_{t/t}$ and C_{ff}^{ij} was given in (12). The partonic matrix elements needed to evaluate those expressions to NNLO are known from [14] for the fragmentation functions and [30] for the PDFs. Rather than give the results separately, we quote only the result for the Laplace-transformed combination of the three functions appearing in (19). Expressed in terms of α_s with five active flavors, the result is

$$\tilde{c}_t^{q\bar{q}}(L, m_t, \mu) = 1 + n_h\Big(\frac{\alpha_s}{4\pi}\Big)^2\Big[\Big(\frac{32}{9}L_m^2 - \frac{320}{27}L_m + \frac{896}{81}\Big)L + \frac{16}{3}L_m^2 - \Big(\frac{16}{9} + \frac{64\pi^2}{27}\Big)L_m + \frac{7592}{243} - \frac{64\pi^2}{81}\Big] + \cdots \quad (60)$$

$$\tilde{c}_t^{gg}(L, m_t, \mu) = 1 - n_h\frac{\alpha_s}{4\pi}\frac{4}{3}L_m + n_h\Big(\frac{\alpha_s}{4\pi}\Big)^2\Big[\Big(\frac{52}{9}L_m^2 - \frac{520}{27}L_m + \frac{1456}{81}\Big)L + \frac{8}{3}L_m^2 - \Big(\frac{32\pi^2}{27} + \frac{200}{9}\Big)L_m + \frac{2228}{243} - \frac{16\pi^2}{9} + \frac{32\zeta_3}{9} + \frac{4n_h}{9}L_m^2\Big] + \cdots \quad (61)$$

If desired, these can be converted to momentum-space by the set of replacements (45) with $\mu = M$.

The RG equations for the heavy-flavor coefficients C_{ff} and $C_{t/t}$ follow from the fact that the parton luminosity and fragmentation functions in the $n_h + n_l$ flavor theory obey the standard Altarelli-Parisi equations in the soft limit. This implies

$$\frac{d}{d\ln\mu}C_{t/t}(z, m_t, \mu) = [P_{qq}^{n_h+n_l}(z, \mu) - P_{qq}^{n_l}(z, \mu)] \otimes C_{t/t}(z, m_t, \mu), \quad (62)$$

$$\frac{d}{d\ln\mu}C_{ff}^{ij}(z, m_t, \mu) = 2[P_{ij}^{n_h+n_l}(z, \mu) - P_{ij}^{n_l}(z, \mu)] \otimes C_{ff}^{ij}(z, m_t, \mu), \quad (63)$$

where we have used that nondiagonal evolution is suppressed by powers of $(1 - z)$. The function P_{gg} is defined in analogy with (58) after the obvious replacements, and both $\Gamma_{\rm cusp}^g = C_A\gamma_{\rm cusp}$ and γ^{ϕ_g} can be read off to two loops from Appendix C. The superscripts indicate the number of active flavors to be used in both α_s and the coefficients of the anomalous dimensions themselves. When expressed in terms of a common five-flavor coupling, the anomalous dimensions $P_{ij}^{n_h+n_l}$ pick up explicit powers of $\ln m_t/\mu$ related to the α_s decoupling relation

$$\alpha_s^{(n_h+n_l)} = \alpha_s^{(n_l)}\Big(1 + n_h\frac{2}{3}L_m\frac{\alpha_s^{(n_l)}}{4\pi} + \ldots\Big). \quad (64)$$

The logarithms associated with this decoupling are the reason why the explicit results (61) look slightly different from what one might expect from the form of the Altarelli-Parisi kernel in the soft limit in (58). One can easily show, however, that the RG equations (63) are indeed satisfied. We note that for the NNLL analysis, we need only the NLO correction from $\tilde{c}_t^{gg}$, which contains no large logarithms for $\mu_t \sim m_t$. Beyond NNLL accuracy, however, such a choice leads to large logarithms in $1 - z$ that are not resummed. While it is conceivable that one could derive a method for resumming logarithms between the scales $m_t(1 - z)$ and m_t within the heavy-flavor coefficients, we will leave this as an open point in our current analysis of resummation in the double soft and small-mass limit.

IV. THE PARTONIC CROSS SECTION AT NNLL AND APPROXIMATE NNLO

In this section we derive the final expression for the resummed partonic cross section at NNLL in the double soft and small-mass limit. We discuss a few points having to do with its practical implementation, and then turn to its approximate NNLO implementation.

A. Partonic cross section at NNLL

To derive the final result for the resummed partonic cross section at a scale μ_f we insert the RG-improved results for the hard, soft, and fragmentation functions presented above into the factorization formula (18). The convolution integrals can be performed analytically using

$$\int_z^1 dz' \frac{1}{(1 - z')^{1-\eta_1}}\frac{1}{(1 - z/z')^{1-\eta_2}} \approx \frac{\Gamma(\eta_1)\Gamma(\eta_2)}{\Gamma(\eta_1 + \eta_2)}\frac{1}{(1 - z)^{1-\eta_1-\eta_2}}, \quad (65)$$

where the approximation is true in the limit $z \to 1$. We can also simplify the various products of evolution matrices by employing the relations

$$\begin{aligned}\boldsymbol{u}(M, \cos\theta, \mu_f, \mu_s)\boldsymbol{u}(M, \cos\theta, \mu_h, \mu_f) &= \boldsymbol{u}(M, \cos\theta, \mu_h, \mu_s),\\ a_A(\mu_s, \mu_h) + a_A(\mu_h, \mu_f) &= a_A(\mu_s, \mu_f),\\ S_A(\mu_h, \mu_f) - S_A(\mu_s, \mu_f) &= S_A(\mu_h, \mu_s) - a_A(\mu_s, \mu_f)\ln\frac{\mu_h}{\mu_s}.\end{aligned} \quad (66)$$

