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Top-quark pair production close and below threshold: parametric and missing higher-order uncertainties

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Abstract

The detection of binding and the search for bound-state effects affecting top-quark pair production close and below threshold at the Large Hadron Collider has just started. In this work we assess the uncertainties on theoretical predictions for the top-quark pair invariant mass distribution in this kinematical regime stemming from variation of the parameters used as input in the computation, working in the NRQCD framework. We consider top-quark mass, width, $\alpha_s(M_Z)$ and renormalization and factorization scale variation, as well as parton distribution function variation. We also discuss and provide a conservative estimate of the uncertainties related to the limited accuracy of the color-singlet and octet Green's functions describing the formation of the quasi-bound $t\bar{t}$ state (colloquially often referred as "toponium"), that we computed so far using as input a NLO QCD potential of Coulomb-like form. We contrast the uncertainties of the NRQCD calculation to those affecting standard QCD calculations valid at large enough top-quark pair invariant mass values. We comment on the relevance and experimental implications of our findings in view of present-day analyses by the ATLAS and CMS collaborations. Finally, we provide predictions for toponium formation at the Future Circular Collider in the hadron-hadron modality, including uncertainties as discussed above. The predictions obtained for fixed values of the various input parameters are released in tables, to facilitate their public use.

I. INTRODUCTION

After the discovery of the top quark at the TeVatron [1, 2], top-quark pair production in hadron-hadron collisions has been the focus of many experimental analyses and further theory efforts (for recent theory and experimental reviews, see e.g. Ref. [3, 4]). This has led to a growing understanding of the extreme importance of the top quark within and beyond the Standard Model (SM), mainly driven by its large mass, that facilitates connections with Beyond-the-Standard-Model (BSM) physics [5], has implications for the electroweak vacuum stability [6–8] and plays a role in the electroweak symmetry breaking process. Furthermore, the top quark decays much faster than hadronizing, implying that processes leading to the production of top quarks can be well described by perturbative QCD (pQCD), thus providing an excellent test of this theoretical framework.

Most of the $t\bar{t}+X$ events at hadron colliders collected so far involve top quarks not at rest. At the Large Hadron Collider (LHC), the bulk contribution to the total inclusive cross section for $t\bar{t}+X$ production comes from events with $t\bar{t}$ pair invariant mass $M_{t\bar{t}} \sim O(400)$ GeV, above the value $2m_t \sim 345$ GeV, computed with a top-quark pole mass value of 172.5 GeV well compatible with recent estimates by the PDG [9] and corresponding to free stable top and antitop quarks produced at rest, but not too far from it. In the case of stable top quark, $2m_t$ is the minimal threshold of the $M_{t\bar{t}}$ distribution. On the other hand, in the most realistic case of non-null top-quark width Γ_t, even the region of lower invariant mass values is populated. Various theory studies in the literature, conducted both in the direct-QCD (d-QCD) and in the Soft-Collinear Effective Theory (SCET) frameworks, have shown that the effects of the resummation of large logarithms associated to real soft gluon emission close to partonic thresholds [1], play an important role in modifying the predictions for total cross sections.

Some theory studies have also investigated the role of Coulomb corrections, encoding the exchange of potential gluons between the t and $\bar{t}$ quarks produced by the hard scattering, in the threshold region. These may lead to binding effects, that, together with long-distance effects [sentence ok ?], may induce the formation of toponium for $M_{t\bar{t}} \lesssim 2m_t$. What we call here toponium is not a long-lived proper bound state like charmonia or bottomonia, due to the fact that the top quark, differently from the charm and bottom quarks, decays quite fast before hadronizing, i.e. even before a top quark may complete an orbit around another one. By toponium we mean instead a fast-decaying quasi-bound state composed by a free [?] top and antitop quark slowing moving one with respect to the other and exchanging gluons among each other. Toponium has been described in the non-relativistic QCD (NRQCD) framework, applicable when the relative velocity between the two quarks is small enough ($v_{t\bar{t}} \to 0$) [2]. So far, it has been studied quite deeply in the case of lepton colliders [], whereas the studies at hadron colliders are much less, both on the theory and on the experimenal side.

