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DOI:

[10.1103/PhysRevLett.121.152002](https://doi.org/10.1103/PhysRevLett.121.152002)

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Document Version

Publisher's PDF, also known as Version of record

Citation for published version (Harvard):

Aaboud, M, Collaboration, ATLAS & Newman, P 2018, 'Probing the quantum interference between singly and doubly resonant top-quark production in $pp\bar{p}$ collisions at $\sqrt{s}=13$ TeV with the ATLAS detector', *Physical Review Letters*, vol. 121, no. 15, 152002. <https://doi.org/10.1103/PhysRevLett.121.152002>

[Link to publication on Research at Birmingham portal](#)

Publisher Rights Statement:

checked for eligibility 20/11/2018

<https://doi.org/10.1103/PhysRevLett.121.152002>

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Probing the Quantum Interference between Singly and Doubly Resonant Top-Quark Production in pp Collisions at $\sqrt{s} = 13$ TeV with the ATLAS Detector

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 (Received 13 June 2018; revised manuscript received 6 August 2018; published 12 October 2018)

This Letter presents a normalized differential cross-section measurement in a fiducial phase-space region where interference effects between top-quark pair production and associated production of a single top quark with a W boson and a b -quark are significant. Events with exactly two leptons (ee , $\mu\mu$, or $e\mu$) and two b -tagged jets that satisfy a multiparticle invariant mass requirement are selected from 36.1 fb^{-1} of proton-proton collision data taken at $\sqrt{s} = 13$ TeV with the ATLAS detector at the LHC in 2015 and 2016. The results are compared with predictions from simulations using various strategies for the interference. The standard prescriptions for interference modeling are significantly different from each other but are within 2σ of the data. State-of-the-art predictions that naturally incorporate interference effects provide the best description of the data in the measured region of phase space most sensitive to these effects. These results provide an important constraint on interference models and will guide future model development and tuning.

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Top-quark pair ($t\bar{t}$) production is one of the most widely studied processes at the Large Hadron Collider (LHC) and is a key background to many searches for physics beyond the standard model (BSM). The differential cross section for $t\bar{t}$ has been measured [1–5] and calculated [6–8] across a wide kinematic range with high accuracy. However, all of these results treat the decay of the top quark to a b -quark and W boson in the narrow-width approximation, separating $t\bar{t}$ production from production of a single top quark in association with a W boson and a b -quark (tWb). Because of their identical $WWb\bar{b}$ final states, processes with one or two timelike top-quark propagators (called singly and doubly resonant, respectively) interfere. Standard *ad hoc* methods of modeling this interference [9–12] are a significant source of uncertainty for many BSM searches [13–18]. Traditional measurements of production of a single top quark with an associated W boson (tW) are designed to be insensitive to such effects [19–21]. Recent fixed-order calculations of the full next-to-leading-order (NLO) $pp \rightarrow \ell^+\nu\ell^-\bar{b}b\bar{b}$ process [22–26] include proper treatment of the interference and have set the stage for corresponding predictions matched to a parton shower [27]. However, there are no measurements available to assess the modeling in a region sensitive to interference effects.

This Letter presents a novel way to test different models of the interference between $t\bar{t}$ and tWb , using 36.1 fb^{-1} of proton-proton (pp) collision data at $\sqrt{s} = 13$ TeV collected with the ATLAS detector in 2015 and 2016. The measurement targets the dilepton final state, characterized by a pair of oppositely charged leptons (ee , $\mu\mu$, or $e\mu$) originating from W -boson decays [28], associated with jets containing b -hadrons (b -jets) and missing transverse momentum due to undetected neutrinos. The contributions from doubly and singly resonant amplitudes (and hence also their interference) to the combined cross section depend on the invariant mass of the bW pairs in the event, m_{bW} . In this analysis, the charged lepton is used as a proxy for the W boson and a differential cross section is measured as a function of the invariant mass of a b -jet and a lepton. There is ambiguity in forming this mass, so