The only subtlety is related to the treatment of heavy-quark threshold effects at $\mu_t \sim m_t$. However, this is a standard problem in RG-improved perturbation theory involving heavy quarks, and we deal with it in the usual way [50]. To understand the logic, it suffices to consider a hypothetical observable involving three widely separated scales $M \gg m_t \gg \mu_0$, which satisfies a factorization formula of the form $C(M, \mu)D(m_t, \mu)F(\mu_0, \mu)$. If C is a coefficient function whose RG running is known, and the goal is to evolve it from a high scale $\mu_M \sim M$ to the scale μ_0 below the heavy-flavor threshold, one uses the following schematic equation:

$$C^{(n_l)}(M, m_t, \mu_0) = U^{(n_l)}(M, \mu_0, \mu_t)M_h(m_t, \mu_t)U^{(n_l+n_h)} \times (M, \mu_t, \mu_M)C^{(n_l+n_h)}(M, \mu_M). \quad (67)$$

In words, one uses six-flavor evolution functions $U^{(n_l+n_h)}$ above the flavor threshold at μ_t, and five-flavor evolution functions $U^{(n_l)}$ below it. The change in the number of flavors induces a matching coefficient M_h at the flavor threshold. It is determined by requiring that the partonic cross section in the n_f and n_f-1 flavor theories be equal at the scale μ_t:

$$C^{(n_f)}(M,\mu_t)\langle DF\rangle^{(n_f)} = C^{(n_f-1)}(M,m_t,\mu_t)\langle DF\rangle^{(n_f-1)}, \quad (68)$$

where the $\langle\rangle^{(f)}$ denotes a partonic matrix element in the theory with f massless flavors evaluated at the scale μ_t.

The generalization of this simple picture to our case is straightforward. The role of the coefficient C is played by the massless hard and soft functions, and that of the heavy-flavor matching coefficient M_h by the convolution of the three functions appearing in the second line of (18). The explicit result reads

$$\begin{aligned} C(z,M,m_t,\cos\theta,\mu_f) &= \exp\Big[4S_{\Gamma^q_{\rm cusp}}(\mu_{ds},\mu_{dh}) + 4a_{\gamma^\phi}(\mu_t,\mu_f) + 4a_{\gamma^{\phi_q}}(\mu_t,\mu_{dh}) + 4a_{\gamma^s}(\mu_{ds},\mu_{dh}) \\ &\quad + 2a_{\Gamma^q_{\rm cusp}}(\mu_{dh},\mu_{ds})\ln\frac{m_t^2}{\mu_{ds}^2}\Big]_{n_f=5} \exp[4a_{\gamma^\phi}(\mu_s,\mu_t) + 4a_{\gamma^{\phi_q}}(\mu_s,\mu_t)]_{n_f=6} \\ &\quad \times \mathrm{Tr}\Big[\boldsymbol{U}(M,t_1,\mu_h,\mu_s)\boldsymbol{H}(M,t_1,\mu_h)\boldsymbol{U}^\dagger(M,t_1,\mu_h,\mu_s)\times\tilde{\boldsymbol{s}}\Big(\ln\frac{M^2}{\mu_s^2}+\partial_{\eta'},M,t_1,\mu_s\Big)\Big]_{n_f=6} \\ &\quad \times\Big[\tilde{c}_t^{ij}(\partial_{\eta'},m_t,\mu_t)\tilde{\boldsymbol{d}}\Big(\ln\frac{m_t^2}{\mu_{ds}^2}+\partial_{\eta'},m_t,\mu_{dh},\mu_{ds}\Big)\Big]_{n_f=5}\frac{e^{-2\gamma_E\eta'}}{\Gamma(2\eta')}\frac{1}{(1-z)^{1-2\eta'}} + \mathcal{O}(1-z) + \mathcal{O}\Big(\frac{m_t}{M}\Big). \end{aligned} \quad (69)$$

We have defined $\eta' = [2a_A(\mu_s,\mu_t)]_{n_f=6} + [2a_A(\mu_t,\mu_f) + 2a_{\Gamma^q_{\rm cusp}}(\mu_f,\mu_{ds})]_{n_f=5}$ and in addition $\tilde{\boldsymbol{d}}(L,m_t,\mu_{dh},\mu_{ds}) = [C_D(m_t,\mu_{dh})\tilde{s}_D(L/2,\mu_{ds})]^2$. We have indicated with the subscripts the number of active massless flavors n_f to be used in evaluating the running coupling constant and perturbative functions in the various parts of the formula. This number of active flavors is chosen according to the physical picture of the schematic example (67) above, namely that of integrating out heavy degrees of freedom until reaching a scale under the flavor threshold below which the remaining degrees of freedom are factorized into the PDFs. However, it is formally true for any value of the factorization scale. It thus provides a convenient way to use the standard PDFs with five light flavors even when μ_f is far above the heavy-flavor threshold at $\mu_t \sim m_t$, as it explicitly resums any large logs in m_t/M in the partonic cross section for such a scale choice.

