Threshold expansion of the $gg(q\bar{q}) \to Q\bar{Q} + X$ cross section at $\mathcal{O}(\alpha_s^4)$

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Abstract

We derive the complete set of velocity-enhanced terms in the expansion of the total cross section for heavy-quark pair production in hadronic collisions at next-to-next-to-leading order. Our expression takes into account the effects of soft-gluon emission as well as that of potential-gluon exchanges. We prove that there are no enhancements due to subleading soft-gluon couplings multiplying the leading Coulomb singularity.

1. Introduction

Hadronic heavy-quark pair production is of interest not only because of its phenomenological relevance in the particular case of top quarks, but also because of the theoretical insights that may be gained into the singularity structure of QCD in the presence of massive partons.

A complete result for the next-to-next-to-leading order (NNLO) $\mathcal{O}(\alpha_s^4)$ corrections is still elusive despite substantial recent progress. First, the virtual corrections at NNLO were obtained in the limit of large invariants $s, -t \gg 4m^2$ [1, 2] thanks to the understanding of this limit as an alternative regularization scheme for collinear divergences [3, 4]. Subsequently, the complete amplitude in the case of quark annihilation was derived with numerical methods [5], followed by partial analytic results [6, 7]. The latest studies of the structure of massive gauge amplitudes [8, 9, 11, 12, 13] led to the derivation of the soft and collinear divergences of the $gg(q\bar{q}) \to Q\bar{Q}$ two-loop amplitudes in analytical form [13]. Despite all this, the NNLO program for the calculation of the heavy-particle pair production cross section will only be completed once these two-loop corrections have been combined with squared one-loop corrections [14, 15, 16], the one-loop corrections to $t\bar{t} + j$ [17], and the real corrections.

In this note we build on our recent work on soft-gluon radiation [12] and soft-gluon radiation in the presence of Coulomb enhancements [11] to derive the complete set of velocity-enhanced terms in the expansion of the total heavy-quark pair production cross section at NNLO. The result contains terms of the form $\beta^i \log^j \beta$, with $\beta = \sqrt{1 - 4m^2/s}$ the velocity of the heavy quark, and $-2 \leq i \leq 0, 0 \leq j \leq 2i + 4$, which we provide, apart from the constant term $i = j = 0$, which remains inaccessible with the methods used. As discussed in [11], the $\ln \beta$ coefficient at NNLO receives contributions from heavy-quark potentials other than the Coulomb potential, and from soft-gluon effects not contained in the standard resummation formula for the total cross section due to subleading soft-gluon couplings multiplying the leading Coulomb singularity. We compute these terms below, and prove that the subleading soft-gluon effects vanish for the total cross section. Our results may be used for improving approximate NNLO top-quark production cross section calculations [18]. We also provide a general formula for the velocity-enhanced terms at NNLO for arbitrary colour representations of the particles involved, which requires as only

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2. Sources of enhancement

There are two general sources of enhancement of the partonic cross section near threshold. One is connected with the emission of soft gluons, resulting in up to two powers of \( \ln \beta \) per emission, whereas the other is due to potential exchanges of gluons (the Coulomb potential being the most prominent example), yielding up to one factor of \( 1/\beta \) and \( \ln \beta \) per loop.

The NNLL soft-gluon effects can be readily derived either by inverting the Mellin-space transform of Ref. [12] or, directly in \( x \)-space, from the resummation formula of Ref. [11]. The latter approach has been studied before [19, 20] in the context of the Drell-Yan and Higgs-boson production processes at hadron colliders. The soft-gluon enhancement of the Coulomb-potential effects has been considered at NLO/NLL in Ref. [21] assuming factorization of the two effects. A priori, there could be a highly non-trivial intertwining between the two. The general factorization of leading soft-gluon and Coulomb effects has been studied recently in Ref. [11] to all orders, resulting in the formula

\[
\sigma_{pp'}(s, \mu) = \sum_{i,i'} H_{ii'}(m, \mu) \int d\omega \sum_{R_n} J_{R_n}(E - \frac{\omega}{2}) W^{R_n}_{ii'}(\omega, \mu)
\]

for the partonic cross sections, which justifies the multiplicative factorization of the two effects in Mellin space to NNLO. In the case at hand, where we are only interested in the NNLO expansion of the resummed result, we can describe the problem as a sum of a pure NNLO soft-gluon exchange (which requires the knowledge of the two-loop anomalous dimension [11, 12]) contained in the two-loop contribution to the soft function \( W^{R_n}_{ii'} \); a soft-gluon enhancement of the Coulomb-potential exchange due to the convolution of the one-loop terms in \( J_{R_n} \) and \( W^{R_n}_{ii'} [22] \); and, finally, two-loop non-Coulomb potential and kinetic-energy corrections as described by non-relativistic effective theory (NRQCD), which for the present purpose may be thought of as two-loop contributions to the non-relativistic function \( J_{R_n} \). By factorizing the “hard” cross sections \( H_{ii'}(m, \mu) \) from the soft and Coulomb effects, one generates not only logarithms of the type \( 1/\beta \times \log^2 \beta \) and \( 1/\beta \times \log \beta \), but also a process-dependent non-logarithmic term proportional to \( 1/\beta \), due to the product of the matching coefficients and the Coulomb potential. Our result below differs from the one given in Ref. [18, 23] and due to this effect, the value of the two-loop soft anomalous dimension [11, 12], and the \( \ln \beta \) terms from the non-Coulomb effects, which we now derive.