$$m_{b\ell}^{\text{minimax}} \equiv \min\{\max(m_{b_1\ell_1}, m_{b_2\ell_2}), \max(m_{b_1\ell_2}, m_{b_2\ell_1})\}$$

is used, where the b_i and ℓ_i represent the two b -jets and leptons, respectively. This choice is inspired by the minimax procedure used to construct the transverse mass [29,30] and measure the top mass [31]. At leading order, for doubly resonant events at parton level, $m_{b\ell}^{\text{minimax}} < \sqrt{m_t^2 - m_W^2}$, where m_t and m_W are the top-quark and W -boson masses, respectively. Because of suppression of the doubly resonant contribution, the differential cross section above this kinematic endpoint has increased sensitivity to interference effects.

ATLAS is a multipurpose particle detector designed with nearly full 4π coverage in a solid angle [32]. Lepton and jet reconstruction and identification used in this paper are

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described in Ref. [33] and are briefly summarized in the following. Electrons and muons are required to have transverse momentum $p_T > 28$ GeV, pseudorapidity [34] η satisfying $|\eta| < 2.47$ (2.5) for electrons (muons), and meet a series of quality criteria [35,36], denoted “tight” in Ref. [33]. Jets are clustered from topologically connected calorimeter cells [37] using the anti- k_r jet algorithm [38] with radius parameter $R = 0.4$ implemented in FASTJET [39] and calibrated to particle level [40]. Jets are identified as originating from b -quarks with a multivariate classifier using observables sensitive to lifetimes, production mechanisms, and decay properties of b -hadrons [41]. The tagging efficiency is determined in simulated $t\bar{t}$ events to be 60% (85%) for the tight (loose) tagging criterion.

Samples of simulated data are used in the design of the measurement, estimation of the background, and the unfolding procedure. POWHEG-BOX [42] v1 and v2 were used to simulate tW and $t\bar{t}$ events, respectively, with PYTHIA 6.428 [43], the five-flavor scheme (5FS) CT10 [44] parton distribution function (PDF) set, and Perugia 2012 [45] collection of tuned parameters. An identical configuration except using PYTHIA 8.183 and POWHEG-BOX-v2 for tW was included for particle-level comparisons. Alternative samples used POWHEG-BOX-v2 or MADGRAPH5_aMC@NLO (MG5_aMC) 2.2.2 [46], each interfaced to Herwig++ 2.7.1 [47] with the UE-EE-5 set of tuned parameters [48] and CT10 PDF set. The $t\bar{t} + b\bar{b}$ process [49] was generated using SHERPA 2.1.1 [50] plus OPENLOOPS [51] with the CT10 four-flavor scheme PDF. The $V + \text{jets}$ and $VV + \text{jets}$ ($V = W, Z$) processes were generated with SHERPA 2.2.1 and the CT10 PDF set. Associated production of $t\bar{t}$ with a boson ($t\bar{t}V$) was generated using MG5_aMC 2.2.2 combined with PYTHIA 8.186 [52], the NNPDF2.3LO PDF set [53] and the A14 set of tuned parameters [54]. All predictions, including the $t\bar{t}$ and tW processes, are normalized to next-to-next-to-leading-order or next-to-leading-order cross sections [6,46,50,55,56]. All samples of simulated data were processed using the full ATLAS detector simulation [57] based on GEANT 4 [58].