The result (69) is the final expression for the resummed partonic cross section in momentum-space. It can be evaluated perturbatively at NNLL order using the results given in the previous section. There are two important issues in terms of its numerical evaluation. The first is a technical one having to do with the choice of matching scales, the second is a practical one having to do with the power corrections away from the soft and small-mass limits. We end this section on the resummed cross section by discussing these in turn.

As alluded to several times in the previous section, the philosophy of RG-improved perturbation theory is to use RG evolution factors to evaluate the matching functions at an arbitrary scale μ_f given their value at an initial scale where they do not involve large logarithms. This RG running then exponentiates large corrections appearing when μ_f is parametrically far from the natural scale. For the hard function and the coefficient C_D, which obey local RG equations, the choice is straightforward: one uses $\mu_h \sim M$ and $\mu_{dh} \sim m_t$. For the massless soft function and the function S_D, the correct choice of this scale is less obvious. If the goal is to resum logarithms of $(1-z)$ in the partonic cross sections, then the natural scales are $M(1-z)$ and $m_t(1-z)$. However, such choices are ill-defined at the level of the momentum-space result (69). Partonic logarithms can be resummed by choosing the scales μ_s and μ_{ds} at the level of the Laplace-transformed functions (19) and performing the inverse transform back to momentum-space numerically, but at the cost of introducing the Landau-pole singularity familiar from Mellin-space implementations of soft-gluon resummation for top-quark pair production [51–57]. An alternate method is to choose the two scales as numerical functions of M, in such a way that the logarithmic corrections to the hadronic cross section arising from those in the partonic one are minimized after convolutions with the PDFs [17]. The fixed-order expansions of the resulting expressions at any finite order in the logarithmic counting are then of a different structure than those in the partonic cross section [26,58]. Studying the numerical differences between these methods would be an interesting exercise, but since we will not do detailed phenomenology in the current paper we leave this issue aside.

Dealing with the power corrections away from the double soft and small-mass limit is also important, although considerably more straightforward technically. The standard method is to include these corrections at

NLO in fixed-order perturbation theory, thus obtaining NLO + NNLL accuracy. This is accomplished by evaluating partonic cross sections $d\hat{\sigma}$ as

$$d\hat{\sigma}(\mu_f) = d\hat{\sigma}^{\rm NNLL}(\{\mu_i\})|_{m_t\to 0, z\to 1} + \Big(d\hat{\sigma}^{\rm NLO}(\mu_f) - d\hat{\sigma}^{\rm NNLL}(\{\mu_i\} = \mu_f\})|_{m_t\to 0, z\to 1}\Big), \tag{70}$$

where by $\{\mu_i\}$ we mean the set of scales μ_h, $\mu_s, \ldots$ appearing in (69). Such a resummation formula is useful only at values of the invariant mass where m_t/M is truly small. It is straightforward to extend the matching procedure to take into account in addition the set of higher-order m_t/M corrections determined from soft-gluon resummation at NNLL with the counting $m_t \sim M$ used in [5], thus yielding a result useful for the full range of M, but we do not give the explicit results here.

B. Partonic cross section at approximate NNLO

The resummed formula from the previous subsection can be used as a means of extracting what can be argued to be dominant part of the full NNLO correction in fixed-order perturbation theory. This truncation of the resummed expansion is of course not valid if the logarithms are truly large, but it is easy to imagine a situation where $(1 - z)$ and m_t/M are good expansion parameters for the fixed-order corrections, but not necessary so small that logarithmic corrections beyond NNLO are numerically important. In this section we focus on such approximate NNLO formulas based on our NNLL results, and explain how the results in this paper can offer an improvement on those previously derived in [4,5].

It is convenient to discuss the approximate NNLO formulas at the level of Laplace-transformed coefficients. The general expression for the NNLO correction in Laplace space reads

$$\tilde{c}(N,M,m_t,\cos\theta,\mu_f) = \alpha_s^2\bigg[\tilde{c}^{(0)}(M,m_t,\cos\theta,\mu_f) + \Big(\frac{\alpha_s}{4\pi}\Big)\tilde{c}^{(1)}(N,M,m_t,\cos\theta,\mu_f) + \Big(\frac{\alpha_s}{4\pi}\Big)^2\tilde{c}^{(2)}(N,M,m_t,\cos\theta,\mu_f) + \mathcal{O}(\alpha_s^3)\bigg],$$
$$\tilde{c}^{(2)}(N,M,m_t,\cos\theta,\mu_f) = \sum_{n=0}^{4} c^{(2,n)}(M,m_t,t_1,\mu_f)\ln^n\frac{M^2}{\bar{N}^2\mu_f^2} + \mathcal{O}\Big(\frac{1}{N}\Big). \tag{71}$$

The terms $c^{(2,n)}$ for $n = 1, 2, 3, 4$ are determined exactly by NNLL soft-gluon resummation for arbitrary m_t [4]. On the other hand, only parts of the $c^{(2,0)}$ coefficient are determined by the NNLL calculation, namely its μ-dependence and the contribution from the product of NLO corrections to the hard and soft functions. To determine this coefficient exactly would require the massive hard and soft functions at NNLO in fixed-order perturbation theory, which are parts of the $\mathrm{N^3LL}$ calculation.

