Higher Order Corrections to Spin Correlations in Top Quark Pair Production at the LHC

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We calculate, for the first time, the next-to-next-to-leading order (NNLO) QCD corrections to spin correlations in top quark pair production at the LHC. The NNLO corrections play an important role in the description of the corresponding differential distributions. We observe that the standard model calculation describes the available $\Delta\phi_{\ell\ell}$ data in the fiducial region but does not agree with the $\Delta\phi_{\ell\ell}$ measurement extrapolated to full phase space. Most likely this discrepancy is due to the difference in precision between existing event generators and NNLO calculations for dilepton top-pair final states.

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Introduction.—Within the standard model (SM) of particle physics, individual top quarks produced in proton-(anti)proton collisions are not polarized. The spins of two *pair-produced* top quarks are, however, correlated to each other. It is possible [1] to study directly such *spin correlations* between top quarks since, due to the very rapid decay of the top quark, its spin is passed to its decay products almost free of nonperturbative effects [2]. This implies that top quark spin correlations are calculable.

The study of top quark spin correlations has a long history. Spin correlations have been long recognized as a powerful tool for probing the nature of the quark sector in the SM [3–14] as well as Higgs and/or beyond the SM (BSM) physics [15–19]. Indeed, a generic BSM contribution to top production will alter the top-pair production spin density matrix. An important example is the case of a light spin zero top quark supersymmetric partner, the stop, decaying to top quarks [16,18]. Seeking deviations between SM predictions and LHC measurements of top quark spin correlations represents a powerful, model-independent search strategy for possible BSM physics coupled to the top quark sector.

Very recently, the ATLAS Collaboration published [20] a very precise measurement of spin correlations in top quark pair production at the LHC (earlier LHC and Tevatron measurements include Refs. [21–25]). A deviation of about 3.2σ with respect to the SM has been observed. This is by far the biggest deviation from the SM observed in the top quark sector at the LHC to date. Given the potential significance of such a discrepancy, in this Letter we calculate for the first time the complete set of NNLO QCD corrections to top quark pair production and decay. Our calculation uses the narrow width approximation. It allows us to qualitatively increase the level of precision of SM predictions for realistic top quark final states, thus making the comparison with the ATLAS data [20] much more predictive.

Generally, top quark spin correlations can be assessed following two strategies. The first strategy, which we call direct, reconstructs the top-pair spin density matrix and is based on kinematic distributions computed in specially designed frames of reference; see Refs. [8,9] for details.

The second strategy, which we call indirect, utilizes differential distributions defined in the laboratory frame. These distributions are best suited for experimental study but they tend to be only partly sensitive to spin correlations. In order to maximize the extracted information about spin

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correlations, the use of a likelihood function was advocated for in Ref. [10]. Clearly, a prerequisite for extracting spin correlations from laboratory frame distributions is good control over theory predictions.

In this Letter we use the *indirect* approach to spin correlations and study the following differential distributions: the angular difference $\Delta\phi_{\ell\ell}$ between the two leptons in the transverse plane and the rapidity difference $|\Delta\eta_{\ell\ell}|$ between the two leptons. Both observables are sensitive to spin correlations and can be measured with high precision since the top quarks need not be reconstructed.

Our main goal in this Letter is to establish whether higher order corrections can account for the 3.2σ discrepancy in the $\Delta\phi_{\ell\ell}$ distribution reported in Ref. [20]. Our finding is in the affirmative. In hindsight, this should not come as a complete surprise given the important role higher order QCD corrections play in the $t\bar{t}$ forward-backward asymmetry [26] and in taming the so-called top p_T discrepancy [27]. We caution, however, that the interpretation of higher order corrections is not completely straightforward since it uncovers possible subtleties in the modeling of realistic top quark final states at hadron colliders. We explain all of this in detail in the results section.

Details about the calculation.—The calculations performed in this Letter are at next-to-next-to-leading order (NNLO) in QCD. This means that NNLO QCD corrections to both top-pair production and top quark decay are included. This is the first time top quark pair production and decay has been consistently computed in NNLO QCD.

As in Ref. [28], where top-pair production was included in approximate NNLO, the present calculation is performed within the narrow width approximation for both the top quark and the W boson. This approximation is known to work well [29] for distributions that are away from kinematic boundaries, which is the case considered in this Letter. Below we also compare our calculation with a more recent NLO study [30]. We recall that this approximation has been used in the existing NNLO QCD calculations for single top production including top decay [31,32].

