

Automatic computations at next-to-leading order in QCD for top-quark flavor-changing neutral processes

Celine Degrande,¹ Fabio Maltoni,² Jian Wang,³ and Cen Zhang⁴

¹*Institute for Particle Physics Phenomenology, Department of Physics, Durham University, Durham DH1 3LE, United Kingdom*

²*Centre for Cosmology, Particle Physics and Phenomenology, Université Catholique de Louvain, B-1348 Louvain-la-Neuve, Belgium*

³*PRISMA Cluster of Excellence & Mainz Institute for Theoretical Physics, Johannes Gutenberg University, D-55099 Mainz, Germany*

⁴*Department of Physics, Brookhaven National Laboratory, Upton, New York 11973, USA*
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Computations at next-to-leading order in the Standard Model offer new technical challenges in the presence of higher dimensional operators. We introduce a framework that, starting from the top-quark effective field theory at dimension six, allows one to make predictions for cross sections as well as distributions in a fully automatic way. As an application, we present the first complete results at next-to-leading order in QCD for flavor-changing neutral interactions including parton shower effects, for tZ , th , ty associated production at the LHC.

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I. INTRODUCTION

The millions of top quarks already produced at the LHC together with the tens of millions expected in the coming years will provide a unique opportunity to search for interactions beyond the Standard Model (SM). Among them flavor-changing neutral (FCN) interactions are of special interest. In the SM, FCN interactions can be generated at one loop, yet they turn out to be suppressed by the Glashow-Iliopoulos-Maiani mechanism [1]. The resulting FCN decay modes of the top quark have branching ratios of order 10^{-12} – 10^{-15} [2–4]. Thus, any signal for top-quark FCN processes at a measurable rate would immediately indicate new physics in the top-quark sector. These processes have been searched for already at different colliders, including LEP2, HERA, Tevatron and more recently at the LHC [5]. So far no signal has been observed and limits have been set on the coupling strengths.

The most important top-quark FCN processes at the LHC include decay processes such as $t \rightarrow qB$ and production processes such as $qg \rightarrow t$ and $qg \rightarrow tB$, where q is a u or c quark and B is a neutral boson, i.e., $B = \gamma, Z, h$. In general, the decay processes are equally sensitive to utB and ctB couplings, while the production modes are less sensitive to ctB , but may provide a better handle on a certain class of utB couplings [6]. In addition, compared to decay modes, single-top production can provide more information. First, it makes a wider range of kinematic variables accessible, helping in the discrimination of the light quark flavors involved and the structure of the qtB couplings. Second, it probes interactions at higher scales where new physics effects could be enhanced. In general, being somewhat complementary, both decay and

production processes are used for setting the most stringent constraints.

Leading order (LO) predictions for the production processes suffer from large uncertainties due to missing higher order corrections. To curb such uncertainties, next-to-leading order (NLO) predictions in QCD for this class of processes have started to be calculated in recent years [7–11], providing a much better, yet incomplete, picture of their relevance. In general, corrections are found to be large, of order 30% to 80%, and to lead to considerable reductions of the residual theoretical uncertainties. Both aspects are important in bounding and possibly extracting top-quark FCN couplings at the LHC.

In this paper we present the first automatic computations for top-quark FCN production processes, $qg \rightarrow tB$ with $B = \gamma, Z, h$, at NLO in QCD, by implementing all flavor-changing dimension-six fully gauge-invariant operators in FEYNRULES [12] and then passing this information into the MADGRAPH5_AMC@NLO framework [13]. Compared to previous works [9–11, 14–17], the salient features of our results can be summarized as follows. Our study is the first where all relevant dimension-six operators for this class of processes (associated production with a boson) are consistently taken into account. In particular the vector-current-like tqZ coupling in $ug \rightarrow tZ$, and the tug and $tugh$ couplings in $ug \rightarrow th$ are included here for the first time. Second, our results are obtained via a fully automatic chain of tools that allows one to go directly from the Lagrangian to the hard events by performing its renormalization at one loop, and then passing the corresponding Feynman rules to the MADGRAPH5_AMC@NLO to generate all the elements necessary for a computation at NLO in QCD. In particular, other processes triggered by the same