We now discuss to what extent the results from this paper can improve the NNLO approximation described above. For the pieces proportional to the Laplace-space logarithms there is no possible improvement to the exact results as a function of m_t. However, it is a nontrivial check on the factorization formula (20) that its expansion in fixed-order reproduces these results in the limit $m_t/M \to 0$. We have confirmed explicitly that this is the case, also for the n_h pieces after converting the results for the massless hard and soft functions to a theory with five active flavors using (64). For the $c^{(2,0)}$ term, on the other hand, we can take the further step of determining exactly the terms enhanced by logarithms of M/m_t. Moreover, since the NNLO fragmentation function is known, and all diagrammatic calculations needed to extract the contribution of the two-loop hard function to this term are in place, the only piece needed to fully determine this coefficient in the limit $m_t/M \to 0$ is the NNLO massless soft function. This is a much simpler calculation than that for generic top-quark mass, and once completed it will provide valuable insight into the uncertainties in approximate NNLO calculations based on NNLL resummation alone.

Given results for the Laplace-space coefficients, we can obtain a result in momentum-space by making the replacements in (45). The momentum-space coefficient then takes the form

$$\begin{aligned} C^{(2)}(z, M, m_t, \cos\theta, \mu) &= D_3\bigg[\frac{\ln^3(1-z)}{1-z}\bigg]_+ + D_2\bigg[\frac{\ln^2(1-z)}{1-z}\bigg]_+ \\ &\quad + D_1\bigg[\frac{\ln(1-z)}{1-z}\bigg]_+ + D_0\bigg[\frac{1}{1-z}\bigg]_+ \\ &\quad + C_0\delta(1-z) + R(z). \end{aligned} \tag{72}$$

The coefficients $D_0, \ldots, D_3$ and C_0 are functions of the variables M, m_t, t_1, and μ. The plus-distributions D_i are determined by the approximate NNLO formula in Laplace-space; explicit results were given in [4]. These plus-distribution coefficients are exact, valid for generic values of the top-quark mass. To determine the delta-function coefficient exactly would also require the unknown pieces of the $c^{(2,0)}$ coefficient, in other words the NNLO hard and soft functions. Without these pieces, there is an ambiguity as to what to include in this term. Parts of these are directly related to those in Laplace-transformed coefficient $c^{(2,0)}$, and parts are related to whether to include the results from inverting the Laplace transform via the replacements (45);

we will always specify our means of dealing with these ambiguities when giving numerical results later on.

The decomposition (72) is the natural one for studying the NNLO correction within the framework of soft-gluon resummation. However, it is worth mentioning that another way to estimate higher-order corrections would be to instead focus on the leading terms in the m_t/M expansion, as determined by factorization formula (14) for the small-mass limit. Given NNLO fragmentation functions and the NLO massless scattering kernels C_{ij} for *generic* values of z, it would then be possible to study to what extent the leading terms in the soft limit reproduce the singular logarithmic corrections in the limit $m_t/M \to 0$. While such a calculation would be interesting and valuable as a means of studying power corrections to soft-gluon resummation, it is clearly beyond the scope of this work to pursue this idea further.

V. NUMERICAL STUDIES

In this section we perform short numerical studies of our results. Since a detailed analysis of soft-gluon resummation for the pair-invariant-mass distribution was carried out with the counting $m_t \sim M$ in [4,5], our main motivation is to study to what extent these results can be improved through the additional layer of resummation in the small-mass limit $m_t \ll M$.

When arguing that resummation is required in a certain limit, a typical first step is to check to what extent the corrections at a given order in perturbation theory are related to the logarithmic pieces. If the logarithms account for the bulk of the corrections, it is an obvious improvement to use the resummed formula to include subsets of higher-order corrections related to them. Comparisons of NLO corrections in the $z \to 1$ limit with exact fixed-order results were performed in [4,5,26]. It was shown there that the logarithmic plus-distributions, determined by an NLL calculation, account for a bit more than half of the NLO corrections, while these logarithms plus the delta-function term, determined by an NNLL calculation, account for essentially all of it. Moreover, it was observed that the perturbative corrections at the scale $\mu_f = M$ are rather large at high values of the invariant-mass. The main question we seek to answer in this section is whether this is due to the small-mass logarithms. If so, it would be necessary to supplement the phenomenological results of [5] with the small-mass resummation derived here.

We address this question at NLO by isolating the terms which can give rise to large logarithms in m_t/M. This is easily done by expanding the resummed formula (69) to NLO in $\alpha_s(\mu_f)$, for the choice $\mu_h = \mu_s = M$, $\mu_{dh} = \mu_{ds} = \mu_t = m_t$. The NLO corrections proportional to mass logarithms are determined by the NLL calculation, and when expressed in a theory with five active massive flavors, they read (normalized to the Born-level Laplace-space coefficient $\tilde{c}^{(0)}$)

$$\frac{2\alpha_s}{4\pi}\bigg\{\bigg(\Gamma^q_{\text{cusp},0}\ln\frac{M^2}{m_t^2}+\Gamma_{\text{cusp},0}\ln\frac{M^2}{\mu_f^2}\bigg)\bigg[\frac{1}{1-z}\bigg]_+ +\bigg(\bigg(\frac{2}{3}\delta_{q\bar{q}}N_h+\gamma_0^{\phi_q}\bigg)\ln\frac{M^2}{m_t^2}+\bigg(-\beta_0+\gamma_0^{\phi}\bigg)\ln\frac{M^2}{\mu_f^2}\bigg)\delta(1-z)\bigg\}. \tag{73}$$

We have checked numerically that for $\mu_f \sim M$ these small-mass logarithms make up only a small part of the NLO corrections in the $z \to 1$ limit (which in turn account for most of the full correction), even for values of M as high as 3–5 TeV at the LHC with $\sqrt{s} = 7$ TeV. The NLL corrections determined by soft-gluon resummation for arbitrary m_t, which include also plus-distributions containing no small-mass logarithms, make up a much larger part of the exact NLO correction. We will therefore view small-mass resummation as supplementary to that, a means of improvement rather than a substitute. The point is that the mass logarithms generated at NLL in the small-mass limit are a subset of the NNLL corrections in soft-gluon resummation for generic m_t, so including them may be advantageous. We now study this statement in more detail.

