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# Search for $t\bar{t}H/A \rightarrow t\bar{t}t\bar{t}$ production in the multilepton final state in proton-proton collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector

The ATLAS Collaboration

A search for a new heavy scalar or pseudo-scalar Higgs boson (H/A) produced in association with a pair of top quarks, with the Higgs boson decaying into a pair of top quarks  $(H/A \rightarrow t\bar{t})$ is reported. The search targets a final state with exactly two leptons with the same-sign electric charge or at least three leptons. The analysed dataset corresponds to an integrated luminosity of 139 fb<sup>-1</sup> of proton-proton collisions collected at a centre-of-mass energy of 13 TeV with the ATLAS detector at the LHC. Two multivariate classifiers are used to separate the signal from the background. No significant excess of events over the Standard Model expectation is observed. The results are interpreted in the context of the two-Higgs-doublet model of type II. The observed (expected) upper limits at 95% confidence level on the  $t\bar{t}H/A$  cross-section times the branching ratio of  $H/A \rightarrow t\bar{t}$  range between 14 (10) fb and 6 (5) fb for a heavy Higgs boson mass between 400 GeV and 1000 GeV, respectively. Assuming that only one particle, either the scalar H or the pseudo-scalar A, contributes to the  $t\bar{t}t\bar{t}$  final state, the values of tan  $\beta$ below 1.2 and 0.5 are excluded for the studied mass range. This exclusion range increases up to tan  $\beta$  between 1.6 and 0.6 when both particles are considered.

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# **1** Introduction

The Higgs boson discovery by the ATLAS and CMS Collaborations in 2012 [1, 2] and later precision measurements [3, 4] of Higgs boson production and decay properties established the Standard Model (SM) of particle physics as an effective description of nature up to the TeV energy scale.

Within the SM, the Brout-Englert-Higgs mechanism [5–10] is responsible for generating the mass of the gauge bosons via electroweak symmetry breaking (EWSB). The Higgs boson emerges from the EWSB as the only physical spin-0 CP-even particle of the SM, while the remaining components of the Higgs field are absorbed into the longitudinal components of the gauge bosons.

In many Beyond the Standard Model (BSM) scenarios, the Higgs sector is typically extended to incorporate new degrees of freedom. A popular and minimal extension of the SM paradigm is provided by two-Higgs-doublet models (2HDM) [11] where the Higgs sector consists of two complex doublets: a mixture of the two doublets fulfills the same role as the SM Higgs field and generates a SM-like Higgs boson (*h*), and the other mixture gives rise to one neutral CP-even (*H*), one neutral CP-odd (*A*), and a charged Higgs boson ( $H^{\pm}$ ). A generic CP-conserving 2HDM with natural flavour conservation, and a lighter CP-even Higgs boson playing the role of the SM Higgs boson, has five free parameters: three Higgs-boson masses ( $m_H$ ,  $m_A$ ,  $m_{H^{\pm}}$ ), the mixing angle of the two CP-even Higgs fields ( $\alpha$ ), and the ratio of the vacuum-expectation-values of the two Higgs doublets (tan  $\beta$ ). A popular realisation of 2HDM is the Minimal Supersymmetric Standard Model (MSSM) [12, 13]. Similar Higgs sectors also arise in axion models [14].

Existing constraints from direct searches for heavy neutral bosons by the ATLAS and CMS Collaborations [15–25] as well as precision measurements of the cross-sections and decay rate of the SM Higgs boson restrict the available parameter-space to the so-called "alignment limit" ( $\sin(\beta - \alpha) \rightarrow 1$ ). In this limit the *h* couplings are the same as for the SM Higgs boson.

For masses of the heavy neutral Higgs bosons above twice the top quark mass, the dominant decay mode is  $H/A \rightarrow t\bar{t}$ . Inclusive searches for  $H/A \rightarrow t\bar{t}$  are challenging because of negative interference effects with the SM background  $gg \rightarrow t\bar{t}$  that largely dilute a resonant peak in the  $t\bar{t}$  invariant mass spectrum [26, 27]. An alternative approach is to search for associated production with third generation quarks [28]; thanks to its sizeable cross-section and striking signature, the  $t\bar{t}H/A$  production mode provides the most promising channel characterised by large experimental acceptance and low SM background rate.

This paper presents a search for a new heavy scalar or pseudo-scalar Higgs boson, H/A, produced in association with a pair of top quarks, with the Higgs boson decaying into a pair of top quarks,  $t\bar{t}H/A(\rightarrow t\bar{t})$ . The Feynman diagram of this process is shown in Figure 1. The mass of the heavy Higgs boson is assumed to be between 400 GeV and 1000 GeV, where a large  $H/A \rightarrow t\bar{t}$  branching ratio and small H/A total widths are expected. The search targets a final state with exactly two leptons<sup>1</sup> with the same-sign electric charge or at least three leptons (SSML). The analysed dataset corresponds to an integrated luminosity of 139 fb<sup>-1</sup> of proton-proton (pp) collisions collected at a centre-of-mass energy  $\sqrt{s} = 13$  TeV with the ATLAS detector at the LHC.

Previous searches for  $t\bar{t}H/A(\rightarrow t\bar{t})$  in the SSML channel were performed by the ATLAS and CMS Collaborations [29, 30]. A similar search for BSM  $t\bar{t}t\bar{t}$  events using an alternative experimental signature featuring exactly one charged lepton or two opposite-sign leptons was performed by the CMS Collaboration [31]. Other related searches include those looking at SM production of four-top-quarks [30, 32, 33]. The ATLAS

<sup>&</sup>lt;sup>1</sup> In this paper, leptons refer either to electrons or muons, which can include those that come from the  $\tau$ -lepton decay.