We consistently truncate the *production* $\times$ *decay* differential cross section through NNLO in QCD:

$$\begin{aligned} d\sigma^{\mathrm{LO}} &= d\sigma^{\mathrm{LO\times LO}}, \\ d\sigma^{\mathrm{NLO}} &= d\sigma^{\mathrm{NLO\times LO}} + d\sigma^{\mathrm{LO\times NLO}} - \frac{2\Gamma_t^{(1)}}{\Gamma_t^{(0)}} d\sigma^{\mathrm{LO}}, \\ d\sigma^{\mathrm{NNLO}} &= d\sigma^{\mathrm{NNLO\times LO}} + d\sigma^{\mathrm{LO\times NNLO}} + d\sigma^{\mathrm{NLO\times NLO}} \\ &\quad - \frac{2\Gamma_t^{(1)}}{\Gamma_t^{(0)}} d\sigma^{\mathrm{NLO}} - \frac{(\Gamma_t^{(1)})^2 + 2\Gamma_t^{(0)}\Gamma_t^{(2)}}{(\Gamma_t^{(0)})^2} d\sigma^{\mathrm{LO}}. \end{aligned} \tag{1}$$

As the above equations imply, the top quark decay width has also been expanded in powers of α_S [as in Eq. (2)]. The contribution containing NLO corrections to the two decays is included in $d\sigma^{\mathrm{LO\times NNLO}}$.

The $d\sigma^{\mathrm{NLO}}$ correction has been known for some time [33–35]. These results were extended in Ref. [36] to include approximate NNLO results in production, while Ref. [28] combined the approximate NNLO correction in production with the complete NNLO correction in decay.

Our calculation uses the STRIPPER framework [37–39] for NNLO calculations in QCD. The only exception is the calculation of the $d\sigma^{\mathrm{NLO\times NLO}}$ contribution, where, purely for convenience, the *decay* correction is computed with the help of Catani-Seymour dipoles [40,41] as implemented in Ref. [42].

We modify the existing calculations of differential top-pair production [27,43,44] in such a way that the information about the helicities of the top quarks is retained. For the double real correction at NNLO, this requires the use of tree-level helicity amplitudes. The real-virtual corrections require the calculation of the one-loop five-point helicity amplitudes for the processes $q\bar{q} \to t\bar{t}g$, $qg \to t\bar{t}q$, and $gg \to t\bar{t}g$. To that end we have used a private version [45] of the OpenLoops2 code [46] which employs the stability and speed improvements of Ref. [47]. We have checked that the result agrees with a modified version of a private code by S. Dittmaier used previously in the calculation of spin-averaged top production. The two-loop amplitudes $q\bar{q} \to t\bar{t}$ and $gg \to t\bar{t}$ have been computed in Ref. [48] using spin projections and the methods used for the derivation of the spin-averaged amplitudes [49].

We have computed independently the NNLO QCD correction to top decay. The two-loop helicity amplitude $t \to bW(\to \ell\nu)$ is known analytically [50–52]. The one-loop helicity amplitude for $t \to bgW(\to \ell\nu)$ has been computed in analytical form in Ref. [53] and has been checked numerically against the OpenLoops and GoSam [54] libraries. Alternatively, we have implemented the results of Ref. [42] and find agreement between the two. We have checked that the assembled fully differential spin-averaged top quark decay width agrees within numerical uncertainties with the program NNTopDec [55] as well as with Ref. [56] (where such a comparison was possible).

For all terms in Eq. (1) but $d\sigma^{\mathrm{NNLO\times LO}}$, we have checked that they agree with Ref. [28].

In the calculation we work in the G_μ scheme and use the following set of numerical inputs:

$$\begin{aligned} m_t &= 172.5\ \mathrm{GeV}, \\ m_W &= 80.385\ \mathrm{GeV}, \\ m_Z &= 91.1876\ \mathrm{GeV}, \\ \Gamma_W &= 2.0928\ \mathrm{GeV}, \\ \Gamma_t &= (1.48063 - 1.18\alpha_S - 2.65\alpha_S^2)\ \mathrm{GeV}, \\ G_F &= 1.166379 \times 10^{-5}\ \mathrm{GeV}^{-2}. \end{aligned} \tag{2}$$

The top quark width is specified as an α_S expansion through NNLO in QCD [55–57], as needed in Eq. (1).