To do so, we define different approximations to the NLO corrections at the level of the Laplace-space coefficient, which reads

$$\tilde{c}^{(1)}(N, M, m_t, \cos\theta, \mu_f) = \sum_{n=0}^{2} c^{(1,n)}(M, m_t, t_1, \mu_f)\ln^n\frac{M^2}{\bar{N}^2\mu_f^2} + \mathcal{O}\bigg(\frac{1}{N}\bigg). \tag{74}$$

Momentum-space results are obtained through the replacement rules (45). The coefficients $c^{(1,2)}$ and $c^{(1,1)}$ thus determine the plus-distribution coefficients. We will take the exact expression for these, valid for arbitrary m_t. We then distinguish between three approximations, which differ only in their treatment of $c^{(1,0)}$:

(1) use no information, i.e. $c^{(1,0)} = 0$;
(2) use the information from the NLO fragmentation function, the heavy-flavor matching coefficients, and α_s decoupling in the massless hard and soft functions, thereby including all terms enhanced by $\ln m_t/M$ for $\mu_f \sim M$;
(3) use the information from approximation 2 plus the constant pieces of the massless NLO hard and soft functions.

These three approximations add progressively more information to the Laplace-space coefficients: the first is NLL in soft-gluon resummation, the second contains parts of the NNLL correction enhanced by small-mass logarithms, and the third includes the entire NNLL correction but expanded in the limit $m_t/M \to 0$. We show the NLO correction to the invariant-mass distribution obtained from these three approximations in Table I. We also show the "exact" result obtained from the leading terms in the $z \to 1$ limit, for

TABLE I. NLO corrections to the differential cross section $d\sigma/dM$ (in pb/GeV) computed using $m_t = 172.5$ GeV, $\mu_f = M$ and MSTW2008NNLO PDFs, at LHC with $\sqrt{s} = 7$ TeV.

	$M = 500$ GeV	$M = 1500$ GeV	$M = 3000$ GeV
Approx. 1	0.074	1.04×10^{-4}	0.70×10^{-7}
Approx. 2	0.085	1.35×10^{-4}	0.94×10^{-7}
Approx. 3	0.126	1.79×10^{-4}	1.19×10^{-7}
Exact ($z \to 1$)	0.154	1.86×10^{-4}	1.20×10^{-7}

arbitrary top-quark mass. We see that the first approximation accounts for about 50%–60% of the exact answer. The second approximation is a small improvement, and can account for up to 75% of the exact answer for high invariant mass. The third is a big improvement over the first two, especially at lower values of the invariant mass, and accounts for nearly the entire correction in the $z \to 1$ limit already at $M = 1500$ GeV.

We now discuss approximate NNLO corrections, and how they change upon including extra information from the small-mass limit. Following our NLO analysis, we take the Laplace-transformed coefficient (71) as the fundamental object. As mentioned in the previous section, the terms $c^{(2,n)}$ for $n = 1, 2, 3, 4$ are known exactly for arbitrary m_t, since they are part of the NNLL calculation. We keep the full mass dependence of these terms in our NNLO approximation, and convert them to momentum-space results as in (45). We then consider two approximations for the constant term $c^{(2,0)}$:

(a) use no information, i.e. $c^{(2,0)} = 0$;

(b) use the information from the NNLO fragmentation function, plus the n_h terms arising from α_s-decoupling and the heavy-flavor coefficients, thereby including all terms enhanced by (up to two) powers of $\ln m_t/M$ for $\mu_f \sim M$.

The first of these is a pure NNLL calculation in soft-gluon resummation for arbitrary m_t, while the second is NNLL plus the part of the N^{3}LL correction enhanced by small-mass logarithms (as well as some unenhanced terms associated with the fragmentation function, heavy-flavor coefficients, and α_s-decoupling to second order). The results for the NNLO correction corresponding to these choices are shown in Table II. The two approximations

TABLE II. NNLO corrections to the differential cross section $d\sigma/dM$ (in pb/GeV) computed using $m_t = 172.5$ GeV, $\mu_f = M$ and MSTW2008NNLO PDFs, at LHC with $\sqrt{s} = 7$ TeV.

	$M = 500$ GeV	$M = 1500$ GeV	$M = 3000$ GeV
Approx. A	5.67×10^{-2}	1.22×10^{-4}	1.11×10^{-7}
Approx. B	6.35×10^{-2}	1.40×10^{-4}	1.26×10^{-7}

are numerically rather close to one another. This shows that logarithms enhanced by powers of $\ln m_t/M$ do not lead to large corrections. Moreover, at higher values of the invariant mass the NNLO corrections can be even larger than the NLO ones. This motivates all-orders soft-gluon resummation instead of NNLO expansions, which was indeed the approach taken in [5]. However, the only way to know the size of the missing N^{3}LL corrections is to calculate them, and it will be interesting to return to this issue once they are known in the $m_t/M \to 0$ limit.