[1] Besides the minimal threshold $\beta = \sqrt{1-4m_t^2/\hat{s}} \to 0$, corresponding to both t and $\bar{t}$ quarks produced at rest, other more general partonic threshold variables have been introduced. Examples of partonic threshold variables often considered in the case of $t\bar{t}+X$ hadroproduction are $s_4 = \hat{s}+\hat{t}+\hat{u}-2m_t^2$ in single-particle-inclusive kinematics and $z = M_{t\bar{t}}^2/\hat{s}$ in pair-invariant-mass kinematics, where $\hat{s}$, $\hat{t}$ and $\hat{u}$ denote the partonic Mandelstam variables. Threshold is approached for $s_4 \to 0$ or $z \to 1$, respectively. These two limits do not constrain the velocities of the top and antitop quarks, thus allowing for $t\bar{t}$ pair not at rest. In this work we will use z as partonic threshold variable appearing in the large logarithms associated to threshold real soft gluon emission.

[2] This does not necessarily imply that the velocity of the the t- and $\bar{t}$-quark is small. The latter can still be large.

In general, in the case of hadron colliders, the NRQCD approach is based on a factorization of the cross section for heavy-flavour bound state (i.e. charmonium or bottomonium) production in terms of PDFs, the hard-scattering cross-section, leading to the production of free heavy quark and antiquark, and long-distance matrix-elements describing the formation of bound states. In the case of wide resonances, like the top quark, these long-distance effects can be expressed in terms of non-relativistic Green's functions. Additionally, as discussed above, in the case of $t\bar{t}$ we can not speak about a "bound" state, considering the top-quark fast decay. The formation of different $t\bar{t}$ ${}^{2S+1}L_J^{[C]}$ states in the $q\bar{q}$, qg and gg channels has been considered, where S, L, and J are the spin, orbital angular momentum and total angular momentum of the $t\bar{t}$ state, respectively, and C denotes its color state (1 for color-singlet and 8 for color-octet, using the decomposition $3 \otimes 3 = 1 + 8$ of the SU(3) representations). It has turned out that some of these states can give a relevant numerical contribution to the $(t\bar{t} + X)$ cross section.

The majority of the studies looking at binding and bound-state effects have focused on total inclusive cross sections, for which an accuracy of approximate N^{3}LL and approximate N^{3}LO has been reached in Ref. [10], including the joint resummation of both the Coulomb and the threshold logarithms. The latter results have been incorporated in the last version of the `TOPIXS` code, which, in its first version [11] was reaching NNLL accuracy in soft and Coulomb resummation, including the contribution from bound-state effects [12]. Previous work by an independent group also considering both Coulomb and threshold corrections on total cross sections has reached NLO+NNLL accuracy in Ref. [13]. [What is the relation of the various papers above with NRQCD ?] On the other hand, some studies have also investigated the $M_{t\bar{t}}$ differential distribution [14, 15], although at a lower accuracy. Ref. [14] has incorporated binding effects and ISR effects at NLO, whereas Ref. [15] have reached NLO + NLL accuracy. At NLL, the Coulomb and threshold logarithms factorize [for the cconsidered distribution or for all ?], greatly simplifying the inclusion of the resummation of both of them in cross-section calculations. The latter papers have explicitly shown that, besides allowing for a non-negligible cross-section for $M_{t\bar{t}}$ values below the minimal threshold, Coulomb corrections [and long-distance effects ?] affect even the cross section above it, playing a role in the $M_{t\bar{t}}$ region up to $\sim$ 400 GeV. In any case, we expect that the NRQCD framework is not applicable anymore above this invariant mass value.

Considering the sophistication, accuracy and precision reached by the present-day experimental analyses at the LHC, it is legitimate to think that these effects are finally measurable, and their proper consideration may affect/modify the interpretation of some of the most recent experimental results. They can, e.g., be critical for both SM and BSM analyses (see e.g. Ref. [16]) and for an improved determination of the top-quark mass value from top-quark differential cross sections with the indirect method (see e.g. Ref. [17, 18]), and, as a consequence of the latter, may even affect the results of simultaneous fits of top-quark mass, Parton Distribution Functions (PDF) and $\alpha_s(M_Z)$ based on multi-differential $t\bar{t} + X$ data, considering the correlations among these quantities (see e.g. Ref. [19]).

Indeed, they will be increasingly important in Run 3 and even in future experimental studies, in the High-Luminosity LHC phase (HL-LHC). We emphasize that nowadays not only total cross sections, but even multi-differential cross-section measurements with uncertainties of the order of $\sim \mathcal{O}(\%)$ are reported by the experimental collaborations, with bins of increasingly small size, even around threshold.