The signal process is combined $t\bar{t} + tWb$ production [59]. A calculation of the $e^\pm \nu \mu^\mp \bar{\nu} b \bar{b}$ process in the four-flavor scheme at NLO was implemented in POWHEG-BOX-RES [27,60] with PYTHIA 8.226. Here, resonance-aware matching allows the inclusion of off-shell top-quark effects at NLO, and the interference term is included. Alternatively, predictions are obtained from the exclusive $t\bar{t}$ and tWb samples described above, where the definition of the tW process is chosen to enable combination with the corresponding $t\bar{t}$ calculation. This is nontrivial at NLO, where care must be taken to avoid double-counting tWb events with $m_{bW} \sim m_t$. The default scheme for combining the $t\bar{t}$ and tW processes at NLO adopted here is diagram removal (DR) [9] in which all doubly resonant amplitudes are removed from the tW sample. Other choices exist where

doubly resonant contributions are canceled out by gauge-invariant subtraction terms (diagram subtraction, DS) [9] or are only included in the interference terms (DR2) [10,12]. For a more detailed review of possible tW definitions, see Ref. [11]. Finally, all $t\bar{t}$ events with b -jets not associated with top-quark decays are classified as $t\bar{t} + \text{heavy flavor}$ ($t\bar{t} + \text{HF}$) and treated separately from the signal process.

Events are selected with single-lepton triggers [61] and required to have a pair of opposite-charge leptons ($e^\pm e^\mp$, $\mu^\pm \mu^\mp$, $e^\pm \mu^\mp$). Events with a same-flavor lepton pair having invariant mass $m_{\ell\ell} < 10$ GeV or within 15 GeV of the Z -boson mass are rejected to suppress contributions from low-mass resonances and $Z + \text{jets}$. Events are required to have exactly two jets with $p_T > 25$ GeV and $|\eta| < 2.5$ which satisfy the tight b -tagging criterion and no additional jets that pass the looser b -tagging requirement. This b -jet veto suppresses $t\bar{t} + \text{HF}$ events, which can have large $m_{b\ell}^{\text{minimax}}$ when a selected b -jet does not originate from a top-quark decay.

A combination of data-driven and simulation-based methods is used to estimate backgrounds to the $t\bar{t} + tWb$ signal process. The dominant background at high $m_{b\ell}^{\text{minimax}}$ is $t\bar{t} + \text{HF}$, where a b -jet from a top-quark decay is not identified. This contribution is estimated from data events with at least three jets that are b -tagged according to the tight criterion. Simulated data is used to extrapolate the $t\bar{t} + \text{HF}$ yield measured in this region to the two- b -tag signal selection, giving a prediction $1.49 \pm 0.05(\text{stat}) \pm 0.20(\text{syst})$ times larger than the prediction obtained using POWHEG+PYTHIA 6. This is consistent with the results of previous measurements, finding scale factors from 1.1 to 1.7 depending on the selection criteria [62–66]. Figure 1(a) shows the $m_{b\ell}^{\text{minimax}}$ distribution for events passing the three- b -tag selection, constructed from the two b -jets with largest p_T . The leading two b -jets are both found to originate from top decays in 60% of simulated $t\bar{t} + \text{HF}$ events when $m_{b\ell}^{\text{minimax}}$ is below 160 GeV and less than 10% when above. Good agreement between data and prediction across the distribution demonstrates that the additional jet from heavy flavor is well modeled. The next largest background is from $Z + \text{jets}$ production, which is estimated in an analogous manner from data events with same-flavor leptons satisfying an inverted $m_{\ell\ell}$ requirement. In both cases, the $t\bar{t}$ contribution is subtracted before estimating the scale factor. Various checks show that this does not bias the measurement in the signal region phase space. Finally, there is a small contribution from non-prompt and misidentified leptons arising from photon conversions, heavy-flavor hadrons decaying leptonically, and jets misidentified as leptons. Following Ref. [67], this background is estimated using events with same-charge lepton pairs, after subtracting the prompt lepton contribution. Minor contributions from $t\bar{t}V$ and $VV + \text{jets}$ are estimated using simulation. Uncertainties in the simulation-based extrapolations are described below. The $t\bar{t} + tWb$ signal