We present two ways to obtain the desired result. The first is based on an explicit calculation of the potential contribution in NRQCD. We first generalize the expression for the colour-singlet heavy-quark potential in momentum space given in Ref. [24] to arbitrary colour representations \( R_n \). To obtain the NNLO \( \ln \beta \) terms it is sufficient to use the four-dimensional potentials. The required terms read

\[
\hat{V}(p, q) = \frac{4\pi D_{R_n}}{q^2} \alpha_s(\mu^2) \left[ 1 + \left( a_1 - \beta_0 \ln \frac{q^2}{\mu^2} \right) \frac{\alpha_s}{4\pi} \right. \\
+ \left. \frac{\pi \alpha_s(\mu^2)}{2m} \left( \frac{D_{R_n}}{2} + C_A \right) + \frac{p^2}{m^2} + \frac{q^2}{m^2} v_{\text{spin}} \right]
\]

where \( D_{R_n} \) is the strength of the Coulomb potential in representation \( R_n \), such that \( D_{R_n} = -C_F \) for the singlet and \( D_{R_n} = -(C_F - C_A)/2 \) for the octet representation (note the sign convention!), and \( v_{\text{spin}} = 0 \) and \(-2/3\) for a \( t\bar{t} \) pair in a spin-singlet and spin-triplet state, respectively. The non-Coulomb potentials, including a new result for the one-loop \( 1/r^2 \)-potential in an arbitrary representation, are those in the second line. The first line refers to the Coulomb potential and its one-loop correction that is already dealt with as described above. To NNLO we need the resummed insertions of the non-Coulomb potentials used in the \( e^+e^- \rightarrow t\bar{t} \) calculation of Ref. [24],
given explicitly in Ref. [25], expanded to NNLO, which results in very simple expressions. Including the relativistic kinetic-energy correction we find the non-Coulomb contribution

$$\sigma_{X^{\text{inc}}} = \sigma_X^{(0)} \alpha_s^2 \langle \mu^2 \rangle \ln \beta \left[-2D_{R_n}(1 + v_{\text{spin}}) + D_{R_n}C_A \right]$$

to the total cross section, with $\sigma_X^{(0)}$ the Born cross section in the spin and colour channel $X$. For top quarks the Born cross section in the $q \bar{q}$ initiated channel is a pure colour-octet spin-triplet, whereas in gluon-gluon fusion the $t \bar{t}$ state is spin-singlet but colour-octet or -singlet.

The second derivation of the non-Coulomb logarithms uses known results on the threshold expansion of the $e^+e^- \rightarrow t \bar{t}$ and $\gamma\gamma \rightarrow t \bar{t}$ processes at NNLO. The potential contributions are implicit in these results, and the two processes cover the singlet-triplet spin dependence of the results for the enhanced terms in exact correspondence to the hadronic case. The only non-trivial issue is the colour dependence since we also need the colour-octet case. It is well known that for an interaction with colour structure $T^a \otimes T^b$, the transition between singlet and octet is obtained by a simple change $C_F \rightarrow C_F - C_A/2$ corresponding to the different value of $D_{R_n}$. But the $1/r^2$ potential comes also from exchanges of two gluons as depicted in Fig. 1. An explicit check proves that each of the diagrams gives the correct contribution (as far as colour is concerned), with the same replacement as before. Thus, we obtain the correct results for hadronic $t \bar{t}$ production by keeping only the velocity-enhanced terms from the respective formulae of $[26, 27]$, making the replacement $C_F \rightarrow C_F - C_A/2$ for colour-octet contributions, and removing the contribution from the hard matching coefficient at one-loop multiplying the one-loop Coulomb potential. The latter step is crucial in obtaining the correct result, since the appropriate matching coefficients corresponding to the processes considered have already been taken into account in the soft gluon enhancement of the Coulomb contribution as described above.