VI. CONCLUSIONS

The pair invariant-mass distribution is an important observable for top-quark physics at hadron colliders. In this paper we set up a framework for dealing with potentially large perturbative corrections at high values of invariant mass. In particular, we gave explicit factorization and resummation formulas appropriate in the double soft ($z \to 1$) and small-mass ($m_t \ll M$) limit of the differential cross section, along with the ingredients needed to evaluate them to NNLL order. While many of the ideas and perturbative calculations needed to accomplish such a resummation were already available in the literature, this is the first time they have all been combined for a description of the invariant-mass distribution in top-quark pair production at hadron colliders. With small modifications the methods can also be used for the double soft and small-mass limit of single-particle inclusive observables such as the p_T or rapidity distribution of the top quark.

We deferred a detailed phenomenological study of our results to future work. However, a short numerical study of the invariant-mass distribution at the LHC with a center of mass energy of 7 TeV revealed the following features. First, it is not obvious that small-mass logarithms of the ratio m_t/M are so large that they need to be resummed, even for values of the invariant mass as high as 3–5 TeV. On the other hand, already for values of the invariant mass of around 1.5 TeV, the leading terms in the $m_t/M \to 0$ limit, including the constant pieces as well as the logarithms, provide an excellent approximation to the full correction within the soft limit. We thus envision the main utility of the results obtained here as a means of adding parts of the N^{3}LL corrections to soft-gluon resummation for arbitrary values of m_t, as an expansion in m_t/M. The missing piece of this analysis is the NNLO soft function for massless two-to-two scattering. Once completed, the calculation of this function will provide valuable information into the importance of higher-order corrections to the NLO + NNLL results for the invariant-mass distribution presented in [5].

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APPENDIX A: SMALL-MASS LIMITS OF MASSIVE HARD AND SOFT FUNCTIONS

Our derivation of the factorization formula (18) used as a starting point the small-mass factorization formula (14) for the differential partonic cross section. In this appendix we briefly discuss the alternative derivation starting from the factorization formula (10) and studying the properties of the massive hard and soft functions in the small-mass limit. For simplicity, we neglect contributions of heavy-quark loops, which give rise to additional terms proportional to n_h taken into account by the heavy-flavor matching coefficient (19)

We begin by recalling that the massive hard matrix is related to UV-renormalized virtual corrections to color-decomposed amplitudes for two-to-two scattering. These IR-divergent quantities are rendered finite through multiplication by a renormalization matrix $\boldsymbol{Z}_m$. We define the bare and renormalized quantities according to

$$\lim_{\epsilon\to 0}\boldsymbol{Z}_m^{-1}(\epsilon, M, m_t, t_1, \mu)|\mathcal{M}(\epsilon, M, m_t, t_1)\rangle = |\mathcal{M}_{\rm ren}(M, m_t, t_1, \mu)\rangle, \tag{A1}$$

where the quantity on the right is finite in the limit $\epsilon \to 0$. We write the analogous relation for massless amplitudes as

$$\lim_{\epsilon\to 0}\boldsymbol{Z}^{-1}(\epsilon, M, t_1, \mu)|\mathcal{M}(\epsilon, M, t_1)\rangle = |\mathcal{M}_{\rm ren}(M, t_1, \mu)\rangle. \tag{A2}$$

We can use these together with the relation between massive and massless scattering amplitudes in the small-mass limit [31] to derive a relation between the massless and massive hard functions. To do so, we first use

$$|\mathcal{M}(\epsilon, M, m_t, t_1)\rangle = Z_{[q]}(\epsilon, m_t, \mu)|\mathcal{M}(\epsilon, M, t_1)\rangle \tag{A3}$$

where $Z_{[q]}$ is the object given to NNLO in Eqs. (37) and (38) of [31]. Here and in the remainder of this appendix we have neglected terms which vanish in the limit $m_t \to 0$. We then multiply both sides of (A3) by the massive renormalization factor, use (A1) to deduce that both sides are finite, and then observe that (A2) implies that

$$Z_{[q]}(\epsilon, m_t, \mu)\boldsymbol{Z}_m^{-1}(\epsilon, M, m_t, t_1, \mu) = f(m_t, \mu)\boldsymbol{Z}^{-1}(\epsilon, M, t_1, \mu). \tag{A4}$$

The function f is a scalar matching correction which is finite in the limit $\epsilon \to 0$. From this relation and the definition of the hard matrix in terms of the IR-renormalized color-decomposed amplitudes, it then follows that

$$\boldsymbol{H}^m_{ij}(M, m_t, t_1, \mu) = f^2(m_t, \mu)\boldsymbol{H}_{ij}(M, t_1, \mu). \tag{A5}$$

Since when neglecting terms proportional to n_h the only m_t dependence in the factorization formula for the partonic cross section is through the fragmentation function, it must also be true that

$$\boldsymbol{S}^m_{ij}(\sqrt{\hat{s}}(1-z), m_t, t_1, \mu) = \boldsymbol{S}_{ij}(\sqrt{\hat{s}}(1-z), t_1, \mu) \otimes \frac{C_D(m_t, \mu)S_D(m_t(1-z), \mu)}{f(m_t, \mu)} \otimes \frac{C_D(m_t, \mu)S_D(m_t(1-z), \mu)}{f(m_t, \mu)}. \tag{A6}$$