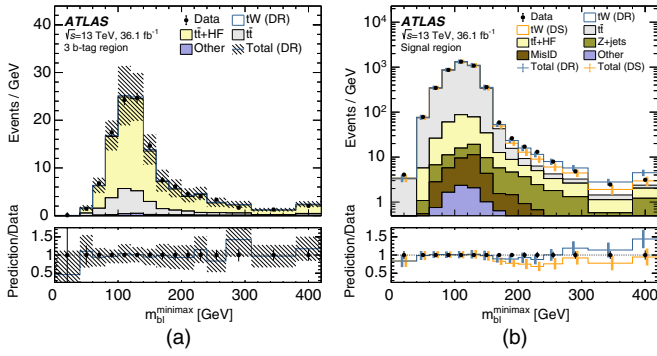


FIG. 1. (a) The $m_{b\ell}^{\text{minimax}}$ distribution in the three- b -tag region, constructed from the two b -jets with largest p_T . The predicted $t\bar{t} + \text{HF}$ contribution from simulation is scaled to match observed data in this region. The hashed band indicates the uncertainty on the total number of predicted events, where the DR scheme is used to estimate the minor contribution from the tW process. (b) The detector-level $m_{b\ell}^{\text{minimax}}$ distribution, with signal selection and background estimation as described in the text. The total predicted events are shown for both the DR and DS definitions of the tW process, with uncertainties on the respective estimates indicated by separate error bars. Uncertainties include all statistical and systematic sources. The rightmost bin of each distribution includes contributions from events beyond the displayed axis limit.

process accounts for 95% of events passing the full selection, with remaining background contributions subtracted from the data before unfolding the signal process to particle level. In Fig. 1(b), the data are compared to the predicted event yields for both the DR and DS schemes.

The unfolding procedure corrects detector-level [68] observables to particle level using a Bayesian method [69] with one iteration, optimized to minimize the average uncertainty per bin. The particle-level selection is defined to be as close as possible to the detector-level selection to minimize simulation-based corrections for acceptance effects and the detector resolution when unfolding. The definitions of particle-level objects are given in Ref. [70] with the following choices and modifications: (1) jets are clustered from all simulated particles with a mean lifetime $\tau > 30$ ps excluding muons and neutrinos to reduce model dependence, (2) jets are identified as b -jets if a b -hadron is found within the jet cone. Particle-level events must pass the same event selection as detector-level events, including the $m_{\ell\ell}$ requirement. To avoid contamination from $t\bar{t} + \text{HF}$ production, events with three or more particle-level b -jets with $p_T > 5$ GeV are rejected.

There are two categories of systematic uncertainties in the measurement: experimental and theoretical modeling. These affect the result via the background prediction that is subtracted from data or through the model used to unfold the data to particle level. Experimental uncertainties result from potential mismodeling in the reconstruction and identification of the jets [40], b -jets [71], and leptons

[35,36]. The background subtraction introduces uncertainty from the limited number of events in the control regions. A suite of simulation samples with alternative settings are used to assess the theoretical uncertainties in modeling the $t\bar{t}$, tW , $t\bar{t} + \text{HF}$, and $Z + \text{jets}$ processes [72,73]. A further uncertainty is assessed by varying the composition of the $t\bar{t} + tWb$ signal according to the uncertainty in the total cross sections of the singly and doubly resonant processes. An additional uncertainty is assessed for $t\bar{t} + \text{HF}$ by comparing the prediction obtained using POWHEG +PYTHIA 6 with that using the SHERPA $t\bar{t} + b\bar{b}$ sample. Furthermore, to ensure that the bias from the choice of interference scheme used in the unfolding is small, the procedure is repeated using the DS scheme. Finally, as another test of the unfolding, the particle-level $m_{b\ell}^{\text{minimax}}$ spectrum is reweighted to attain better agreement between the corresponding detector-level distribution and the data. Unfolding this reweighted distribution using the nominal unweighted simulation gives a measure of the method non-closure, which is assessed as an additional uncertainty [74]. The systematic uncertainty due to experimental sources ranges from 1% to 14%, with leading contributions from the jet energy scale and resolution and the b -tagging efficiency. Theoretical uncertainties associated with the modeling of processes with top quarks are generally the most important and range from 1% to 22% of the unfolded yields. The separate uncertainty due to the interference treatment is subdominant (22% in the largest bin of $m_{b\ell}^{\text{minimax}}$, elsewhere 1%–8%), and everywhere much smaller than the raw difference between the DR and DS scheme predictions. The size of the data set leads to statistical uncertainties of up to 20%.