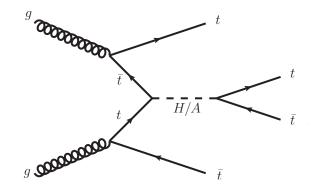


Figure 1: Feynman diagram showing the production of a heavy scalar or pseudo-scalar Higgs boson, H/A, produced in association with a pair of top quarks, with the Higgs boson decaying into a pair of top quarks.

and CMS measurements of the SM four-top-quarks production cross-section were found to be  $24^{+7}_{-6}$  fb and  $13^{+11}_{-9}$  fb, respectively, compared to a SM expectation of  $\sigma_{t\bar{t}t\bar{t}} = 12.0 \pm 2.4$  fb [34].

The results obtained in this search are interpreted in the context of the 2HDM type-II; upper limits are placed on the  $t\bar{t}H/A$  production cross-section times the branching ratio of  $H/A \rightarrow t\bar{t}$  as well as on tan  $\beta$  as a function of the heavy Higgs boson mass. By using a significantly larger dataset and improved analysis techniques including multivariate classifiers based on Boosted Decision Trees (BDTs) used to distinguish the signal from the SM background, the  $t\bar{t}H/A(\rightarrow t\bar{t})$  search presented in this paper improves the expected sensitivity of the previous  $t\bar{t}H/A(\rightarrow t\bar{t})$  ATLAS search with 36 fb<sup>-1</sup> [29] by about a factor four.

This paper is structured as follows. The ATLAS detector is presented in Section 2. The data and samples of simulated events are described in Section 3. The object and event selections are detailed in Section 4. The analysis strategy is presented in Section 5. This is followed by the description of the systematic uncertainties in Section 6. The statistical analysis and the results are presented in Sections 7 and 8, respectively. Finally, the conclusion is presented in Section 9.

# 2 ATLAS detector

The ATLAS detector [35] at the LHC covers nearly the entire solid angle around the collision point.<sup>2</sup> It consists of an inner tracking detector surrounded by a thin superconducting solenoid, electromagnetic and hadron calorimeters, and a muon spectrometer incorporating three large superconducting air-core toroidal magnets.

The inner-detector system (ID) is immersed in a 2 T axial magnetic field and provides charged-particle tracking in the range  $|\eta| < 2.5$ . The high-granularity silicon pixel detector covers the vertex region and typically provides four measurements per track, the first hit normally being in the insertable B-layer (IBL)

<sup>&</sup>lt;sup>2</sup> ATLAS uses a right-handed coordinate system with its origin at the nominal interaction point (IP) in the centre of the detector and the *z*-axis along the beam pipe. The *x*-axis points from the IP to the centre of the LHC ring, and the *y*-axis points upwards. Cylindrical coordinates  $(r, \phi)$  are used in the transverse plane,  $\phi$  being the azimuthal angle around the *z*-axis. The pseudorapidity is defined in terms of the polar angle  $\theta$  as  $\eta = -\ln \tan(\theta/2)$ . Angular distance is measured in units of  $\Delta R \equiv \sqrt{(\Delta \eta)^2 + (\Delta \phi)^2}$ .

installed before Run 2 [36, 37]. It is followed by the silicon microstrip tracker (SCT), which usually provides eight measurements per track. These silicon detectors are complemented by the transition radiation tracker (TRT), which enables radially extended track reconstruction up to  $|\eta| = 2.0$ . The TRT also provides electron identification information based on the fraction of hits (typically 30 in total) above a higher energy-deposit threshold corresponding to transition radiation.

The calorimeter system covers the pseudorapidity range  $|\eta| < 4.9$ . Within the region  $|\eta| < 3.2$ , electromagnetic calorimetry is provided by barrel and endcap high-granularity lead/liquid-argon (LAr) calorimeters, with an additional thin LAr presampler covering  $|\eta| < 1.8$  to correct for energy loss in material upstream of the calorimeters. Hadron calorimetry is provided by the steel/scintillator-tile calorimeter, segmented into three barrel structures within  $|\eta| < 1.7$ , and two copper/LAr hadron endcap calorimeters. The solid angle coverage is completed with forward copper/LAr and tungsten/LAr calorimeter modules optimised for electromagnetic and hadronic energy measurements respectively.

The muon spectrometer (MS) comprises separate trigger and high-precision tracking chambers measuring the deflection of muons in a magnetic field generated by the superconducting air-core toroidal magnets. The field integral of the toroids ranges between 2.0 and 6.0 T m across most of the detector. A set of precision chambers covers the region  $|\eta| < 2.7$  with three layers of monitored drift tubes, complemented by cathode-strip chambers in the forward region, where the background is highest. The muon trigger system covers the range  $|\eta| < 2.4$  with resistive-plate chambers in the barrel, and thin-gap chambers in the endcap regions.

Interesting events are selected by the first-level trigger system implemented in custom hardware, followed by selections made by algorithms implemented in software in the high-level trigger [38]. The first-level trigger accepts events from the 40 MHz bunch crossings at a rate below 100 kHz, which the high-level trigger further reduces in order to record events to disk at about 1 kHz.

An extensive software suite [39] is used in the reconstruction and analysis of real and simulated data, in detector operations, and in the trigger and data acquisition systems of the experiment.

## **3** Data and samples of simulated events

This analysis uses pp collision data collected between 2015 and 2018 by the ATLAS detector at  $\sqrt{s} = 13$  TeV. The full dataset corresponds to an integrated luminosity of 139 fb<sup>-1</sup>. Only data recorded during stable beam conditions in which all detector subsystems were operational [40] have been included. Events were collected using single-lepton or dilepton triggers. The trigger  $p_T$  threshold depends on the lepton flavour and the data-taking period [41, 42]. The lowest  $p_T$  threshold for the single-lepton trigger varies from 20 to 26 GeV, while for the dilepton trigger it varies from 7 to 24 GeV.