In the light of all considerations above, the main aim of this work is revisiting the predictions for the $M_{t\bar{t}}$ distributions presented in Ref. [15, 20], by considering a more comprehensive assessment of uncertainties, including not only scale variation (already considered in Ref. [15, 20]), but even, top-quark mass and width, PDF+$\alpha_s(M_Z)$ variation, plus uncertainties associated to missing higher orders in the QCD potential used for Green's function calculation. After a description/recap of the theory framework in Section II, we present our predictions with uncertainties in Section III, we discuss implications for state-of-the-art experimental analyses in Section IV, we consider future scenarios (HL-LHC and FCC-hh) in Section V, and we draw our Conclusions in Section VI. In order to facilitate the incorporation of binding, bound-state and real soft gluon resummation effects in the ongoing experimental analyses and the comparisons with predictions from other theory frameworks, this work is accompanied by public tables of our predictions for various input parameters, downloadable from the web.

II. THEORY FRAMEWORK

In this section we summarize the theory framework adopted in this paper, largely based on the one already presented and used by some of us in Ref. [15], with a few updates.

A. Fixed-order calculations

To compute fixed-order predictions, we apply two different methodologies: the NRQCD effective field theory, which allows to account for bound-state effects, and whose validity is limited to low v, i.e. low enough $M(t\bar{t})$, and standard conventional QCD at large $M(t\bar{t})$. The two theories should produce same or very similar predictions in a range of intermediate $M(t\bar{t})$ values, where they should both be valid. One of the aims of this work is to provide quantitative information on this interval, where a matching between the two theories should be performed.

In conventional perturbation theory (QCD), we obtain fixed-order predictions of the $M_{t\bar{t}}$ inclusive distribution with the `MATRIX` framework, up to NNLO accuracy. We use an in-house modified version of `MATRIX` [21, 22], that we interfaced to `PineAPPL` [23] to facilitate the computation of PDF+$\alpha_s(M_Z)$ uncertainties and the generation of predictions with different PDF+$\alpha_s(M_Z)$ sets. More detail on this interface are discussed in Ref. [18]. `MATRIX` is based on q_T-subtraction [24, 25], a (N)NLO infrared (IR) divergence subtraction method, potentially subject to power corrections, due to its non-locality. We explicitly verify that, for the distributions of interest of this paper, the size of these corrections is indeed within the numerical accuracy of Monte Carlo integration ($\sim 1\%$), by comparing predictions with `MATRIX` with those obtained with the `HighTEA` framework [26], based on the local IR subtraction method STRIPPER [27–29]. In the q_T-subtraction framework, a slicing-parameter cut is introduced in practical computation, i.e. calculations are performed for $q_T > q_{T,0}$ and the cross section corresponds to the limit $q_{T,0} \to 0$. We perform our computations by fixing $r_0 \equiv q_{T,0}/m_{t\bar{t}} = 0.0XXX$ and we explicitly verify that the limit above still lead to predictions compatible to those obtained with this cut, even in the threshold region.

In NRQCD, we use the NLO input extracted from Ref. [30]. Although P-wave states are also discussed in this work, we limit ourselves to S-wave (i.e. $L = 0$) states, being the contribution of P-wave ones suppressed by powers of v. Our master formulas are summarized in Ref. [20] See Ref. [15] for a more extended discussion.

B. Resummation of large logarithms associated with real soft-gluon emission close to threshold

Resummation, applied to the three most relevant contributions to cross-sections, corresponding to the channels $gg \to {}^1S_0^{[1]}, {}^1S_0^{[8]}, {}^3S_1^{[8]}$, causes an enhancement of predictions of some percent. We treat it according to the methodology discussed in Section 4 of Ref. [15], also used in Ref. [20]

III. PREDICTIONS

Based on the theory framework summarized in section II, in the following we present our predictions for the invariant mass distribution at the LHC, using state-of-the-art inputs and considering their variation, which allow for a comprehensive estimates of their current uncertainties.

A. Setup, input and variations

For our central default predictions, we focus on LHC at $\sqrt{S}$ = 13 TeV, using as input $\mu_R = \mu_F = m_t$ (or $m_t/2$? [We decide this after seeing the central predictions with the various scales]), m_t = 172.5 GeV, the NNPDF31_nnlo_as_0118 PDF set (303600), with its accompanying $\alpha_s(M_Z)$ = 0.118 value. In the NRQCD Green's functions we use m_t = ... and Γ_t = ... [Please, Matthias, make compatible choices for what you use in Green's functions with what we use in the hard functions, if possible].