Figure 2 presents the differential cross section observed in data, normalized to the total observed cross section with this selection. Various predictions are also shown, with uncertainties included from varying the PDF set [75] and the renormalization and factorization scales. A χ^2 test statistic is constructed for the various models to assess the level of agreement with the data. Correlations among uncertainties of the unfolded distribution are included, as well as theory uncertainties on the signal predictions. Results of the test are presented in Table I as p values, corresponding to the observed level of agreement over the full distribution as well as the subset $m_{b\ell}^{\text{minimax}} > 160$ GeV where the predicted differences due to interference are largest.

The tWb prediction using the DR scheme gives a better description of the relative normalization of the region $m_{b\ell}^{\text{minimax}} \gtrsim m_t$ than the DS scheme. However, the DS scheme better models the $m_{b\ell}^{\text{minimax}}$ shape over the same range of values. The DR and DS predictions generally bracket the data in the region of large $m_{b\ell}^{\text{minimax}}$, justifying the practice of applying their difference as a systematic uncertainty. The DR2 scheme describes the data well up to the top-quark mass, but significantly underpredicts the data

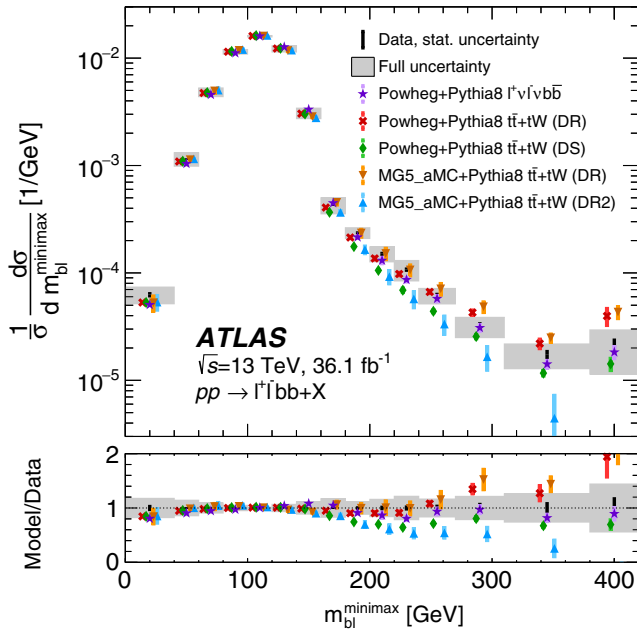


FIG. 2. The unfolded normalized differential $m_{b\ell}^{\text{minimax}}$ cross section compared with theoretical models of the $t\bar{t} + tWb$ signal with various implementations of interference effects. The uncertainty of each data point includes all statistical and systematic sources, while uncertainties for each of the MC predictions correspond to variations of the PDF set and renormalization and factorization scales. The rightmost bin of the distribution includes contributions from events beyond the displayed axis limit.

at higher masses [76]. The calculation from MG5_aMC using the DR scheme is presented alongside the corresponding DR2 calculation to directly compare the two interference treatments with other inputs held constant. The full $\ell^+\nu\ell^-\nu bb$ prediction [77] obtained from POWHEG-BOX-RES models $m_{b\ell}^{\text{minimax}}$ well across the full distribution, including the region beyond the top-quark mass where predictions using traditional models of the interference diverge.