Monte Carlo (MC) simulation samples are used for the different signal and background processes. The generated events were processed through the simulation [43] of the ATLAS detector geometry and response using GEANT4 [44], and through the same reconstruction software as data. Corrections are applied to the simulated events so that particle selection efficiencies, energy scales and energy resolutions match those determined from data. For the parton shower and hadronisation, unless otherwise stated, samples generated with MADGRAPH5\_aMC@NLO [45] and POWHEG BOX v2 [46–52] were interfaced to PYTHIA 8.230, 8.210 or 8.212 [53], using the A14 set of tuned parameters [54] and the NNPDF2.3LO [55] parton distribution function (PDF). The decays of bottom and charm hadrons were simulated using the EvtGen 1.6.0 or EvtGen 1.2.0 program [56].

Signal MC samples were generated using the MADGRAPH5\_AMC@NLO 2.3.3 generator at leading order (LO) with the NNPDF3.1L0 [55] PDF; in order to account for the spin correlation of the particles in the final state, the full matrix-element for the  $2 \rightarrow 12$  parton-level scattering is generated. The signal MC events are generated assuming a 2HDM type-II model. A total of seven signal MC samples were generated with  $m_H$  ranging from 400 GeV to 1000 GeV with regular 100 GeV spacing. The heavy Higgs boson total width is assumed to be narrow throughout the mass range, varying from 5 GeV to 30 GeV, consistent with the expected heavy Higgs boson width in the 2HDM type-II model for tan  $\beta \sim 1$ . Interference between the signal and SM production of four-top-quarks was not simulated. In the mass range of interest for this search, the interference leads to up to 20% change of the signal cross-section for a signal with  $m_H$ =400 GeV and width of 50 GeV, and the kinematic properties of the signal are found to be consistent between A and H. For tan  $\beta \sim 1$ , the  $t\bar{t}H(\rightarrow t\bar{t})$  and  $t\bar{t}A(\rightarrow t\bar{t})$  production cross-sections are found to differ at most by 1%.

The SM production of *tītī* events was modelled as described in the following. The nominal sample was generated using the MADGRAPH5\_AMC@NLO 2.3.3 generator, which provides matrix elements at next-to-leading order (NLO) in the strong coupling constant  $\alpha_s$  with the NNPDF3.1NLO PDF. The functional form of the renormalisation and factorisation scales are set to  $\mu_r = \mu_f = m_T/4$  where  $m_T$  is defined as the scalar sum of the transverse masses  $\sqrt{m^2 + p_T^2}$  of the particles generated from the matrix element calculation, following the Ref. [34]. The decay of the top quark is done at LO using MADSPIN [57, 58] to preserve all spin correlations. In order to avoid the use of negative weights present in the nominal sample in the multivariate discriminant used to separate SM  $t\bar{t}t\bar{t}$  events from background (see Section 5.2), a sample with similar settings as the nominal one, but produced at LO was generated. An additional  $t\bar{t}t\bar{t}$  sample was produced with the parton shower of the nominal sample replaced by HERWIG 7.04 [59, 60] to evaluate the impact of using a different parton shower and hadronisation model. The H7UE set of tuned parameters [60] and the MMHT2014Lo PDF set [61] were used. In order to assess the uncertainty associated to the choice of the event generator, a sample with  $t\bar{t}t\bar{t}$  events modelled using the SHERPA v2.2.10 [62] generator with the NNPDF3.0NNLO [55] PDF set has been used. A sample including electroweak (EW) corrections has been generated with the same settings as the one of SHERPA v2.2.10 but using SHERPA v2.2.11. This sample is used to evaluate the systematic uncertainty associated to the missing EW corrections in the nominal sample. The production of  $t\bar{t}t\bar{t}$  events is normalised to a cross-section of 12 fb computed at NLO in QCD including EW corrections [34].

The production of  $t\bar{t}W$  events was modelled at NLO in QCD using the SHERPA v2.2.10 generator with the NNPDF3.0NNLO PDF set with up to one extra parton at NLO and up to 2 extra partons included at LO. The additional partons are matched and merged with the SHERPA parton shower based on Catani-Seymour dipole factorisation [63] using the MEPS@NLO prescription [64–67] with a merging scale of 30 GeV. The virtual QCD correction for matrix elements at NLO accuracy are provided by the OpenLoops 2 [68–70] library. The renormalisation and factorisation scales are set to  $\mu_r = \mu_f = m_T/2$ . The production of  $t\bar{t}W$  events with only EW corrections ( $O(\alpha_S^2\alpha^2) + O(\alpha_S\alpha^3)$ ) is modelled at LO in QCD using the same generator and PDF set as in the QCD-only production. The  $t\bar{t}W$  cross-section predicted by these MC generator settings, including EW corrections, is 639 fb. The impact of the systematic uncertainty associated to the choice of the generator is evaluated with an alternative  $t\bar{t}W$  sample generated at NLO in QCD with no additional partons using the MADGRAPH5\_aMC@NLO v2.3.3 generator with the NNPDF3.0NLO as PDF. The production of  $t\bar{t}W$  events in MADGRAPH5\_aMC@NLO with only EW corrections ( $O(\alpha_S\alpha^3)$ ) is modelled at LO in QCD with the NNPDF3.0NLO as

The production of  $t\bar{t}(Z/\gamma^*)$  events was modelled using the SHERPA v2.2.1 generator at NLO with the NNPDF3.0NNLO PDF set. The invariant mass of the lepton pair is requested to be  $m_{\ell^+\ell^-} > 5$  GeV. For the low mass range, i.e.  $m_{\ell^+\ell^-} \in (1, 5)$  GeV, events are modelled using the MADGRAPH5\_aMC@NLO v2.3.3

generator at NLO with the NNPDF3.0NLO PDF set. These two samples are combined and together they form the " $t\bar{t}(Z/\gamma^*)$  (high mass)" sample. In order to assess the uncertainty associated to the choice of the generator, a MADGRAPH5\_aMC@NLO sample generated exactly with the same settings as the nominal low mass range sample but with  $m_{\ell^+\ell^-} > 5$  GeV has been used.