We consider the following variations:

- **renormalization and factorization scale variation**:
  - a factor of two up and down with respect to central scale $\mu_R = \mu_F$ (see above)
  - [shall we also try 7-point scale variation, or we are sure that 2-point is enough ? Giovanni's code will allow for a check.]
- **PDF variation**: we consider central PDFs from the following NNLO sets, together with their associated $\alpha_s(M_Z)$ values:
  - ABMPtt_5_nnlo_0118 (XXXXX) special PDF with $\alpha_s(M_Z) = 0.118$,
  - CT18NNLO (14000) with $\alpha_s(M_Z) = 0.118$,
  - MSHT20nnlo_as118 (27400) with $\alpha_s(M_Z) = 0.118$,
  - NNPDF30_nnlo_as_0118 (261000) with $\alpha_s(M_Z) = 0.118$ (elective choice by ATLAS)

  - For one of these PDFs (possibly the default one NNPDF31_nnlo_as_0118), we should also do the full band from its own variation. This should at least be done in the QCD part (before thinking to do it in the NRQCD part).

  General Note:
  Please observe that if we use μ_R and μ_F sufficiently low, NLL effects are negligible (probably not true! To be better verified), and, therefore we can do the study of PDF uncertainties just at NLO. We can study PDF uncertainties just at NLO in any case.

- **α_s variation**:

  we perform two studies

- NNPDF31_nnlo_as_0118 (303600) with its central $\alpha_s(M_Z) = 0.118$ is compared to the results from the NNPDF3.1 variants with $\alpha_s(M_Z) = 0.116$ and 0.120, called NNPDF31_nnlo_as_0116 (319300) and NNPDF31_nnlo_as_0120 (319500), respectively.
- do the same with another input PDF, e.g. running the eigenvectors of 1,2,3,4,5,6 of MSHT20nnlo_as_smallrange (27500), corresponding to variations $\alpha_s(M_Z) = 0.115$, 0.116, 0.117, 0.119, 0.120, 0.121, respectively.

Same General Note as before I think applies even for α_s variation.

- m_t **variation**:

  Considering the typical variations of m_t by ± 1 GeV applied in experimental analyses,

  - NNPDF31_nnlo_as_0118 with $m_t = 172.5$ GeV, is compared to the case where one uses the same PDF and $m_t = 173.5$ GeV and $m_t = 171.5$ GeV.

  Additionally:

  - ABMPtt_5_mnlo_0118 with $m_t = 172.5$ GeV used above, is compared to ABMPtt_5_nnlo (43560) (with $\alpha_s(M_Z)$ =0.118 or its proper $\alpha_s(M_z)$?) with its proper m_t value ($m_t = 170.2$ GeV).

- **simultaneous PDF +** $\alpha_s(M_Z)$ **+** m_t **variation, accounting for correlations**

  - ABMPtt_5_nnlo (43560) with its default $\alpha_s(M_Z) = 0.1150$ and $m_t = 170.2$ GeV value is compared to the special set ABMPtt_5_nnlo_0.118 (XXXXX) with $\alpha_s(M_Z) = 0.118$ and relevant $m_t = YYY$ GeV value.

- Γ_t **variation**

  In all previous cases we use a Γ_t value compatible with the m_t value.

  - Additionally, for the central default prediction we vary Γ_t by $\pm XXX$ GeV [Matthias, up to you to decide this variation]

- **Uncertainties due to missing higher-orders in the Green's function**

  Green's functions are computed using a soft scale $\mu_s = 30$ GeV. [Shall we vary it or keep fixed ?]

  - For our default predictions, we consider the uncertainties stemming from the use of the NNLO Coulomb Green's functions, instead of the NLO one. (The general NNLO Green's function is divergent, but the Coulomb one is not, so we can use it.)

B. Estimate of uncertainties

Plots with uncertainties and discussion on them.

IV. PHENOMENOLOGY IMPLICATIONS FOR PRESENT LHC ANALYSES

In this section we discuss the implications of our uncertainty estimate, considering selected present setups of $t\bar{t}+X$ experimental analyses developed and/or under development within the ATLAS and CMS collaborations.

V. FUTURE SCENARIOS

In this section we examine the degree of relevance of our results for precision physics studies at HL-LHC and at possible future colliders, considering in particular the possible setups currently under discussion for the FCC-hh.

A. HL-LHC

B. FCC-hh

We consider the following center-of-mass energies....for which integrated luminosities of .....are expected.

VI. CONCLUSIONS

We made a comprehensive study of uncertainties affecting the $M_{t\bar{t}}$ distribution close and below threshold.

We found that the most dominant uncertainties are related to.... whereas the uncertainties related to ....only have a minor effects.

Our predictions for different inputs are publicly available at the website ....

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