There could be another enhanced single or double logarithm of velocity at NNLO from the product of a $\alpha_s / \beta$ Coulomb term multiplying an $\alpha_s \ln^2 \beta$ or $\alpha_s \ln \beta$ term from a beta-suppressed subleading soft-gluon coupling $[11]$. Such suppressed couplings exist for the emission of soft gluons from the initial state as well as from the final state. We now show that such terms do not appear in the total pair production cross section. To this end we imagine obtaining the cross section by evaluating the imaginary part of forward-scattering graphs such as those of Fig. 2. We first consider the subleading coupling to the heavy-quark loop, so the gluon coupling to the external line in Fig. 2 is the standard eikonal coupling. In the framework of non-relativistic effective theory the subleading gluon coupling corresponds to the $x \cdot E$ interaction $[29, 30]$. An expansion of the heavy-quark loop in the velocity can be extracted directly by the strategy of regions $[31]$. As described in the latter work, it is sufficient to consider the following regions of integration momenta in the partonic cms frame where the sum of the heavy-particle momenta is $(2m, \vec{0})$: hard $(k \sim m$, with $m$ the heavy-quark mass and $k$ a loop momentum), potential $(k^0 \sim m \beta^2, k \sim m \beta)$, soft $(k^0 \sim m \beta, k \sim m \beta)$ and ultrasoft $(k^0 \sim m \beta^2, k \sim m \beta^2)$. At NNLO the diagrams corresponding to the soft region vanish, as they generate only scaleless integrals. The source of singular terms is in the potential and ultrasoft regions. By the velocity scaling only terms corresponding to the potential three-momentum contribute odd powers of $\beta$. The same scaling arguments also show that, in any

$^1$This can be anticipated from the known expansion of the NLO cross section $[28]$. From this result one can readily verify that the logarithms of velocity appear in terms suppressed by even powers of $\beta$ relative to the leading terms, i.e. no $\alpha_s \log \beta$ terms of the mentioned origin are generated.
denominator containing a combination of a potential and an ultrasoft momentum, the ultrasoft momentum will be (multipole) expanded. Therefore, the denominators containing potential three-momenta will not depend on the direction of any external three-momentum (unlike denominators containing an ultrasoft three-momentum). In consequence, rotational invariance implies that all integrals with an odd number of potential three-momenta in the numerator vanish. Thus, given a term with a specified power of $\beta$, the next higher-order contribution will be suppressed by a relative factor of $\beta^2$, smaller than the terms we seek.

Next, regarding the subleading soft-gluon couplings to the initial state, the relevant expansion is one in transverse momentum. The effective Lagrangian for the corrections to the eikonal approximation is given in soft-collinear effective theory by $\xi \left( x_\perp^2 n_\mu W_c \gamma F^{\mu\nu} W^\nu \right) \frac{2}{x_\perp^2} \xi$ for quarks [32, 33], and similar terms involving transverse derivatives or factors of $x_\perp$ for the couplings to collinear gluons, and of soft quarks. None of these terms can contribute a beta-suppressed term, since the initial-state momenta in Fig. 2 can always be chosen to have zero transverse momentum, implying that loop integrals with transverse-momentum factors in the numerator vanish by arguments similar to those applied to the heavy-quark couplings. This completes the proof, that we have correctly taken into account all possible sources of singular terms in the expansion of the cross sections for heavy-quark pair production at NNLO by including the extra terms from the non-Coulomb potentials.

Note that some of the cuts of Fig. 2 correspond to three-particle colour correlations at the amplitude level, for which the infrared divergence structure has recently been given in Ref. [13]. The latter work shows that the infrared-singular three-particle correlations may not vanish in the limit $\beta \to 0$ in the amplitude, but that they do in the virtual contributions to the total cross section at NNLO in the particular case of top quarks because of colour projections [12, 13]. Our arguments above prove that there are no contributions to the $\ln \beta$ terms from three-particle correlations in both, the virtual and real corrections. This holds independent of particular colour representations for purely kinematic reasons.

### 3. Results

Next we present the main result of this paper, namely the expansion of the two-loop partonic cross section close to the partonic threshold $\beta = 0$. As we emphasized above, our result is complete up to the so-called constant terms $C_{gq}^{(2)}$, $C_{gg,1}^{(2)}$, $C_{gg,8}^{(2)}$. Their derivation requires a dedicated calculation that goes beyond the scope of the present work. Setting $\mu_R = \mu_F = \mu$, the result for the total cross-section close to threshold reads:

$$
\sigma_{ij,1}(\beta, \mu, m) = \begin{pmatrix}
\sigma_{ij,1}^{(0)} \\
\sigma_{ij,1}^{(1,0)} + \sigma_{ij,1}^{(1,1)} \ln \left( \frac{\mu^2}{m^2} \right) \\
\left( \frac{\alpha_s(\mu^2)}{4\pi} \right)^2 \left( \sigma_{ij,1}^{(2,0)} + \sigma_{ij,1}^{(2,1)} \ln \left( \frac{\mu^2}{m^2} \right) + \sigma_{ij,1}^{(2,2)} \ln^2 \left( \frac{\mu^2}{m^2} \right) \right) + \mathcal{O}(\alpha_s^3) 
\end{pmatrix}
$$