set of operators can be seamlessly computed within the same framework. Third, event generation is also automatically available at NLO accuracy, by matching it to the parton shower via the MC@NLO formalism [18] so that results can be employed in realistic experimental simulations. Finally, another important aspect of this work is that it provides a proof of principle that fully automatic computation of cross sections at NLO in QCD is possible in the context of the full dimension-six Lagrangian of the SM. Higher order computations in effective field theories, which are renormalizable only order by order in $1/\Lambda$, Λ being the scale of new physics, present novel technical challenges. In general, UV divergences generated by one operator at a certain order of $1/\Lambda$ have to be absorbed also by other effective operators. As a result, the full set of relevant operators together with their operator mixing effects need to be considered simultaneously, and appropriate UV counterterms have to be implemented in the calculation. Our method and its implementation are fully general and can cover arbitrary NLO calculations in the complete dimension-six Lagrangian of the SM.

II. FRAMEWORK

The FCN couplings of the top quark can be parametrized using either fully gauge-symmetric dimension-six operators [19,20] or dimension-four and dimension-five operators in the electroweak broken phase [6,21]. The latter approach has some intrinsic limitations [22], and we will use the dimension-six operators throughout the paper. The effective Lagrangian can be written as

$$\mathcal{L}_{\text{EFT}} = \mathcal{L}_{\text{SM}} + \sum_i \frac{C_i}{\Lambda^2} O_i + \text{H.c.} \quad (1)$$

In this work we consider qtB couplings at the dimension-six level. The relevant operators must involve one top quark and one light quark. They are

$$\begin{aligned} O_{\varphi q}^{(3,i+3)} &= i(\varphi^\dagger \overleftrightarrow{D}_\mu \varphi)(\bar{q}_i \gamma^\mu \tau^I Q), \\ O_{\varphi q}^{(1,i+3)} &= i(\varphi^\dagger \overleftrightarrow{D}_\mu \varphi)(\bar{q}_i \gamma^\mu Q), \\ O_{\varphi u}^{(i+3)} &= i(\varphi^\dagger \overleftrightarrow{D}_\mu \varphi)(\bar{u}_i \gamma^\mu t), \\ O_{uB}^{(i3)} &= g_Y(\bar{q}_i \sigma^{\mu\nu} t) \tilde{\varphi} B_{\mu\nu}, \quad O_{uW}^{(i3)} = g_W(\bar{q}_i \sigma^{\mu\nu} \tau^I t) \tilde{\varphi} W_{\mu\nu}^I, \\ O_{uG}^{(i3)} &= g_s(\bar{q}_i \sigma^{\mu\nu} T^A t) \tilde{\varphi} G_{\mu\nu}^A, \quad O_{u\varphi}^{(i3)} = (\varphi^\dagger \varphi)(\bar{q}_i t) \tilde{\varphi}, \end{aligned}$$

where the operator notation is consistent with Ref. [23], with additional flavor indices. On the right hand side, the subscript $i = 1, 2$ represents the generation of the light quark fields. u_i and q_i are single and doublet quark fields of the first two generations, respectively, while t and Q are of the third generation. φ is the Higgs doublet. A diagonal Cabibbo-Kobayashi-Maskawa matrix is assumed.