It is treated as a fixed parameter throughout this Letter, and its value in Eq. (2) corresponds to a fixed scale $\mu = m_t$.

In this Letter we take the b quark to be massless and renormalize with $n_F = 5$ active flavors. The top quark is renormalized on shell; i.e., we use the top quark pole mass. Its value $m_t = 172.5$ GeV is lower than the world average. It is chosen such that it agrees with the value used by the ATLAS Collaboration. This way our predictions can be directly compared with Ref. [20].

We use the NNPDF3.1 [58] family of parton distributions but have also checked the CT14 set [59]. The default renormalization and factorization scales are chosen dynamically as proposed in Ref. [44]:

$$\mu_{F,R} = \frac{H_T}{4}, \qquad H_T = \sqrt{m_t^2 + p_{T,t}^2} + \sqrt{m_t^2 + p_{T,\bar{t}}^2}. \quad (3)$$

In the evaluation of the scales equation (3) we have used the true top momenta, not the reconstructed ones.

Although our setup allows us to output FASTNLO tables [60,61] in this first NNLO calculation with top decay, we have chosen for simplicity not to do so. We plan to use this capability in future calculations as with our results [62] of stable top quark production. All results derived in this Letter, together with some extra plots, are available for download from Ref. [63].

Results.—In this Letter we calculate two differential distributions—namely, the two leptons' angular difference in the transverse plane $\Delta\phi_{\ell\ell}$ and their rapidity difference $|\Delta\eta_{\ell\ell}|$.

We have two selection criteria for each distribution. The first one, called *inclusive*, does not assume any selection cuts. The second one, called *fiducial*, is based on the ATLAS selection cuts [20]: an electron and a muon of opposite electric charge with $p_T > 27(25)$ GeV for the harder (softer) lepton and $|\eta| < 2.5$. In addition, we require at least two jets (at least one of which is a b-flavored jet) with $p_T > 25$ GeV and $|\eta| < 2.5$. All jets are defined with the anti-k_T algorithm [64] with $R = 0.4$.

The normalized fiducial and inclusive $\Delta\phi_{\ell\ell}$ and $|\Delta\eta_{\ell\ell}|$ distributions are shown in Figs. 1 and 3, respectively. Each curve is normalized with respect to the corresponding visible cross section; i.e., the integral under it equals unity. The $\Delta\phi_{\ell\ell}$ distribution is compared with the published ATLAS data [20]; the $|\Delta\eta_{\ell\ell}|$ one is not since the corresponding data have not been published yet.

A number of observations can be made from Fig. 1. The most interesting feature is the different behavior of the NNLO/NLO $\Delta\phi_{\ell\ell}$ K factor between the fiducial and inclusive cases. With respect to the inclusive case, in the fiducial case the K factor is much larger, the NNLO distribution is in good agreement with the data, and the scale uncertainty is much larger. Notably, the NNLO inclusive prediction does not agree well with the data.

Since both the fiducial and inclusive data originate from the same measurement, it is not *a priori* clear why the

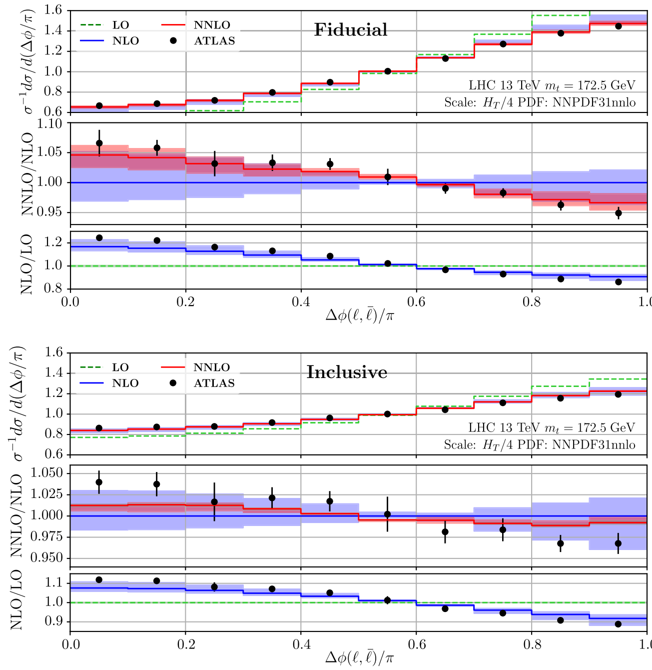

FIG. 1. NNLO QCD predictions for the (top panels) fiducial and (bottom panels) inclusive selections of the normalized $\Delta\phi_{\ell\ell}$ distribution versus the ATLAS data [20]. Uncertainty bands are from seven-point scale variation.