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where I = 1, 8 is a colour index and \(ij = (q\bar{q}, gg)\), whereas \(\alpha_s(\mu^2)\) is defined in the \(\overline{\text{MS}}\) scheme with \(n_f\) (number of massless quarks) flavours. The derivation of the coefficients of \(\ln^n(\mu^2/m^2)\) with \(n = 1, 2\) from one-loop results and splitting functions is given in Appendix B. The non-trivial scale-independent two-loop contributions \(\sigma^{(2,0)}_{ij,1}\) read:

\[
\sigma^{(2,0)}_{q\bar{q},1} = \frac{(2C_F - C_A)^2\pi^4}{3\beta^2} + \frac{(2C_F - C_A)^2\pi^2}{9\beta} \left[ 288C_F \ln^2 \beta + 6(48C_F \ln 2 - 23C_A + 2n_l) \ln \beta + 12C_F (-24 + 9 \ln 2 + \pi^2) + 3C_A (89 - 58 \ln 2 - 3\pi^2) + 6n_l (-5 + 6 \ln 2) - 32 \right] \\
+ 512C_F^2 \ln^4 \beta + \frac{128}{9} C_F \left[ 72C_F (-2 + 3 \ln 2) - 29C_A + 2n_l \right] \ln^3 \beta \\
+ \frac{16}{9} \left[ 2C_F (12C_F (120 - 207 \ln 2 + 156 \ln^2 2 - 7\pi^2) + 3C_A (217 - 198 \ln 2 - 4\pi^2) \\
+ 6n_l (-9 + 10 \ln 2) - 32) + 3C_A (17C_A - 2n_l) \right] \ln^2 \beta \\
+ \frac{8}{27} \left[ 2C_F (18C_F (-960 + \ln 2 (1368 - 84\pi^2) - 1140 \ln^2 2 + 576 \ln^3 2 + 55\pi^2 + 336\zeta_3) \\
+ C_A (-7582 + 108 \ln 2 (115 - 2\pi^2) - 5886 \ln^2 2 + 360\pi^2 + 189\zeta_3) \\
+ 2n_l (338 - 630 \ln 2 + 378 \ln^2 2 - 9\pi^2) + 192 (2 - 3 \ln 2) \right] \ln \beta + C^{(2)}_{q\bar{q}} ,
\]

\[
\sigma^{(2,0)}_{gg,1} = \frac{4C_F^2\pi^4}{3\beta^2} + \frac{2C_F^2\pi^2}{9\beta} \left[ 288C_A \ln^2 \beta + 6(C_A (-11 + 48 \ln 2) + 2n_l) \ln \beta + 9C_F (-20 + \pi^2) + C_A (66 - 66 \ln 2 + 3\pi^2) + 2n_l (-5 + 6 \ln 2) \right] + 512C_A^2 \ln^4 \beta \\
+ \frac{128}{9} C_A \left[ C_A (-155 + 216 \ln 2) + 2n_l \right] \ln^3 \beta + \frac{32}{9} C_A \left[ 9C_F (-20 + \pi^2) \right] \\
+ C_A (1963 - 2790 \ln 2 + 1872 \ln^2 2 - 90\pi^2) + 2n_l (-17 + 18 \ln 2) \right] \ln^2 \beta \\
+ \frac{16}{27} \left[ 27C_F (-2C_F \pi^2 + C_A (80 + 6 \ln 2 (-20 + \pi^2) - 5\pi^2)) + C_A (C_A (-23758 \\
+ 18 \ln 2 (1963 - 96\pi^2) - 24246 \ln^2 2 + 10368 \ln^3 2 + 1251 \pi^2 + 6237\zeta_3) \\
+ 2n_l (218 - 306 \ln 2 + 162 \ln^2 2 - 9\pi^2) \right] \ln \beta + C^{(2)}_{gg,1} ,
\]

\[
\sigma^{(2,0)}_{gg,8} = \frac{(2C_F - C_A)^2\pi^4}{3\beta^2} + \frac{(2C_F - C_A)^2\pi^2}{18\beta} \left[ 576C_A \ln^2 \beta + 12(C_A (-23 + 48 \ln 2) + 2n_l) \ln \beta + 18C_F (-20 + \pi^2) + C_A (278 - 132 \ln 2 - 3\pi^2) + 4n_l (-5 + 6 \ln 2) \right] + 512C_A^2 \ln^4 \beta \\
+ \frac{128}{9} C_A \left[ C_A (-173 + 216 \ln 2) + 2n_l \right] \ln^3 \beta + \frac{16}{9} C_A \left[ 18C_F (-20 + \pi^2) \right] \\
+ C_A (4553 - 6156 \ln 2 + 3744 \ln^2 2 - 201\pi^2) + 2n_l (-37 + 36 \ln 2) \right] \ln^2 \beta \\
+ \frac{4}{27} \left[ 54C_F (-4C_F \pi^2 + C_A (180 + 12 \ln 2 (-20 + \pi^2) - 7\pi^2)) + C_A (C_A (-111418 \\
+ 36 \ln 2 (4499 - 201\pi^2) - 105624 \ln^2 2 + 41472 \ln^3 2 + 5823 \pi^2 + 24840\zeta_3) \\
+ 4n_l (505 - 666 \ln 2 + 324 \ln^2 2 - 18\pi^2) \right] \ln \beta + C^{(2)}_{gg,8} .
\]