The group generators are normalized such that $\text{Tr}(T^A T^B) = \delta^{AB}/2$ and $\text{Tr}(\tau^I \tau^J) = 2\delta^{IJ}$, and $\varphi^\dagger \overleftrightarrow{D}_\mu \varphi \equiv \varphi^\dagger D_\mu \varphi - D_\mu \varphi^\dagger \varphi$, $\varphi^\dagger \overleftrightarrow{D}_\mu \varphi \equiv \varphi^\dagger \tau^I D_\mu \varphi - D_\mu \varphi^\dagger \tau^I \varphi$. For operators with $(i3)$ superscript, a similar set of operators with $(3i)$ flavor structure can be obtained by interchanging $(i3) \leftrightarrow (3i)$, $t \leftrightarrow u_i$ and $Q \leftrightarrow q_i$. The first three operators give rise to V/A couplings of Z to a flavor-changing current, which were not considered in previous calculations of Ref. [10]. The $O_{uB}^{(i3,3i)}$, $O_{uW}^{(i3,3i)}$ and $O_{uG}^{(i3,3i)}$ operators correspond to weak- and color-dipole couplings. In particular, $O_{uG}^{(i3,3i)}$ could induce the production $pp \rightarrow th$, and it was not included in [11]. The last operator gives rise to flavor-changing Yukawa couplings. This operator is actually implemented as $O_{u\varphi}^{(i3)} = (\varphi^\dagger \varphi - v^2/2)(\bar{q}_i t) \tilde{\varphi}$ to avoid any need for a field redefinition in order to remove the tree-level $q-t$ mixing. It is interesting to note that all qtB interactions receive contributions from operators that involve the Higgs field; therefore they are also relevant for constraining new physics in the Higgs sector. Finally, we stress that four-fermion operators should also be taken into account for a complete phenomenological study of FCN interactions; see Ref. [22]. Their implementation in the current framework is possible and is left for future work.

In calculations at NLO in QCD, a renormalization scheme needs to be specified, in particular for the dimension-six operators. We adopt the $\overline{\text{MS}}$ scheme in general, except for masses and wave functions that are renormalized on shell. Specifically, this requires the introduction of off-diagonal wave function counterterms to cancel the $u-t$ or $c-t$ two-point functions generated by $O_{u\varphi}^{(i3,3i)}$. We work in the five-flavor scheme where the b -quark mass is neglected, and we subtract the massless modes according to the $\overline{\text{MS}}$ scheme and the top at zero momentum for the strong coupling constant renormalization [24]. At order α_S these operators will not mix with the SM terms, but mix among themselves. The running of these coefficients is given by the renormalization group equations

$$\frac{dC_i(\mu)}{d\ln\mu} = \gamma_{ij} C_j(\mu), \quad (2)$$

where γ_{ij} for $C_{uG}^{(13)}$, $C_{uW}^{(13)}$, $C_{uB}^{(13)}$ and $C_{u\varphi}^{(13)}$ can be written as a matrix [17,25]:

$$\gamma = \frac{\alpha_S}{\pi} \begin{pmatrix} \frac{1}{3} & 0 & 0 & 0 \\ \frac{2}{3} & \frac{2}{3} & 0 & 0 \\ \frac{10}{9} & 0 & \frac{2}{3} & 0 \\ 4y_t^2 & 0 & 0 & -2 \end{pmatrix}, \quad (3)$$

where y_t is the top-quark Yukawa coupling. The same γ_{ij} matrix applies for the operators with either $(i3)$ or $(3i)$ superscript. The operators $O_{\varphi q}^{(3,i+3)}$, $O_{\varphi q}^{(1,i+3)}$ and $O_{\varphi u}^{(i+3)}$ do

not have any anomalous dimension due to current conservation and do not mix with other operators.

III. IMPLEMENTATION AND CHECKS

The operators are implemented in the universal feynrules output format [26], using the FEYNRULES package [12]. The evaluation of the loop corrections in MADGRAPH5_AMC@NLO requires two additional elements, the UV counterterms and the rational R2 terms which are required by the OPP technique [27]. These are computed fully automatically by the NLOCT [28] package, which has been extended to handle effective field theory's (EFT's) i.e., to compute the R2 and UV divergent parts of amplitudes with integrals of arbitrary high ranks. Currently, such calculations are limited to operators with up to two fermion fields. The determination of the UV divergent part of the counterterms is obtained by simply changing the sign of the UV divergent part of the corresponding amplitude. This avoids the translations of the counterterms vertices in the operator renormalization constants and the associated basis reduction. However, it is only valid when the dimension-six operators are renormalized in the $\overline{\text{MS}}$ scheme.