The production of  $t\bar{t}H$  events was modelled using the POWHEG BOX v2 generator, which provided matrix elements at NLO in the strong coupling constant  $\alpha_s$  in the five-flavour scheme with the NNPDF3.0NLO PDF set. The cross-section was calculated at NLO QCD and NLO EW accuracy using MADGRAPH5\_AMC@NLO as reported in Ref. [71]. An alternative sample generated with MADGRAPH5\_aMC@NLO v2.3.3 has been used to evaluate the impact of the uncertainty associated to the generator choice.

The production of  $t\bar{t}$  and single-top-quark events was modelled using the POWHEG Box v2 generator at NLO in QCD with the NNPDF3.0NLO PDF set. For the  $t\bar{t}$  sample, the  $h_{damp}$  parameter<sup>3</sup> is set to 1.5  $m_{top}$  [72]. The diagram removal scheme [73] was used to remove interference and overlap between the  $t\bar{t}$  and tWproduction. For these two processes, the contribution from internal photon conversions ( $\gamma^* \rightarrow \ell^+ \ell^-$ ) with  $m_{\ell^+\ell^-} < 1$  GeV is modelled by QED multiphoton radiation via the parton shower. This contribution will be referred in the following as the "Low  $m_{\gamma^*}$ " sample.

The production of tWZ, tZ,  $t\bar{t}$ ,  $t\bar{t}WW$  and other rare top-quark processes, namely the production of  $t\bar{t}ZZ$ ,  $t\bar{t}WZ$ ,  $t\bar{t}HH$ , and  $t\bar{t}WH$  was modelled using the MADGRAPH5\_aMC@NLO generator. The tWZ sample was modelled at NLO, while the remaining processes were modelled at LO in QCD. The contribution of  $t\bar{t}WW$  is normalised to the NLO QCD theoretical cross-section [71].

The *WH* and *ZH* processes were generated using the PYTHIA 8.230 generator with the A14 tune and NNPDF2.3L0 PDF set and normalised to their theoretical cross-sections calculated at NNLO in QCD and NLO EW accuracies [74–80].

The production of Z+jets, W+jets, diboson (VV) and triboson (VVV) events was modelled with the SHERPA 2.2.1 or 2.2.2 generator depending on the process. The NNPDF3.0NNLO set of PDFs was used, along with the dedicated set of tuned parton-shower parameters developed by the SHERPA authors.

The effect of multiple interactions in the same and neighbouring bunch crossings (pile-up) was modelled by overlaying the simulated hard-scattering event with inelastic *pp* events generated with PYTHIA 8.186 [81] using the NNPDF2.3LO set of PDFs and the A3 set of tuned parameters [82].

## 4 Object and event selections

Events are required to contain at least one primary vertex (PV) reconstructed from at least two ID tracks, each with  $p_T > 0.5$  GeV. If more than one PV candidate satisfies these criteria, then the PV with the largest sum of  $p_T^2$  over all associated ID tracks is selected [83].

Electron candidates are reconstructed from energy deposits in the electromagnetic calorimeter matched to a track in the ID [84]. The identification working point for the nominal selection in this analysis is "TightLH" [84]. Only electron candidates with a  $p_T > 28$  GeV and within  $|\eta| < 2.47$ , excluding the calorimeter transition region,  $1.37 < |\eta| < 1.52$ , are selected. Electrons are required to be well isolated using the criteria based on the properties of the topological clusters in the calorimeter and of the ID tracks

<sup>&</sup>lt;sup>3</sup> The  $h_{damp}$  parameter is a resummation damping factor and one of the parameters that controls the matching of PowHEG matrix elements to the parton shower and thus effectively regulates the high- $p_T$  radiation against which the  $t\bar{t}$  system recoils.

around the reconstructed electron. Standard requirements on the longitudinal ( $z_0$ ) and transverse ( $d_0$ ) impact parameters are used to select electrons originating from the primary vertex. The requirements are  $|z_0 \sin \theta| < 0.5 \text{ mm}$  and  $|d_0|/\sigma(d_0) < 5$ .

Muon candidates are reconstructed by combining tracks in the ID with tracks in the MS [85]. The identification working point used in this analysis is "Medium" [85]. Only muon candidates with a  $p_{\rm T} > 28$  GeV and within  $|\eta| < 2.5$  are selected. Muons are required to satisfy the isolation requirements based on the properties of the ID tracks around the reconstructed muon. As for electrons, requirements on the longitudinal,  $|z_0 \sin \theta| < 0.5$  mm, and transverse impact parameters,  $|d_0|/\sigma(d_0) < 3$ , are also applied.

An additional requirement is imposed to electrons in the  $e^{\pm}e^{\pm}$  and  $e^{\pm}\mu^{\pm}$  channels to reduce the background coming from electron charge misidentification. This requirement is based on a BDT discriminant which uses the calorimeter and tracking variables to remove approximately 90% of electrons with the wrong charge assignment while selecting 98% of electrons with the correctly measured charge [84].

The constituents for jet reconstruction are identified by combining measurements from both the ID and the calorimeter using a particle-flow algorithm [86]. Jet candidates are reconstructed from these particle-flow objects using the anti- $k_t$  algorithm [87] with a radius parameter of R = 0.4. They are calibrated using simulation with corrections obtained from data using in situ techniques [88]. Only jet candidates with a  $p_T > 25$  GeV and within  $|\eta| < 2.5$  are selected. To reduce the effect from pile-up, each jet with  $p_T < 60$  GeV and  $|\eta| < 2.4$  is required to satisfy the "Tight" working point of the Jet Vertex Tagger (JVT) [89] criteria used to identify the jets as originating from the selected primary vertex. A set of quality criteria is also applied to reject events containing at least one jet arising from non-collision sources or detector noise [90].