In order to construct the two-loop correction to the colour-averaged cross section from the
colour-state specific components given above, one has to first multiply the two-loop contributions Eqs. (54) and (58) by, respectively, $\sigma^{(0)}_{13}$ and $\sigma^{(0)}_{11}$ (see Eq. (41)), and then add them together. The singlet/octet Born terms can be found in Appendix B. Finally, by setting $\mu = m$, all colour factors to their numerical values, and $n_t = 5$ as applicable to top-quark production, we get the following result for the colour-averaged total inclusive cross-section close to partonic threshold:

$$
\sigma^{(2)}_{qq} = \frac{3.60774}{\beta^2} + \frac{1}{\beta} \left( -140.368 \ln^2 \beta + 32.106 \ln \beta + 3.95105 \right) + 910.222 \ln^4 \beta - 1315.53 \ln^3 \beta + 592.292 \ln^2 \beta + 528.557 \ln \beta + C^{(2)}_{qq},
$$

$$
\sigma^{(2)}_{gg} = \frac{68.5471}{\beta^2} + \frac{1}{\beta} \left( 496.3 \ln^2 \beta + 321.137 \ln \beta - 8.62261 \right) + 4608 \ln^4 \beta - 1894.91 \ln^3 \beta - 912.349 \ln^2 \beta + 2456.74 \ln \beta + C^{(2)}_{gg},
$$

which differs in the coefficients of the $1/\beta$ and $\ln \beta$ terms from the expressions given in [22] for the reasons mentioned in section 2.

In conclusion, the above formulae contain all velocity-enhanced terms in the total hadronic production of heavy quarks at NNLO near the partonic threshold. A compact general result for the velocity-enhanced terms in the production of equal-mass heavy-particle pairs in the collisions of massless particles for arbitrary colour representations is provided in appendix A.

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Appendix A. A formula for arbitrary representations

Here we provide the velocity-enhanced terms at NNLO for the production of a pair of heavy particles with equal mass $m$ in the scattering of massless partons in colour representations $r$ and $r'$, respectively, under the assumption that the Born cross section (which is factored out as in Eq. (41)) admits an $S$-wave term proportional to $\beta$. The heavy-particle pair is in colour representation $R_a$ and a definite spin state. The threshold expansion reads

$$
\sigma^{(2)}_{X} = \frac{4\pi^4 D^2_{R_a}}{3\beta^2} + \pi^2 D_{R_a} \beta \left\{ \left( -8 \right) (C_r + C_{r'}) \left[ \ln^2 \left( \frac{2m\beta^2}{\mu} \right) - \frac{\pi^2}{8} \right] + 2 \left( \beta_0 + 4C_{R_a} \right) \ln \left( \frac{2m\beta^2}{\mu} \right) - 8C_{R_a} - 2a_1 - 4 \Re[C_X^{(1)}] + 2\beta_0 \ln \left( \frac{2m}{\mu} \right) \right\} + 128 (C_r + C_{r'})^2 \ln^4 \beta + 64 (C_r + C_{r'}) \left\{ 4 (C_r + C_{r'}) (L_8 - 2) - \frac{\beta_0}{3} - 2C_{R_a} \right\} \ln^3 \beta
$$

$$
+ \frac{8}{3} (C_r + C_{r'}) \left\{ \left[ 72 L_8^2 - 288 L_8 + 576 - 35\pi^2 \right] + \frac{16}{9} (C_r + C_{r'}) \left[ 18 \Re[C_X^{(1)}] + 18\beta_0 (L_8 - 2) + 36C_{R_a} (-3L_8 + 7) + C_A (67 - 3\pi^2) - 20n_l T_f \right] + 16C_{R_a} (\beta_0 + 2C_{R_a}) \right\} \ln^2 \beta
$$