We have extensively checked our implementation by evaluating the virtual contributions of $ug \rightarrow t$, $u\gamma \rightarrow t$, $uZ \rightarrow t$, $uh \rightarrow t$ and $ug \rightarrow th$ (with uth coupling only) and comparing them with corresponding known analytical expressions numerically. In each case the results agree. In addition we have checked the gauge invariance of all virtual contributions, as well as the pole cancellation when combining virtual and real contributions. When possible, we have also made comparisons with the results for total cross sections for $pp \rightarrow t\gamma, tZ, th$ at the fixed order of Refs. [9–11], finding consistent results.

IV. CALCULATION

As an application of our general framework to the phenomenology of the top quark FCN at the LHC, we consider three processes, $pp \rightarrow t\gamma$, $pp \rightarrow tZ$ and $pp \rightarrow th$. The LO diagrams are shown in Fig. 1. Each process receives contributions from two different interactions, one from utg coupling and the other from utB coupling. At NLO in QCD the utg operator will mix with other operators, and as a result a NLO calculation needs to be carried out with the full set of operators.

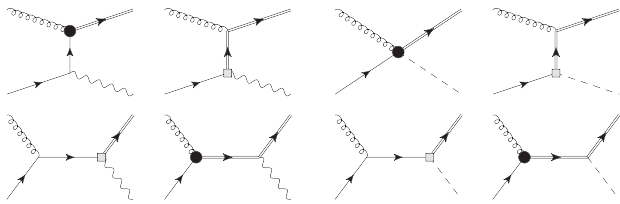


FIG. 1. Tree-level diagrams for $pp \rightarrow tV$ and $pp \rightarrow th$. The black dots represent contributions from color dipole operators $O_{uG}^{(i3,3i)}$, while the shaded squares represent other operators.

Our numerical results are obtained by employing the following input parameters:

$$\begin{aligned}
 m_Z &= 91.1876 \text{ GeV}, & \alpha &= 1/127.9, \\
 G_F &= 1.166370 \times 10^{-5} \text{ GeV}^{-2}, \\
 m_t &= 172.5 \text{ GeV}, & m_h &= 125 \text{ GeV}, & \Lambda &= 1 \text{ TeV}.
 \end{aligned}
 \tag{4}$$

We use CTEQ6M for NLO and CTEQ6L for LO calculations, respectively, with their respective values of α_S [29]. The renormalization scale μ_r and factorization scale μ_f are chosen to be $m_t + m_B$ for the $pp \rightarrow tB$ process, and are allowed to vary independently by a factor of 0.5 to 2. In $pp \rightarrow t\gamma$, we require the photon $p_T > 50$ GeV and its pseudorapidity $|\eta| < 2.5$. For the photon, we employ the isolation criterium of Ref. [30] with a radius of 0.4. The events are then showered with PYTHIA6 [31] or HERWIG6 [32]. Finally, we have checked that the doubly resonant diagrams with the antitop decaying through FCN interactions have a small impact, yet they have been removed from the real contributions; see Ref. [33].

Currently the best limits on top FCN couplings are from the decay searches of $t \rightarrow qZ$ [34], $t \rightarrow qh$ [35,36], and the production searches of $qg \rightarrow t$ [37] and $qg \rightarrow t\gamma$ [38]. To make a viable choice for the operator coefficients in our calculation, we exploit the results of Ref. [22] that are based on a global fit on the full set of current limits,