Finally, we recall that the soft function is related to real gluon emission in the soft limit, a statement independent of whether the final-state quarks are massive or massless. Since all real emission contributions in the fragmentation function are associated with the function S_D, we expect

$$f(m_t, \mu) \stackrel{?}{=} C_D(m_t, \mu), \tag{A7}$$

which would imply a simple relation between the massive and massless soft functions in (A6) through a double convolution with partonic shape functions. We have checked that (A6) and (A7) are satisfied for the NLO functions, and for the part of the NNLO functions determined by approximate NNLO formulas. In addition, we can use (A7) as a consistency check between various NNLO calculations available in the literature, namely those for the renormalization factors in (A4), that for the fragmentation function, and that for the shape-function. We find nearly total agreement, with the exception of a piece related to the $C_A C_F$ color factor. In particular, we find that direct evaluation of (A4) to NNLO yields

$$f(m_t, \mu) = C_D(m_t, \mu) - 4\pi^2 C_A C_F\left(\frac{\alpha_s}{4\pi}\right)^2. \tag{A8}$$

Unfortunately, we have not been able to resolve the source of this discrepancy.

APPENDIX B: CONVOLUTIONS OF PLUS-DISTRIBUTIONS

Let us define the function

$$f(z, \eta) \equiv \frac{e^{-2\eta\gamma_E}}{2\Gamma(2\eta)}\frac{1}{(1-z)^{1-2\eta}}. \tag{B1}$$

Representations of plus-distributions can be obtained by taking derivatives of f with respect to η and by subsequently expanding the result in the limit $\eta \to 0$. One finds for example, with a test function g,

$$\int_0^1 dz\delta(1-z)g(z) = 2\int_0^1 dz f(z,\eta)g(z)\Big|_{\eta\to 0},$$
$$\int_0^1 dz\left[\frac{1}{1-z}\right]_+ g(z) = \partial_\eta \int_0^1 dz f(z,\eta)g(z)\Big|_{\eta\to 0},$$
$$\int_0^1 dz\left[\frac{\ln(1-z)}{1-z}\right]_+ g(z) = \frac{1}{4}\partial_\eta^2 \int_0^1 dz f(z,\eta)g(z)\Big|_{\eta\to 0} + \frac{\pi^2}{6}\int_0^1 dz f(z,\eta)g(z)\Big|_{\eta\to 0}. \tag{B2}$$

These representations are useful when one wants to calculate the convolution of plus-distributions. Consider for example the following convolution:

$$\left[\frac{1}{1-z}\right]_+ \otimes \left[\frac{1}{1-z}\right]_+ = \int_z^1 \frac{dx}{x}\left[\frac{1}{1-x}\right]_+\left[\frac{1}{1-z/x}\right]_+. \tag{B3}$$

By employing the differential representation found above one finds

$$\left[\frac{1}{1-z}\right]_+ \otimes \left[\frac{1}{1-z}\right]_+ = \partial_{\eta_1}\partial_{\eta_2}\int_z^1 \frac{dx}{x} f(x,\eta_1) f\left(\frac{z}{x},\eta_2\right)\Big|_{\eta_1\to 0,\,\eta_2\to 0}. \tag{B4}$$

The integration gives

$$\int_z^1 \frac{dx}{x} f(x,\eta_1) f\left(\frac{z}{x},\eta_2\right) = \frac{e^{-2(\eta_1+\eta_2)\gamma_E}}{4\Gamma(2\eta_1+2\eta_2)^2} F_1(2\eta_1, 2\eta_2, 2(\eta_1+\eta_2), 1-z) \times (1-z)^{-1+2(\eta_1+\eta_2)}. \tag{B5}$$

Since we are only interested in the terms which are singular in the $z \to 1$ limit, for the purposes of our calculation one can actually set ${}_2F_1 \to 1$. The limits for $\eta_i \to 0$ are then considerably easier to evaluate. To do so, one makes the following analytic continuation in the integral in (B5):

$$(1-z)^{-1+2(\eta_1+\eta_2)} \to (1-z)^{-1+2(\eta_1+\eta_2)} + \frac{\delta(1-z)}{2(\eta_1+\eta_2)}. \tag{B6}$$

One can then safely take the derivatives with respect η_1 and η_2 in Eq. (B4) and take the limit for vanishing η_i to obtain

$$\left[\frac{1}{1-z}\right]_+ \otimes \left[\frac{1}{1-z}\right]_+ = 2\left[\frac{\ln(1-z)}{1-z}\right]_+ - \zeta_2\delta(1-z). \tag{B7}$$

The same kind of procedure can be employed to calculate other convolutions. For example

$$\left[\frac{\ln(1-z)}{1-z}\right]_+ \otimes \left[\frac{1}{1-z}\right]_+ = \partial_{\eta_2}\left[\left(\frac{\partial_{\eta_1}^2}{4}+\zeta_2\right)\int_z^1 \frac{dx}{x} f(x,\eta_1) f\left(\frac{z}{x},\eta_2\right)\Big|_{\eta_1\to 0}\right]\Big|_{\eta_2\to 0} = \frac{3}{2}\left[\frac{\ln^2(1-z)}{1-z}\right]_+ - \zeta_2\left[\frac{1}{1-z}\right]_+ + \zeta_3\delta(1-z), \tag{B8}$$

$$\left[\frac{\ln(1-z)}{1-z}\right]_+ \otimes \left[\frac{\ln(1-z)}{1-z}\right]_+ = \left(\frac{\partial_{\eta_2}^2}{4}+\zeta_2\right)\left[\left(\frac{\partial_{\eta_1}^2}{4}+\zeta_2\right) \times \int_z^1 \frac{dx}{x} f(x,\eta_1) f\left(\frac{z}{x},\eta_2\right)\Big|_{\eta_1\to 0}\right]\Big|_{\eta_2\to 0} = \left[\frac{\ln^3(1-z)}{1-z}\right]_+ - 2\zeta_2\left[\frac{\ln(1-z)}{1-z}\right]_+ + 2\zeta_3\left[\frac{1}{1-z}\right]_+ - \frac{\zeta(4)}{4}. \tag{B9}$$