$$
+ \left\{ 8 (C_r + C_{r'}) \left[ 8L_8^3 - 48 L_8^2 + \left( 192 - \frac{35\pi^2}{3} \right) L_8 - 384 + \frac{70\pi^2}{3} + 112\zeta_3 \right] \right\}
$$
\[ + 2 \{ C_r + C_{r'} \} \left[ -16 \text{Re} \left[ C_X^{(1)} \right] \left( -L_8 + 2 \right) + \beta_0 \left( -8L_8^2 + 32L_8 - 64 + \frac{11\pi^2}{3} \right) \right] \]
\[ + 2C_{R_n} \left( -24L_8^2 + 112L_8 - 224 + \frac{35\pi^2}{3} \right) \]
\[ + C_A \left( \frac{8}{3} \left( \frac{67}{3} - \pi^2 \right) L_8 - \frac{4024}{27} + \frac{59\pi^2}{9} + 28\zeta_3 \right) + \frac{4n_f T_f}{9} \left( -40L_8 + \frac{296}{3} - \pi^2 \right) \]
\[ + 4C_{R_n} \left[ -4 \text{Re} \left[ C_X^{(1)} \right] - 4 \left( \beta_0 + 2C_{R_n} \right) \left( -L_8 + 3 \right) + C_A \left( \frac{98}{9} + \frac{2\pi^2}{3} - 4\zeta_3 \right) \right] \]
\[ + \frac{40}{9} n_f T_f \right] + 16\pi^2 D_{R_n} \left[ C_A - 2D_{R_n} (1 + v_{\text{spin}}) \right] \right\} \ln \beta + \mathcal{O}(1) . \] (A.1)

We obtained this result by expanding the resummation formula (1) to NNLO and adding the non-Coulomb terms according to Eq. (3). \( C_r, C_{r'} \) and \( C_{R_n} \) denote the quadratic Casimir operators of the colour representations, \( \beta_0 = \frac{1}{3} C_A - \frac{1}{3} n_f T_f \) is the one-loop beta-function coefficient, and \( L_8 = \ln(8m/\mu) \). The quantities \( D_{R_n}, a_1 = \frac{31}{9} C_A - \frac{20}{9} n_f T_f \) and \( v_{\text{spin}} \) are connected with the heavy-quark potentials as discussed in the main text. \( C_X^{(1)} \) is the one-loop hard matching coefficient in the resummation formula for hadronic heavy-particle pair production at threshold (11), when the heavy-particle pair is in colour and spin state \( X \). Alternatively, it can be deduced from the constant term in the threshold limit of the NLO production cross section \( \sigma_X^{(1)} \) in colour and spin channel \( X \) by comparing the expansion of \( \sigma_X^{(1)} \) to the formula

\[ \sigma_X^{(1)} = \frac{2\pi^2 D_{R_n}}{\beta} + 4 \{ C_r + C_{r'} \} \left[ \text{Re} \left[ \frac{8m\beta}{\mu} \right] \right] + 4 \{ C_{R_n} + 4 \{ C_r + C_{r'} \} \} \ln \left( \frac{8m\beta}{\mu} \right) + 12C_{R_n} + 2 \left\{ \text{Re} \left[ C_X^{(1)} \right] + \mathcal{O}(\beta) \right\} . \] (A.2)

The results for \( t\bar{t} \) production in the main text can be generated from the general formula by inserting the relevant colour and spin factors. The required matching coefficients \( \text{Re} C_X^{(1)} \) can be determined from (31) (for convenience of the reader, the NLO cross sections are reproduced in Appendix B below) and (A.2). Note that the cubic \( \ln \mu \) dependence in the \( L_8^2 \) term in (A.1) cancels with a corresponding term in the product \( \text{Re} \left[ C_X^{(1)} \right] L_8 \) as required since \( \sigma_X^{(2)} \) can depend on \( \ln \mu \) at most quadratically.

### Appendix B. Derivation of the scale dependence

The scale-dependent terms in Eq. (4) can be obtained from Eq. (A.1). Here we give an independent derivation from the known LO and NLO results; the procedure has been detailed, for example, in Ref. (33) and we adopt it in the following. To the best of our knowledge, these terms are not available in the literature in completely analytical form.

We consider the case \( \mu_R = \mu_F = \mu \). To simplify the following discussion, we introduce the functions \( s_{(a,b)}^{(0,1)} = 2^{-a} \beta s_{(a,b)}^{(0,1)} \) with \( s_{(0,0)}^{(0,1)} = \beta \). We then rewrite Eq. (4) as:

\[ \sigma_{ij,1}(\beta, \mu, m) = \frac{\sigma_{ij,1}^{(0)}}{\beta} \left\{ \beta + \frac{\alpha_s(\mu^2)}{2\pi} \left[ s_{ij,1}^{(0,0)} + s_{ij,1}^{(0,1)} \ln \left( \frac{\mu^2}{m^2} \right) \right] \right\} + \left( \frac{\alpha_s(\mu^2)}{2\pi} \right)^2 \left[ s_{ij,1}^{(2,0)} + s_{ij,1}^{(2,1)} \ln \left( \frac{\mu^2}{m^2} \right) + s_{ij,1}^{(2,2)} \ln^2 \left( \frac{\mu^2}{m^2} \right) + \mathcal{O}(\alpha_s^3) \right] \] (B.1)