Jets containing b-hadrons are identified (b-tagged) using the DL1r algorithm [91]. It consists of a deep-learning neural network based on the distinctive features of the *b*-hadrons in terms of the impact parameters of tracks and the displaced vertices reconstructed in the ID. The input to the DL1r network also includes discriminant variables constructed by a recurrent neutral network [92], which exploits the spatial and kinematic correlations between tracks originating from the same b-hadron. A jet is b-tagged if the DL1r score is above a certain threshold, referred to as an operating point (OP). Four OPs are defined with average expected efficiencies for *b*-jets of 60%, 70%, 77% and 85%, as determined in simulated  $t\bar{t}$  events. The DL1r *b*-tagging score is divided into five exclusive bins according to the OPs, the distribution obtained by ordering these five bins from higher to lower *b*-jet efficiency is referred to as "pseudo-continuous" *b*-tagging score, and it is used as input for the BDT discriminant described in Section 5.2. In this analysis, a jet is considered b-tagged if it passes the OP corresponding to 77% average efficiency for jets containing b-hadrons, with a misidentification rate of 1/130 (1/4.9) for light-flavour (charm) jets. Correction factors are applied to the simulated event samples to compensate for differences between data and simulation in the *b*-tagging efficiency for *b*-, *c*- and light-jets. The correction for *b*-jets is derived from  $t\bar{t}$  events with final states containing two leptons, and the corrections are consistent with unity with uncertainties at the level of a few percent over most of the jet  $p_{\rm T}$  range [93].

An overlap removal procedure is applied in order to avoid the same calorimeter energy deposit or the same track being used in two different objects. First, an electron found within a track of another electron with higher  $p_T$  is removed. Next, electrons sharing their track with a muon candidate are removed. Then, jets are removed if they are within a  $\Delta R = 0.2$  of an electron. Subsequently, in order to remove electrons arising from *b*- or *c*-decays, electrons are removed if they are within a  $\Delta R = 0.4$  of a jet. Next, jets with less than

three tracks within a  $\Delta R = 0.2$  of a muon are removed. Finally, in order to remove muons arising from *b*-or *c*-decays, muons are removed if their tracks are within  $\Delta R = 0.4 + 10 \text{ GeV}/p_T^{\mu}$  of any remaining jets.

The missing transverse momentum of the event  $\vec{p_T}^{\text{miss}}$  is defined as the negative vector sum of the  $p_T$  of all selected and calibrated objects in the event. This sum includes a term to account for momentum of ID tracks matched to the selected PV but which are not associated with any of the selected objects in the event [94]. The magnitude of  $\vec{p_T}^{\text{miss}}$  is denoted as  $E_T^{\text{miss}}$ .

Events are required to have exactly two leptons with the same electric charge or at least three leptons without any charge requirement. Each event must have at least one reconstructed lepton that matches a lepton that fired the trigger. In order to reduce the background coming from electron charge misidentification in the same-sign dilepton channel, and the contamination from the Z-boson decay in the trilepton channel, a Z-veto is applied requiring  $m_{\ell\ell} \notin [81, 101]$  GeV, where  $m_{\ell\ell}$  is checked for the two electrons defining the  $e^{\pm}e^{\pm}$  channel, and for all opposite-sign same-flavour lepton pairs in the trilepton channel. In addition, events with a final state of  $e^{\pm}e^{\pm}$  are also required to satisfy  $m_{ee} > 15$  GeV to reduce the background coming from low-mass resonances with electron charge misidentification.

## **5** Analysis strategy

The analysis strategy follows the one from the past ATLAS  $t\bar{t}t\bar{t}$  measurement [33], using dedicated control regions to constrain the dominant background processes, and multivariate techniques to separate the signal from background. The background estimation is detailed in Section 5.1.

The signal-enriched region is defined by exploiting the high multiplicity of light-flavour and *b*-tagged jets as well as the high overall momentum of final states with  $t\bar{t}t\bar{t}$  events. Thus, events are required to have at least six jets, among which at least two are *b*-tagged, and  $H_T > 500$  GeV, where  $H_T$  is defined as the scalar sum of  $p_T$  of all leptons and jets in the event. This signal region (SR) will be referred in the following as the *baseline SR*.

The signal is separated from the SM background by using two sequential BDT classifiers (see Section 5.2). Those BDTs are trained in the *baseline SR*, inclusively in both lepton flavour and multiplicity. The first one, the "SM BDT", is used to separate SM  $t\bar{t}t\bar{t}$  events from the remaining backgrounds. Due to the similar kinematics of the signal and SM  $t\bar{t}t\bar{t}$  events, signal events are expected to be located in the same region of the BDT score distribution as the SM  $t\bar{t}t\bar{t}$  events. Therefore, the final signal region is built on top of the *baseline SR*, and it is defined by the cut SM BDT > 0.55. This definition will be referred in the following as the *BSM SR*. The full selection for the *BSM SR* can be found in Table 1.

Then, the discrimination of the signal versus all background processes in the *BSM SR* is managed via a mass-parametrised BDT, called "BSM pBDT". The presence of the signal is then tested by fitting the distribution of the BSM pBDT score in the *BSM SR* jointly to the control regions defined in Section 5.1.