Coefficient	Limit	Coefficient	Limit	Relevant production
$C_{qq}^{(j,i+3)}$	1.05	$C_{qu}^{(i+3)}$	1.05	tZ
$C_{uG}^{(13,31)}$	0.041	$C_{uG}^{(23,32)}$	0.093	$t\gamma, tZ, th$
$C_{uW}^{(13,31)}$	0.92	$C_{uW}^{(23,32)}$	1.1	$t\gamma, tZ$
$C_{uB}^{(13,31)}$	1.0	$C_{uB}^{(23,32)}$	1.9	$t\gamma, tZ$
$C_{uq}^{(13,31)}$	3.5	$C_{uq}^{(23,32)}$	3.5	th

where $i = 1, 2, j = 1, 3$, and the limits apply to the moduli of the coefficients, assuming $\Lambda = 1$ TeV. Each limit is obtained by marginalizing over all the other operator coefficients. In this work, we choose real and positive values for the coefficients that do not exceed these bounds. The total cross sections at the LHC at $\sqrt{s} = 13$ TeV corresponding to each operator are displayed in Tables I, II and III. The scale uncertainties are also displayed. As expected the K factors are generally sizable and the scale uncertainties are significantly reduced at NLO. This is the case for all operators except for $O_{uG}^{(i3,3i)}$ in $t\gamma$ production. This process has an unusually large K factor when the flavor-changing coupling is coming from $O_{uG}^{(i3,3i)}$. As shown in Table I, vetoing any extra jet with $p_T > 50$ GeV reduces the K factor from 2.3 (3.3) to 1.6 (2.3) for utg (ctg) coupling as well as the uncertainties for this production mechanism. Note also that a jet veto can help to improve the signal over the SM background ratio, for all three processes.

TABLE I. Total cross sections for $pp \rightarrow t\gamma$. Contributions from operators with (31), (32) superscripts are not displayed, but they are the same as their (13), (23) counterparts. Contributions from $O_{uW}^{(i3),(3i)}$ are equal to those from $O_{uB}^{(i3),(3i)}$.

Coefficient	LO		NLO	
	σ [fb]	Scale uncertainty	σ [fb]	Scale uncertainty
$C_{uB}^{(13)} = 1.0$	546	+14.4% - 11.8%	764	+6.9% - 6.4%
$C_{uG}^{(13)} = 0.04$	1.00	+12.0% - 10.2%	2.34	+15.2% - 11.5%
$C_{uG}^{(13)}$, veto	0.739	+11.50% - 9.8%	1.19	+7.7% - 6.5%
$C_{uB}^{(23)} = 1.9$	152	+10.6% - 9.6%	258	+6.8% - 6.0%
$C_{uG}^{(23)} = 0.09$	0.590	+12.1% - 11.1%	1.95	+16.4% - 12.3%
$C_{uG}^{(23)}$, veto	0.457	+12.2% - 11.2%	1.04	+10.3% - 8.9%

TABLE II. Total cross sections for $pp \rightarrow tZ$. Contributions from operators $O_{uW}^{(31),(32)}$ are the same as those from $O_{uW}^{(13),(23)}$. Contributions from $O_{uB}^{(i3),(3i)}$ are equal to those from $O_{uW}^{(i3),(3i)}$ times $\tan^4 \theta_W$. Contributions from $O_{\phi q}^{(j,i+3)}$ are the same as those from $O_{\phi u}^{(i+3)}$.

Coefficient	LO		NLO	
	σ [fb]	Scale uncertainty	σ [fb]	Scale uncertainty
$C_{\phi u}^{(1+3)} = 1.0$	905	+12.9% - 10.9%	1163	+6.2% - 5.6%
$C_{uW}^{(13)} = 0.9$	1737	+11.5% - 9.8%	2270	+6.6% - 6.2%
$C_{uG}^{(13)} = 0.04$	30.1	+17.5% - 13.8%	36.0	+3.8% - 5.2%
$C_{uG}^{(31)} = 0.04$	29.4	+17.7% - 13.9%	34.9	+3.4% - 5.1%
$C_{\phi u}^{(2+3)} = 1.0$	73.2	+10.4% - 9.3%	107	+6.5% - 5.9%
$C_{uW}^{(23)} = 1.1$	172	+7.5% - 7.2%	255	+6.1% - 5.2%
$C_{uG}^{(23)} = 0.09$	6.92	+11.3% - 9.9%	10.6	+5.8% - 5.4%
$C_{uG}^{(32)} = 0.09$	6.58	+11.5% - 10.1%	10.0	+5.7% - 5.3%

TABLE III. Total cross sections for $pp \rightarrow th$. Contributions from operators $O_{u\phi}^{(3i)}$ and $O_{uG}^{(3i)}$ are equal to those from $O_{u\phi}^{(i3)}$ and $O_{uG}^{(i3)}$, respectively.