NNLO calculation would agree with only one of them. In our view the most plausible explanation for this discrepancy lies in the extrapolation of the fiducial measurement to the full phase space.

Such a conclusion should not come as a complete surprise since the extrapolation to full phase space is performed with event generators that have accuracy different than the one in this Letter. In fact an early indication about the importance of higher order corrections in top quark production came from the long-standing top quark p_T discrepancy—namely, that NLO-accurate event generators do not model well the LHC top quark p_T distribution (see, e.g., Refs. [65–67]), while the NNLO QCD correction significantly improves the agreement with data [27].

Anatomy of higher order corrections to $\Delta\phi_{\ell\ell}$: —In the following we offer a detailed analysis quantifying a number of possible contributions to this observable. We show that they are too small to affect the behavior of this observable in the SM.

(i) Is the NNLO correction large?: —NLO analyses [20] indicate that higher order effects are likely not going to bridge the 3.2σ discrepancy with the ATLAS $\Delta\phi_{\ell\ell}$ data. Yet we see that the NNLO QCD prediction agrees well with the data in the fiducial region. From this one cannot directly conclude that the NNLO correction is unusually large. The reason is that our NNLO prediction uses scales different from the ones in most event generators.

For our preferred choice of scales we find that the fiducial NNLO/NLO K factor is no larger than 5%. This is a perfectly reasonable NNLO correction which, moreover, is consistent with the NLO scale uncertainty band. The NLO/LO K factor is larger by a factor of about 3. In the inclusive case one observes smaller K factors and less scale variation, which is reasonable to expect since the observable is more inclusive. We note that in both cases the smallness of the LO uncertainty band is due to a cancellation between the normalization factor and is not representative of the true uncertainty in the differential distribution.

We conclude that the behavior of $\Delta\phi_{\ell\ell}$ is consistent with good perturbative convergence. The NNLO correction plays an important role: in the fiducial case it reduces the scale uncertainty by more than a factor of 2 and modifies the slope of the theory prediction in a direction that improves the agreement with data.

(ii) Choice of scales: —All calculations in this Letter are performed with three scales: the one in Eq. (3) as well as $\mu_{F,R} = m_t$ and $\mu_{F,R} = m_t/2$. As can be seen in Fig. 2, the result with scale $m_t/2$ behaves similarly to the one in Eq. (3) and is even closer to the data. On the other hand, the calculation with scale m_t has a larger NNLO/NLO K factor, and the agreement with data in the fiducial case is not as good as with the other two scales.

To understand this behavior, we recall that the scale $\mu_{F,R} = m_t/2$ was found in Ref. [44] to lead to fast perturbative convergence for the total cross section. This behavior is similar to the default dynamic scale of Eq. (3). However, perturbative convergence with the canonical scale $\mu_{F,R} = m_t$ is slower. We conclude that the pattern of higher order corrections for the fiducial $\Delta\phi_{\ell\ell}$ distribution is in line with our previous findings for generic top quark differential distributions. We expect that the predictions based on the default dynamic scale as well as on the scale $\mu_{F,R} = m_t/2$ will not have significant corrections beyond NNLO. By contrast, the scale $\mu_{F,R} = m_t$ may lead to non-negligible corrections beyond NNLO, which is the reason, we believe, that it does not describe the data as well.

(iii) Value of m_t: —With the help of a NLO calculation, we have checked that the value of the top quark mass does not affect the $\Delta\phi_{\ell\ell}$ distribution in a significant way. This may be expected on purely dimensional grounds ($\Delta\phi_{\ell\ell}$ is a dimensionless variable). Nevertheless, a dedicated analysis is warranted in light of the findings of Ref. [68], where it was found that the treatment of spin correlations in certain lepton distributions does have a substantial impact on the extracted top mass.

(iv) Parton distribution function (PDF) dependence: —The effect on the normalized $\Delta\phi_{\ell\ell}$ distribution is at the level of 1% and thus is marginal. We have checked this by comparing two different PDF sets (NNPDF3.1 and CT14), including their PDF errors.