#### 5.1 Background estimation

Several SM processes can mimic a final state of two leptons with the same electric charge or three leptons. They can be classified into two different categories depending on the origin of the lepton:

- **Irreducible:** All selected leptons are prompt. They are mainly originating from *W* or *Z*-boson decays. The main contribution in the signal region is given by  $t\bar{t}t\bar{t}$ ,  $t\bar{t}W$ +jets,  $t\bar{t}(Z/\gamma^*)$ +jets (high mass) and  $t\bar{t}H$ +jets production. Smaller contributions are coming from diboson (*VV*), triboson (*VVV*), *VH* production, and rare processes ( $t\bar{t}VV$ , tWZ, tZq and ttt). This background is estimated using the samples of simulated events described in Section 3 and normalised to the theory cross-section. The  $t\bar{t}W$ +jets contribution is split between its QCD and its EW component.<sup>4</sup> As the normalisation of  $t\bar{t}W$ +jets has been found to be underestimated in the simulation in recent measurements [95], the normalisation of the QCD component is corrected using data in a dedicated control region as explained in Section 5.1.1. The background from processes with a virtual photon  $\gamma^*$  leading to an  $e^+e^-$  pair is also included into this category, accounting only for the contribution of  $m_{\ell^+\ell^-} < 1$  GeV (Low  $m_{\gamma^*}$ ). Since the normalisation of this background might not be correct in simulation, its normalisation is also estimated in a dedicated control region as explained in Section 5.1.1. This search targets BSM production of four-top-quarks, therefore the background originating from SM four-top-quarks is normalised to its SM prediction with a Gaussian constraint given by the theoretical uncertainty.
- **Reducible:** At least one of the leptons is fake/non-prompt or it is a prompt lepton with its charge misidentified. It originates mainly from  $t\bar{t}$ +jets, V+jets and tW+jets. The fake/non-prompt lepton background is estimated together with  $t\bar{t}W$  QCD and processes with a virtual photon leading to an  $e^+e^-$  pair using the template fit method as described in Section 5.1.1. The background coming from electron charge misidentification (QmisID) is estimated using data-driven techniques as described in Section 5.1.2.

#### 5.1.1 Fake/non-prompt lepton background, virtual photon decay and $t\bar{t}W$ QCD+jets normalisations

Fake/non-prompt lepton background arises from different sources:

- Events with one lepton coming from material photon conversion (Mat. Conv.).
- Events with one electron (muon) coming from heavy-flavour meson decay (HF  $e/\mu$ ).
- Events with one lepton coming from light-meson decay or with a jet misidentified as a lepton (LF).
- Events with one fake/non-prompt lepton falling into none of the above (other fake).

The true information from the  $t\bar{t}$ +jets, V+jets and single-top samples described in Section 3 is used to separate the different sources of fake/non-prompt leptons. The last two components are very small and are fully estimated with samples of simulated events. The contributions from material photon conversion and HF  $e/\mu$  are estimated with the template fit method. This method relies on the simulation to model the kinematic distributions of the different sources of the fake/non-prompt leptons and uses dedicated control regions to determine their normalisations.

Several control regions have been defined, with each region designed to try to enhance as much as possible the background component that is predominantly fitted in each region. The variable to be fitted in each region has been chosen to bring the most possible discrimination for the targeted dominant background. The normalisation of the irreducible background coming from processes with a virtual photon leading to an  $e^+e^-$  pair is predominantly estimated in the same control region enriched in background from material

<sup>&</sup>lt;sup>4</sup> The  $t\bar{t}W$  QCD and EW samples are calculated at different orders: QCD is NLO in QCD, and EW is LO in QCD. Therefore the QCD and EW components are decorrelated and treated as two independent samples with their own systematic uncertainties.

photon conversion. A dedicated control region has been defined for  $t\bar{t}W$  QCD+jets production. An extra control region has been defined, which is designed to be as close as possible to the *BSM SR*. In total, five control regions are used in the analysis, following closely the definitions of Ref. [33]. They are described in Table 1 and summarised below.

- "CR Conv": It is enriched in material photon conversion and processes with a virtual photon leading to an  $e^+e^-$  pair. Events are required to have an  $e^\pm e^\pm$  or  $e^\pm \mu^\pm$  pair. For each electron in the event, the invariant mass of the system formed by the track associated with the electron and the closest track at the conversion (primary) vertex  $m_{ee}^{CV}(m_{ee}^{PV})$  is computed. The conversion vertex is defined at the point where the track from the electron and its closest track in  $\Delta R$  have the same  $\phi$ . Virtual photons lead to a lepton pair originating from the primary vertex, having a low  $m_{ee}^{PV} \sim m_{\gamma^*}$ . Material conversions have large conversion radius, and the track extrapolation induces a large apparent  $m_{ee}^{PV}$ . The control region is then obtained by selecting events with low  $m_{ee}^{CV}$  and fitting the  $m_{ee}^{PV}$  distribution to separate the material photon conversion and virtual photon decay from each other. Events are also required to have four or five jets, at least one *b*-tagged jet, and low  $H_T$ .
- "CR HF e" ( "CR HF  $\mu$ "): It is enriched in events with one electron (muon) coming from heavyflavour decay. The selection targets  $t\bar{t}$  dilepton decays with an extra non-prompt lepton. This region is then defined by selecting events with three leptons, namely *eee* and *ee* $\mu$  (*e* $\mu\mu$  and  $\mu\mu\mu$ ) for CR HF e (CR HF  $\mu$ ), with low  $H_T$  and exactly one b-jet. The number of events in this region is used as the fitted variable.
- "CR  $t\bar{t}W$ ": It is enriched in  $t\bar{t}W$ +jets events. Events are required to have an  $e^{\pm}\mu^{\pm}$  or  $\mu^{\pm}\mu^{\pm}$  pair, at least four jets and at least two *b*-jets. In order to reduce the background coming from electron charge misidentification, events containing electrons with  $|\eta| > 1.5$  are removed. This region is also required to be orthogonal to the "CR Conv" region and to the *baseline SR*. The fitted variable is the sum of the lepton  $p_{\rm T}$ .
- "CR lowBDT": It is not enriched in any particular background, but rather used as a control region which is very close to the *BSM SR*. Events are required to be in the *baseline SR*, but with SM BDT < 0.55. The fitted variable is the SM BDT.

These control regions are fitted simultaneously with the *BSM SR* to determine the signal strength for the BSM  $t\bar{t}t\bar{t}$  signal and the five normalisation factors:  $\lambda_{t\bar{t}WQCD}$  for the  $t\bar{t}W$  QCD+jets production,  $\lambda_{Mat. Conv.}$  for the background from detector material conversion,  $\lambda_{Low m_{\gamma^*}}$  for the contribution of virtual photon leading to an  $e^+e^-$  pair, and  $\lambda_{HFe}$  ( $\lambda_{HF\mu}$ ) for the non-prompt electron (muon) background from heavy-flavour decays.