In summary, a measurement of a region sensitive to the interference between doubly and singly resonant top-quark pair production is presented. This is an original constraint on this interesting region of phase space that will be important for future model development and tuning.

TABLE I. p values comparing data and predictions from events simulated with various models of the interference, all interfaced to PYTHIA 8. Test statistics are constructed from the full $m_{b\ell}^{\text{minimax}}$ distribution and for the subset $m_{b\ell}^{\text{minimax}} > 160$ GeV.

Model	All bins	$m_{b\ell}^{\text{minimax}} > 160$ GeV
POWHEG-BOX $t\bar{t} + tW$ (DR)	0.71	0.40
POWHEG-BOX $t\bar{t} + tW$ (DS)	0.77	0.56
MG5_aMC $t\bar{t} + tW$ (DR)	0.14	0.17
MG5_aMC $t\bar{t} + tW$ (DR2)	0.02	0.08
POWHEG-BOX $\ell^+\nu\ell^-\nu bb$	0.92	0.95

The results are presented as a normalized fiducial differential cross section, giving constraints on predictions for the full $t\bar{t} + tWb$ process.

We thank CERN for the very successful operation of the LHC, as well as the support staff from our institutions without whom ATLAS could not be operated efficiently. We acknowledge the support of ANPCyT, Argentina; YerPhI, Armenia; ARC, Australia; BMWFW and FWF, Austria; ANAS, Azerbaijan; SSTC, Belarus; CNPq and FAPESP, Brazil; NSERC, NRC and CFI, Canada; CERN; CONICYT, Chile; CAS, MOST and NSFC, China; COLCIENCIAS, Colombia; MSMT CR, MPO CR and VSC CR, Czech Republic; DNRF and DNSRC, Denmark; IN2P3-CNRS, CEA-DRF/IRFU, France; SRNSFG, Georgia; BMBF, HGF, and MPG, Germany; GSRT, Greece; RGC, Hong Kong SAR, China; ISF, I-CORE and Benoziyo Center, Israel; INFN, Italy; MEXT and JSPS, Japan; CNRST, Morocco; NWO, Netherlands; RCN, Norway; MNiSW and NCN, Poland; FCT, Portugal; MNE/IFA, Romania; MES of Russia and NRC KI, Russian Federation; JINR; MESTD, Serbia; MSSR, Slovakia; ARRS and MIZŠ, Slovenia; DST/NRF, South Africa; MINECO, Spain; SRC and Wallenberg Foundation, Sweden; SERI, SNSF and Cantons of Bern and Geneva, Switzerland; MOST, Taiwan; TAEK, Turkey; STFC, United Kingdom; DOE and NSF, United States of America. In addition, individual groups and members have received support from BCKDF, the Canada Council, CANARIE, CRC, Compute Canada, FQRNT, and the Ontario Innovation Trust, Canada; EPLANET, ERC, ERDF, FP7, Horizon 2020 and Marie Skłodowska-Curie Actions, European Union; Investissements d’Avenir Labex and IDEX, ANR, Région Auvergne and Fondation Partager le Savoir, France; DFG and AvH Foundation, Germany; Herakleitos, Thales and Aristeia programmes co-financed by EU-ESF and the Greek NSRF; BSF, GIF and Minerva, Israel; BRF, Norway; CERCA Programme Generalitat de Catalunya, Generalitat Valenciana, Spain; the Royal Society and Leverhulme Trust, United Kingdom. The crucial computing support from all WLCG partners is acknowledged gratefully, in particular from CERN, the ATLAS Tier-1 facilities at TRIUMF (Canada), NDGF (Denmark, Norway, Sweden), CC-IN2P3 (France), KIT/GridKA (Germany), INFN-CNAF (Italy), NL-T1 (Netherlands), PIC (Spain), ASGC (Taiwan), RAL (UK) and BNL (USA), the Tier-2 facilities worldwide and large non-WLCG resource providers. Major contributors of computing resources are listed in Ref. [78].

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