(v) Finite width and electroweak corrections: —We have performed a qualitative check of these effects at NLO using the results of Ref. [30]. While the setup for that reference is different from ours, the comparison indicates that the effects on the $\Delta\phi_{\ell\ell}$ distribution are small, perhaps of the order of 1%. It will be very valuable to investigate such effects in detail in the future.

(vi) Top production versus top decay: —We find that radiative corrections to top quark decay have a small impact on the $\Delta\phi_{\ell\ell}$ distribution.

Observables other than inclusive $\Delta\phi_{\ell\ell}$: —Following Refs. [8,20], we have also investigated the $\Delta\phi_{\ell\ell}$ distribution for several "slices" of the $t\bar{t}$ invariant mass $m_{t\bar{t}}$. Owing to space limitations, we present no results here (however, see Ref. [63]) but only remark that the NNLO corrections are small, in the sense that they are well within the NLO scale uncertainty band and have a much reduced scale variation relative to NLO. Interpreting such results is, however, subtle since our definition of $m_{t\bar{t}}$ is based on the true top momenta, unlike the experimental setup, where

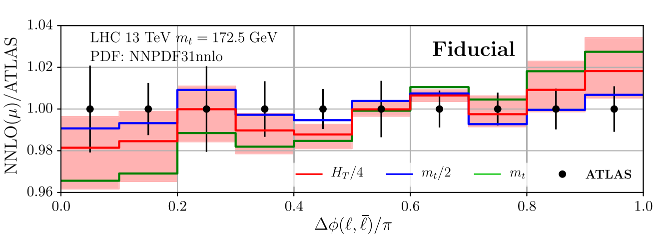

FIG. 2. Three NNLO QCD predictions utilizing different scales versus the ATLAS data [20]. The red band represents the seven-point scale variation for the default scale choice, Eq. (3).

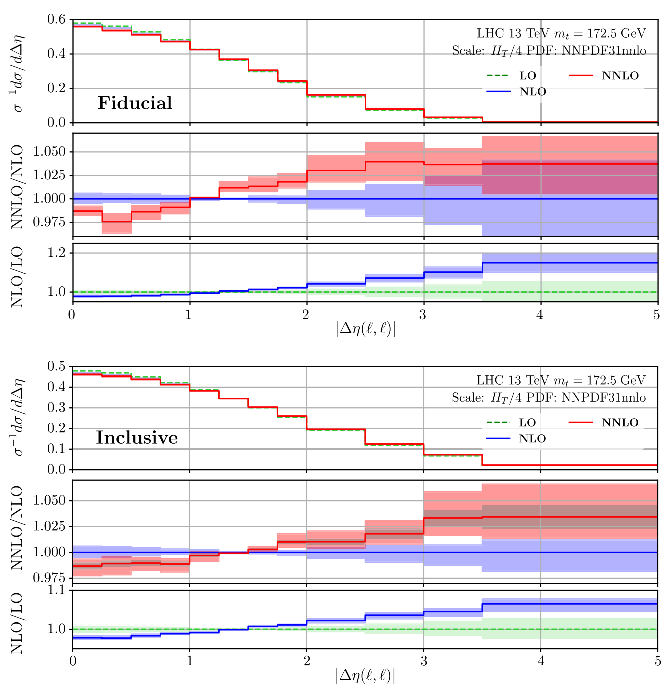

FIG. 3. NNLO QCD predictions for the (top panels) fiducial and (bottom panels) inclusive selections of the normalized $|\Delta\eta_{\ell\ell}|$ distribution. Uncertainty bands are from seven-point scale variation.

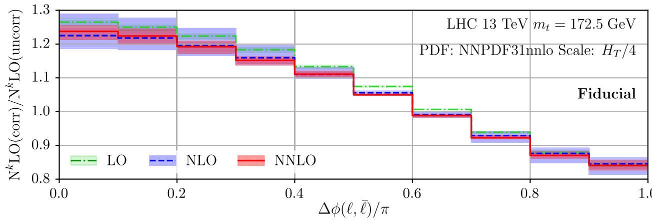

FIG. 4. Size of spin correlations in the fiducial $\Delta\phi_{\ell\ell}$ distribution at each order through NNLO in QCD.

the tops are reconstructed (see also Refs. [8,10] for a discussion of this point).