#### 5.1.2 Electron charge misidentification background

Background from electron charge misidentification is relevant only in the same-sign dilepton channel. It arises when the sign of the electric charge of one of the two leptons in the selected same-sign pair has been misreconstructed either because of bremsstrahlung photon emission followed by its conversion  $(e^{\pm} \rightarrow e^{\pm} \gamma \rightarrow e^{\pm} e^{+} e^{-})$  or due to mismeasured track curvature. In the signal region, it is mainly coming from  $t\bar{t}$ +jets production. Due to the low probability of bremsstrahlung for muons and because of the large lever arm of the MS, the misidentification rates of the muon charge are very low. Thus, this background is only relevant for the  $e^{\pm}e^{\pm}$  and  $e^{\pm}\mu^{\pm}$  channels.

Table 1: Definition of the signal region and control regions used in the analysis. The first column shows the region name as used in the text. The event selection requirements are defined in the middle columns. The last column shows the fitted variable in every region. The variable  $m_{ee}^{CV}$  ( $m_{ee}^{PV}$ ) is defined as the invariant mass of the system formed by the track associated with the electron and the closest track at the conversion (primary) vertex.  $N_j$  ( $N_b$ ) indicates the jet (*b*-tagged jet) multiplicity.  $H_T$  is defined as the scalar sum of the transverse momenta of the isolated leptons and jets. The *baseline SR* is equal to the *BSM SR* + CR lowBDT.

Region	Channel	N <sub>j</sub>	N <sub>b</sub>	Other selection cuts	Fitted variable
CR Conv	$e^{\pm}e^{\pm} \parallel e^{\pm}\mu^{\pm}$	$4 \le N_j < 6$	≥ 1	$m_{ee}^{\text{CV}} \in [0, 0.1] \text{ GeV}$ 200 < $H_{\text{T}}$ < 500 GeV	$m_{ee}^{\rm PV}$
CR HF e	еее    ееµ		= 1	$100 < H_{\rm T} < 250 { m ~GeV}$	Yield
CR HF $\mu$	еµµ    µµµ		= 1	$100 < H_{\rm T} < 250 { m ~GeV}$	Yield
CR tłW	$e^{\pm}\mu^{\pm} \mid\mid \mu^{\pm}\mu^{\pm}$	≥ 4	≥ 2	$m_{ee}^{CV} \notin [0, 0.1] \text{ GeV},  \eta(e)  < 1.5$ for $N_{b} = 2, H_{T} < 500 \text{ GeV}$ or $N_{j} < 6;$ for $N_{b} \ge 3, H_{T} < 500 \text{ GeV}$	$\sum p_{\mathrm{T}}^{\ell}$
CR lowBDT	SS+3L	≥ 6	≥ 2	$H_{\rm T} > 500 \text{ GeV}, \text{SM BDT} < 0.55$	SM BDT
BSM SR	SS+3L	≥ 6	$\geq 2$	$H_{\rm T} > 500 \text{ GeV}, \text{SM BDT} \ge 0.55$	BSM pBDT

The probability for an electron to have its charge incorrectly reconstructed is measured in a data sample of dielectron events with invariant mass within 10 GeV of the Z-boson mass. The side-band method is used to subtract the background contamination. The electron charge misidentification probability is calculated in bins of electron  $|\eta|$  and  $p_T$ . In order to apply it to the conversion region defined in Section 5.1.1, it is also parameterised in bins of  $m_{ee}^{PV}$ . A likelihood fit that adjusts these binned probabilities is used to find the best agreement with the observed number of same-charge and opposite-charge electron pairs. The electron charge misidentification rates vary from 0.002% for low- $p_T$  electrons ( $p_T \le 60$  GeV) at  $|\eta| \le 0.6$ , to ~ 10% for high- $p_T$  electrons ( $p_T \ge 200$  GeV) at  $|\eta| \in [2.3, 2.5]$ .

To estimate the event yields in the  $e^{\pm}e^{\pm}$  and  $e^{\pm}\mu^{\pm}$  channels, *ee* and  $e\mu$  events are selected using all the criteria applied in the analysis, with the exception that the leptons are required to have opposite charge. Then, the final background yield is obtained by weighting this opposite-sign dilepton events by the probability of one electron charge to be misreconstructed.

#### 5.2 Signal discrimination

Multivariate techniques are used to separate the signal from the SM backgrounds. This is done through two sequential BDT classifiers: the first one, the background rejection BDT, namely SM BDT, separates SM  $t\bar{t}t\bar{t}$  events from other SM backgrounds. Then, the second one, the BSM mass-parametrised BDT (BSM pBDT) discriminates BSM  $t\bar{t}t\bar{t}$  events against all background. The BSM pBDT is parametrised as a function of the heavy Higgs boson mass by introducing the mass as input label in the training [96]. Both SM BDT and BSM pBDT are trained in the *baseline SR* with the XGBoost (Extreme Gradient Boosting) algorithm [97]. In both cases, the input variables have been optimised to maximise the integral under the receiver operating characteristic (ROC) curve of each BDT.