Note that as follows from Eq. (B.5) below, the overall factor \( \sigma_{ij,1}^{(0)}/\beta \) is a beta independent constant. It is factored out for later convenience. We will not consider the \( ij = qg \) subprocess since \( \sigma_{qg,1} = \)
$O(\beta^3)$. The scaling functions appearing in Eq. (B.1) read:

$$s_{ij,1}^{(1)}(\rho) = \beta_0 s_{ij,1}^{(0,0)}(\rho) - P_{ik}^{(0)} \otimes s_{kj,1}^{(0,0)}(\rho) - s_{ik,1}^{(0,0)} \otimes P_{kj}^{(0)}(\rho),$$

$$s_{ij,1}^{(2,2)}(\rho) = \frac{3}{4} \beta_0 s_{ij,1}^{(1,1)}(\rho) - \frac{3}{4} P_{ik}^{(0)} \otimes s_{kj,1}^{(1,1)}(\rho) - \frac{1}{2} s_{ik,1}^{(1,1)} \otimes P_{kj}^{(0)}(\rho),$$

$$s_{ij,1}^{(2,1)}(\rho) = \frac{3}{2} \beta_0 s_{ij,1}^{(1,0)}(\rho) + \frac{1}{2} \beta_1 s_{ij,1}^{(0,0)}(\rho) - 2 P_{ik}^{(0)} \otimes s_{kj,1}^{(1,0)}(\rho) - 2 P_{ik}^{(1)} \otimes s_{kj,1}^{(0,0)}(\rho) + O(\beta^3).$$

In the above equation we need to consider the cross sections as functions of the dimensionless variable $\rho = 4 m^2/\bar{s}$, and with $\beta = \sqrt{1-\rho}$. We have also introduced the “hat” notation such that for any function $f(\rho)$ we have $\hat{f}(\rho) = f(\rho)/\rho$; for its origin see the discussion in Ref. [36].

Also, summation over repeated indexes $k = q, \bar{q}, g$ is understood and $\beta_0$ and $\beta_1$ are the QCD beta function coefficients

$$\beta_0 = \frac{11}{3} C_A - \frac{2}{3} n_t, \quad \beta_1 = \frac{34}{3} C_A^2 - \frac{10}{3} C_A n_t - 2 C_F n_t,$$

with $C_A = 3$ and $C_F = 4/3$. Throughout this letter we take the number of active quarks to be equal to the number of light quarks $n_t$. The functions $P^{(n)}$ are the one- and two-loop space-like DGLAP evolution kernels defined as an expansion in $\alpha_s/(2\pi)$.

For the reactions of interest, and neglecting terms that contribute beyond $O(\beta)$, Eqs. (B.2) reduce to:

$$s_{qq,1}^{(1)}(\rho) = \beta_0 s_{qq,1}^{(0,0)}(\rho) - 2 P_{qq}^{(0)} \otimes s_{qq,1}^{(0,0)}(\rho),$$

$$s_{qq,1}^{(2,2)}(\rho) = \frac{3}{4} \beta_0 s_{qq,1}^{(1,1)}(\rho) - P_{qq}^{(0)} \otimes s_{qq,1}^{(1,1)}(\rho) + O(\beta^3),$$

$$s_{qq,1}^{(2,1)}(\rho) = \frac{3}{2} \beta_0 s_{qq,1}^{(1,0)}(\rho) + \frac{1}{2} \beta_1 s_{qq,1}^{(0,0)}(\rho) - 2 P_{qq}^{(0)} \otimes s_{qq,1}^{(1,0)}(\rho) - 2 P_{qq}^{(1)} \otimes s_{qq,1}^{(0,0)}(\rho) + O(\beta^3).$$

The results for the $gg$ initiated subprocess can be obtained from Eqs. (B.3) by replacing everywhere the pairs $qq$ and $\bar{q}q$ by $gg$, see also Ref. [37].

The above convolutions can be performed in a straightforward manner, by expanding the splitting functions around $x = 1$ and keeping only the $1/[1-x]_+$ terms and $\delta$-functions. To make our presentation self contained, in the following we present all terms from Eq. (4) that are not already given in Eqs. (3.6). We do not present the terms $O(1)$, i.e. the terms that are not enhanced by inverse power of $\beta$ or by a power of $\ln \beta$, since they are at the same level as the presently unknown coefficients $c_{qq}^{(2)}$, $c_{gg}^{(2)}$ and $c_{gg,8}^{(2)}$ appearing in Eqs. (5.6.7). Nevertheless, we have calculated these $O(1)$ terms and they can be found in electronic form available with the preprint of this paper.