Finally, in Fig. 3 we show the fiducial and inclusive predictions for the $|\Delta\eta_{\ell\ell}|$ distribution. Unlike the $\Delta\phi_{\ell\ell}$ distribution, the NNLO corrections are significant both in the fiducial and inclusive cases. It will be very interesting to compare these predictions with the data once they become available. An agreement of our NNLO prediction with future data is likely to validate our interpretation of higher order corrections in the $\Delta\phi_{\ell\ell}$ distribution discussed in the subsection pertaining to the anatomy of higher order corrections.

Quantifying spin correlations: —In Fig. 4 we show the magnitude of spin correlations in the $\Delta\phi_{\ell\ell}$ distribution through NNLO in QCD. To that end we take the ratio of the calculations with and without spin correlations at a given order. The former calculation is performed by taking spin-averaged top-production times spin-averaged top decay. We observe that spin correlations are large and change little at higher orders.

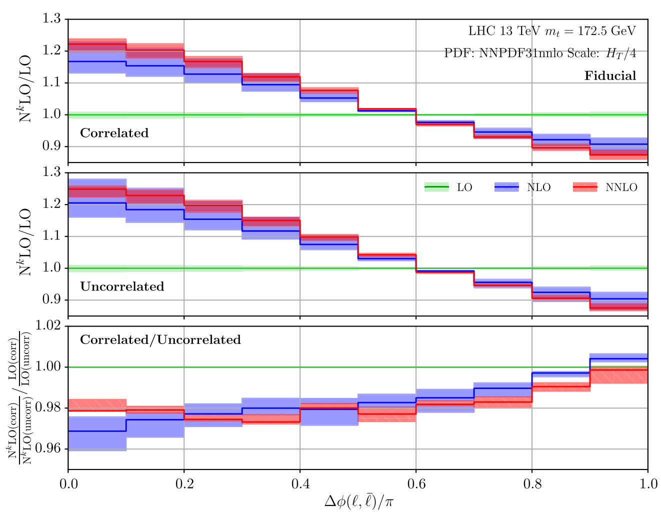

FIG. 5. Disentangling radiative corrections from spin correlations for the fiducial $\Delta\phi_{\ell\ell}$ distribution. Shown is the ratio N^kLO/LO, for $k = 0$, 1, 2, (top panel) for the spin-correlated calculation, (middle panel) for the calculation without spin correlation, and (bottom panel) for their ratio. The bands represent the spread of the ratios for each of the seven scale variations.

In order to disentangle the effect of kinematics from spin correlations, in Fig. 5 we show the ratios NLO/LO and NNLO/LO separately for the exact (top panel) and spin-uncorrelated (middle panel) cases. We observe that all of these K factors are significant in size and nearly identical to each other at a given perturbative order. This means that while higher order corrections are substantial they largely decouple from spin correlations. Indeed, the difference between the two NLO/LO and NNLO/LO bands is much smaller than their individual magnitudes. This can be seen more clearly in the bottom panel, where their ratio is taken.

Our analysis shows that the control of higher order corrections in the $\Delta\phi_{\ell\ell}$ distribution is essential for interpreting spin correlations with high precision. This is because in this observable spin correlations and kinematics are mixed in a very nontrivial way, and therefore a detailed analysis of spin correlations requires a good understanding of kinematic effects.

Conclusions.—In this Letter we compute, for the first time, the complete set of NNLO QCD corrections to top-pair production and decay at hadron colliders. We work in the narrow width approximation for both the top quark and the W boson. We utilize this calculation for the study of spin correlations in top-pair production in the dilepton channel.

Our calculation shows that NNLO QCD corrections to realistic dilepton top quark pair final states play an important role: they increase the SM prediction, significantly decrease the dominant scale uncertainty, and improve the agreement with data.

Using the scales advocated for previously in the context of stable top production, we find that NNLO QCD agrees with the recent 13 TeV ATLAS data, thus alleviating, or perhaps removing altogether, the earlier reported 3.2σ discrepancy with respect to the SM.

An important finding of this Letter is that data extrapolation to full phase space with existing event generators seems not to be compatible with the direct NNLO QCD calculation. We believe that, thanks to the very high precision of both theory predictions and experimental measurements, we begin to see clear evidence that top quark measurements begin to resolve and constrain such delicate modeling effects.

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