APPENDIX C: ANOMALOUS DIMENSIONS

The anomalous dimension $\gamma_{\rm cusp}$, introduced in (28) and (29), has the following expansion in powers of α_s:

$$\gamma_{\rm cusp}(\alpha_s) = \frac{\alpha_s}{4\pi}\left[\gamma_0^{\rm cusp} + \left(\frac{\alpha_s}{4\pi}\right)\gamma_1^{\rm cusp} + \left(\frac{\alpha_s}{4\pi}\right)^2\gamma_2^{\rm cusp} + \mathcal{O}(\alpha_s^3)\right]. \tag{C1}$$

Completely analogous expansions hold for γ^q, γ^g, γ^S, and γ^ϕ. The coefficients of the expansion in (B8) are [59]

$$\gamma_0^{\rm cusp} = 4, \qquad \gamma_1^{\rm cusp} = \left(\frac{268}{9} - \frac{4\pi^2}{3}\right)C_A - \frac{80}{9}T_F n_f,$$
$$\gamma_2^{\rm cusp} = C_A^2\left(\frac{490}{3} - \frac{536\pi^2}{27} + \frac{44\pi^4}{45} + \frac{88}{3}\zeta_3\right) + C_A T_F n_f\left(-\frac{1672}{27} + \frac{160\pi^2}{27} - \frac{224}{3}\zeta_3\right) + C_F T_F n_f\left(-\frac{220}{3} + 64\zeta_3\right) - \frac{64}{27}T_F^2 n_f^2. \tag{C2}$$

The coefficients in the expansion of γ^q and γ^g up to $\mathcal{O}(\alpha_s^2)$ are [60,61]

$$\gamma_0^q = -3C_F,$$
$$\gamma_1^q = C_F^2\left(-\frac{3}{2} + 2\pi^2 - 24\zeta_3\right) + C_F C_A\left(-\frac{961}{54} - \frac{11\pi^2}{6} + 26\zeta_3\right) + C_F T_F n_f\left(\frac{130}{27} + \frac{2\pi^2}{3}\right), \tag{C3}$$

and [17,60]

$$\gamma_0^g = -\frac{11}{3}C_A + \frac{4}{3}T_F n_f,$$
$$\gamma_1^g = C_A^2\left(-\frac{692}{27} + \frac{11\pi^2}{18} + 2\zeta_3\right) + C_A T_F n_f\left(\frac{256}{27} - \frac{2\pi^2}{9}\right) + 4C_F T_F n_f. \tag{C4}$$

The coefficients in the expansion of γ^S up to $\mathcal{O}(\alpha_s^2)$ are [12,13,48]

$$\gamma_0^S = -2C_F,$$
$$\gamma_1^S = C_F\left[\left(\frac{110}{27} + \frac{\pi^2}{18} - 18\zeta_3\right)C_A + \left(\frac{8}{27} + \frac{2}{9}\pi^2\right)T_F n_f\right]. \tag{C5}$$

The coefficients in the expansion of PDF anomalous dimensions up to $\mathcal{O}(\alpha_s^2)$ are

$$\gamma_0^{\phi_q} = 3C_F,$$
$$\gamma_1^{\phi_q} = C_F^2\left(\frac{3}{2} - 2\pi^2 + 24\zeta_3\right) + C_F C_A\left(\frac{17}{6} + \frac{22\pi^2}{9} - 12\zeta_3\right) - C_F T_F n_f\left(\frac{2}{3} + \frac{8\pi^2}{9}\right), \tag{C6}$$

and

$$\gamma_0^{\phi_g} = \frac{11}{3}C_A - \frac{4}{3}T_F n_f,$$
$$\gamma_1^{\phi_g} = C_A^2\left(\frac{32}{3} + 12\zeta_3\right) - \frac{16}{3}C_A T_F n_f - 4C_F T_F n_f. \tag{C7}$$

for the gluon and quark PDFs respectively.

Finally, we define expansion coefficients for the QCD β function as

$$\beta(\alpha_s) = -2\alpha_s\left[\beta_0\frac{\alpha_s}{4\pi} + \beta_1\left(\frac{\alpha_s}{4\pi}\right)^2 + \beta_2\left(\frac{\alpha_s}{4\pi}\right)^3 + \ldots\right], \tag{C8}$$

where to three-loop order we have

$$\beta_0 = \frac{11}{3}C_A - \frac{4}{3}T_F n_f,$$
$$\beta_1 = \frac{34}{3}C_A^2 - \frac{20}{3}C_A T_F n_f - 4C_F T_F n_f,$$
$$\beta_2 = \frac{2857}{54}C_A^3 + \left(2C_F^2 - \frac{205}{9}C_F C_A - \frac{1415}{27}C_A^2\right)T_F n_f + \left(\frac{44}{9}C_F + \frac{158}{27}C_A\right)T_F^2 n_f^2. \tag{C9}$$

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