Coefficient	LO		NLO	
	σ [fb]	Scale uncertainty	σ [fb]	Scale uncertainty
$C_{u\phi}^{(13)} = 3.5$	2603	+13.0% - 11.0%	3858	+7.4% - 6.7%
$C_{uG}^{(13)} = 0.04$	40.1	+16.5% - 13.2%	50.7	+4.0% - 5.2%
$C_{u\phi}^{(23)} = 3.5$	171	+9.7% - 8.7%	310	+7.3% - 6.3%
$C_{uG}^{(23)} = 0.09$	9.53	+11.0% - 9.7%	16.6	+5.5% - 5.1%

V. DIFFERENTIAL CROSS SECTIONS

The p_T distributions of the top quark in $pp \rightarrow t\gamma$ and $pp \rightarrow th$ are shown in Fig. 2. Both LO and NLO signals are displayed, together with the SM backgrounds from $pp \rightarrow tj$ and thj , which are generated at NLO with the same

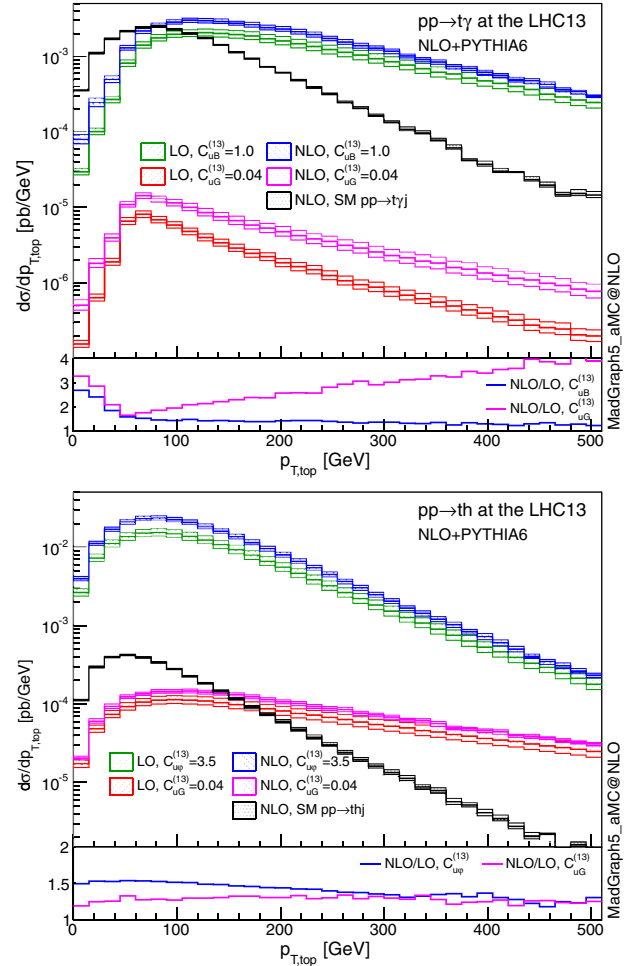


FIG. 2 (color online). The p_T distribution of top quark in $pp \rightarrow t\gamma$ (top) and in $pp \rightarrow th$ (bottom).

parameters. In all cases the $O_{uG}^{(13)}$ contributions are very small due to the stringent limit from $ug \rightarrow t$ production. Therefore, the $pp \rightarrow tX$ processes appear more as confirmation than as a discovery channel for the chromomagnetic operator.