The leading-order (Born) terms appearing in Eq. (4) read:

$$\sigma_{qq,8}^{(0)} = \frac{\pi \beta}{8N^2} \frac{(N^2 - 1)}{m^2} \alpha_s^2(\mu^2),$$

$$\sigma_{gg,8}^{(0)} = \frac{\pi \beta}{8N(N^2 - 1)} \frac{\alpha_s^2(\mu^2)}{m^2},$$

$$\sigma_{qq,1}^{(0)} = \frac{\pi \beta}{4N(N^2 - 1)} \frac{\alpha_s^2(\mu^2)}{m^2},$$

with $N = 3$ the number of colours. The NLO terms appearing in Eq. (4) read:

$$\sigma_{qq,8}^{(1,1)} = -\frac{22}{3} C_A - \frac{4}{3} n_t + C_F (10 - 16 \ln 2) - 16 C_F \ln \beta,$$

$$\sigma_{qq,8}^{(1,0)} = (2C_F - C_A) \frac{\pi^2}{\beta} + 32 C_F \ln^2 \beta + [32 C_F (-2 + 3 \ln 2) - 8 C_A] \ln \beta.$$
\[-\frac{4}{3} C_F (\!\! - 24 + \pi^2 + 63 \ln 2 - 48 \ln^2 2) + \frac{1}{9} C_A (308 - 9 \pi^2 - 180 \ln 2)
+ \frac{4}{9} n_l (-5 + 6 \ln 2) - \frac{32}{9} ,\]

\[\sigma_{gg,8}^{(1,1)} = -16 C_A (-1 + \ln 2) - 16 C_A \ln \beta ,\]

\[\sigma_{gg,8}^{(1,0)} = (2 C_F - C_A) \frac{\pi^2}{\beta} + 32 C_A \ln^2 \beta + 24 C_A (-3 + 4 \ln 2) \ln \beta
+ C_F (-20 + \pi^2) + \frac{1}{6} C_A (504 - 17 \pi^2 - 624 \ln 2 + 384 \ln^2 2) ,\]

\[\sigma_{gg,1}^{(1,1)} = \sigma_{gg,8}^{(1,1)} ,\]

\[\sigma_{gg,1}^{(1,0)} = 2 C_F \frac{\pi^2}{\beta} + 32 C_A \ln^2 \beta + 32 C_A (-2 + 3 \ln 2) \ln \beta
+ C_F (-20 + \pi^2) + \frac{1}{3} C_A (204 - 7 \pi^2 - 288 \ln 2 + 192 \ln^2 2) .\] (B.6)

Finally, the NNLO terms in Eq. (21) proportional to \(\ln^2 (\mu^2/m^2)\) read:

\[\sigma_{gg,8}^{(2,2)} = 128 C_F^2 \ln^2 \beta + \frac{32 C_F^2 (-5 + 8 \ln 2) - 440}{3} C_F C_A + \frac{80}{3} C_F n_l \ln \beta + O(1) ,\]

\[\sigma_{gg,8}^{(2,1)} = \frac{\pi^2}{\beta} \left[ (16 C_A C_F - 32 C_F^2) \ln \beta - 11 C_A^2 - 12 C_F^2 - 4 C_F n_l + C_A (28 C_F + 2 n_l) \right]
- 512 C_F^2 \ln^3 \beta + \left[ 480 C_F C_A - 64 C_F n_l - 64 C_A^2 (-21 + 32 \ln 2) \right] \ln^2 \beta
+ \left[ -88 C_A^2 + 16 C_A n_l + \frac{64}{3} C_F^2 (-102 + 7 \pi^2 + 156 \ln 2 - 120 \ln^2 2) \right] \ln \beta + O(1) ,\]

\[\sigma_{gg,8}^{(2,1)} = \frac{\pi^2}{\beta} \left[ (16 C_F C_A - 32 C_F C_F) \ln \beta - \frac{11}{3} C_A^2 + C_F \left( \frac{22}{3} C_A - \frac{4}{3} n_l \right) + \frac{2}{3} C_A n_l \right]
- 512 C_A^2 \ln^3 \beta + \left[ -\frac{32}{3} C_A^2 (-167 + 192 \ln 2) - \frac{64}{3} C_A n_l \right] \ln^2 \beta
+ \left[ -16 C_F C_A (-20 + \pi^2) - \frac{16}{9} C_A n_l (-37 + 36 \ln 2) \right] \ln \beta + O(1) ,\]

\[\sigma_{gg,1}^{(2,2)} = \sigma_{gg,8}^{(2,2)} ,\]

\[\sigma_{gg,1}^{(2,1)} = \frac{\pi^2}{\beta} \left[ -32 C_F C_A \ln \beta + \frac{22}{3} C_F C_A - \frac{4}{3} C_F n_l \right] - 512 C_A^2 \ln^3 \beta + \left[ -\frac{64}{3} C_A n_l \right.
+ \frac{32}{3} C_A^2 (155 - 192 \ln 2) \right] \ln^2 \beta + \left[ 16 C_F C_A (20 - \pi^2) + \frac{32}{9} C_A n_l (17 - 18 \ln 2) \right.
+ \frac{16}{9} C_A^2 (-1963 + 96 \pi^2 + 2502 \ln 2 - 1440 \ln^2 2) \right] \ln \beta + O(1) .\] (B.7)

Eqs. (B.7) are in agreement with the partially numerical results provided in Ref. [23].

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