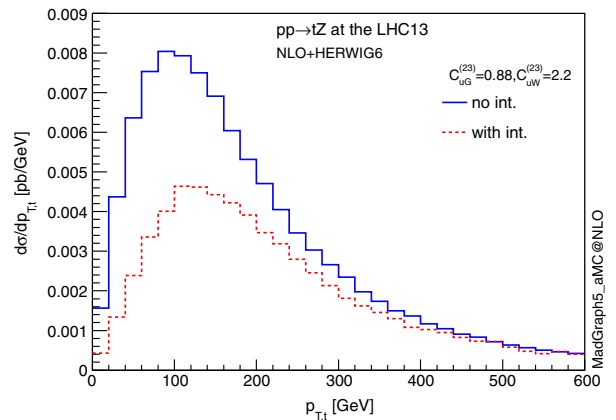


FIG. 3 (color online). The interference effect in $pp \rightarrow tZ$, as a function of top p_T .

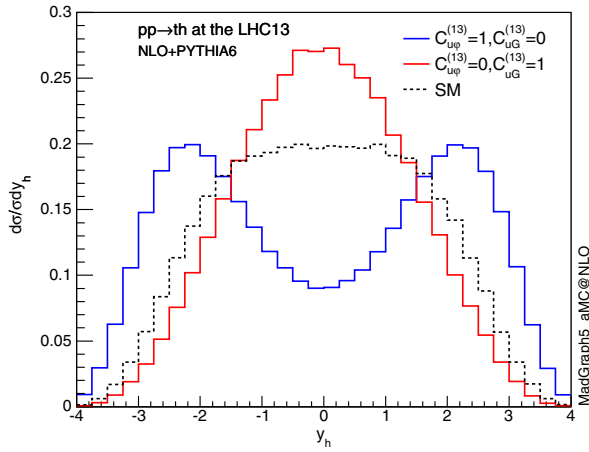


FIG. 4 (color online). Normalized rapidity distribution of the Higgs boson in $pp \rightarrow th$ induced by operators $O_{uq}^{(13)}$ and $O_{uG}^{(13)}$.

To illustrate the importance of keeping all operators possibly contributing to a given final state, we illustrate in Fig. 3 the interference effect between $O_{uW}^{(23)}$ and $O_{uG}^{(23)}$, in $pp \rightarrow tZ$ production. As a matter of fact, the interference between these two operators is large and gives rise to a significant change in the rate as well as in the distributions.

Finally, Fig. 4 shows an example where kinematic variables can be used to distinguish the contributions between different operators. The Higgs boson rapidity distribution in $pp \rightarrow th$ for tuh coupling induced production is more forward than that induced by the tug coupling. The reason is that an incoming up quark, which is in general more energetic than a gluon, can emit a forward Higgs boson and turn into an off-shell top quark via a uth vertex, while the same mechanism is not possible for the utg mediated production. The same observable may also be used to discriminate between uth and cth couplings, as proposed in Ref. [39], because c and g have similar PDFs.

VI. SUMMARY

Precision top-quark physics will be one of the priorities at the next run of the LHC. The detection of new interactions and in particular of FCN ones, will be among

the most promising searches for new physics. A consistent framework to perform such searches is provided by the dimension-six SM, i.e., the SM Lagrangian augmented by all operators of dimension-six compatible with the gauge symmetries of the SM. Bounding the coefficients of such operators first (and possibly determining them in case of deviations) requires accurate predictions for both SM and beyond processes. NLO accurate predictions in QCD are required in order to correctly extract FCN couplings from measurements or to set reasonable limits on their sizes. In this paper we have presented the first complete NLO computation for the single top production processes $u(c) + g \rightarrow t + B$, $B = \gamma, Z, h$, i.e., including all dimension-six flavor-changing (two fermion) operators. In particular, the chromomagnetic operators with their extra nontrivial effects have been added. Our computation is based on the MADGRAPH5_AMC@NLO framework, and thus the computation is fully automatic and can be applied to other FCN processes. The matching of the NLO results to the parton shower is included as well. The K factors in all the FCN processes are found to be large, and are in general not constant over the phase space. Our work is a first step toward the automation of NLO computations relevant for searches of new interactions through the effective field theory framework.

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