The input variables for the SM BDT are the same as those from the SM  $t\bar{t}t\bar{t}$  search [33], with the difference that the highest ranked variable, the sum of the pseudo-continuous *b*-tagging score, takes into account only the four jets with the highest score. The jet multiplicity is also a new input variable for the discriminant, and

it is introduced to further distinguish SM  $t\bar{t}t\bar{t}$  events from the other SM backgrounds. The distributions of these two variables are shown in Figure 2. Other input variables to the SM BDT are the minimum distance  $\Delta R$  between two leptons among all possible pairs, the leading lepton  $p_T$ ,  $E_T^{\text{miss}}$ , the  $p_T$  of the leading and sub-leading jets, the  $p_T$  of the sixth jet, the  $p_T$  of the leading *b*-jet, the scalar sum of the transverse momenta over all leptons and jets excluding the leading  $p_T$  jet, the sum of distances  $\Delta R$  between two leptons for all possible pairs, and the minimum distance  $\Delta R$  between a jet and a *b*-jet among all possible pairs. The SM BDT is used to split the *baseline SR*: the high SM BDT region defines the *BSM SR* (SM BDT  $\geq 0.55$ ), while the low part defines the CR lowBDT (SM BDT < 0.55). The SM BDT is used as an input variable to build the BSM pBDT and as the fitted variable in the CR lowBDT.

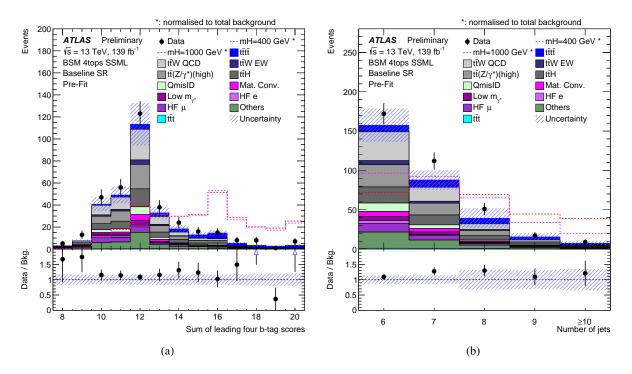


Figure 2: Pre-fit comparison between data and background in the *baseline SR* for two of the variables used as input for the SM BDT: sum of the leading four jet's *b*-tagging scores (a) and the number of jets (b). The signal samples corresponding to  $m_H = 400$  GeV and 1000 GeV are also shown. The signal distributions have been normalised to the total background to compare the shapes. The dashed band includes the total background uncertainty. The first and last bins contain underflow and overflow events, respectively. Upward arrows indicate that the value is out of the plotted range of the *y*-axis.

The BSM pBDT is used in the BSM SR, but to the lack of statistics it is trained in the *baseline SR*. As the *BSM SR* is  $t\bar{t}t\bar{t}$  enriched, the training is done after reweighting the SM  $t\bar{t}t\bar{t}$  events to mimic the fraction with respect to the total background that they have in the *BSM SR*. The remaining background processes are reweighted so that they preserve the total background yield. The SM BDT is the most discriminant input variable for the BSM pBDT. The second most discriminant is  $H_{\rm T}$ . The distributions of these two variables in the *baseline SR* are shown in Figure 3. Other variables used as input are the event shape variable associated to hadronic activity (sphericity) [98], the sphericity in the transverse plane, the minimum distance  $\Delta R$  between two leptons among all possible pairs, the sum of distances  $\Delta R$  between two leptons for all possible pairs, and the  $E_{\rm T}^{\rm miss}$  of the event. The BSM pBDT output score is used as the fitted variable in the *BSM SR*.

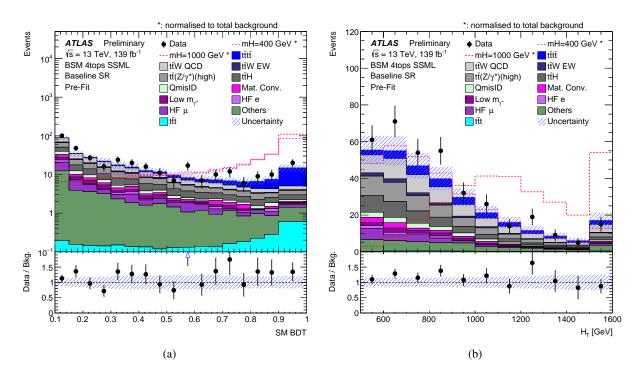


Figure 3: Pre-fit comparison between data and background in the *baseline SR* for two of the variables used as input for the BSM pBDT: SM BDT (a) and  $H_T$  (b). The signal samples corresponding to  $m_H = 400$  GeV and 1000 GeV are also shown. The signal distributions have been normalised to the total background to compare the shapes. The dashed band includes the total background uncertainty. The first and last bins contain underflow and overflow events, respectively. Upward arrows indicate that the value is out of the plotted range of the *y*-axis.

## **6** Systematic uncertainties

Systematic uncertainties arise from the reconstruction of the various physics objects and from theoretical and/or modelling uncertainties affecting the predictions for both the background and signal processes. They can be classified into experimental uncertainties and modelling uncertainties on the signal, irreducible, and reducible backgrounds. These uncertainties manifest themselves as uncertainties in both the overall yield and shape of the final observable.

#### 6.1 Experimental uncertainties

The uncertainty on the integrated luminosity of the combined 2015-2018 dataset is 1.7% [99], obtained using the LUCID-2 detector [100] for the primary luminosity measurements. The uncertainties related to the reweighting factors that correct the pile-up profile in simulations to match that one in data are also included.

Uncertainties on the modelling of leptons arise from their momentum resolution and scale, as well as the trigger, reconstruction, identification and isolation efficiencies used to correct for the difference between the simulation and data [41, 42, 84, 85].

Uncertainties on the modelling of jets come from their energy scale and resolution, containing the effect of jet flavour composition, single-particle response, and pile-up [88]. The uncertainty in the efficiency to pass the JVT requirement for pile-up suppression is also applied [101]. Uncertainties from the calibration of the *b*-tagging efficiencies, including the efficiencies of tagging *b*-jets as well as the rates of mis-tagging *c*-jets and light-flavour jets are also considered [91].

The uncertainty on  $E_{\rm T}^{\rm miss}$  arising due to a possible mis-calibration of its soft-track component is also included [94].

#### 6.2 Modelling uncertainties on the signal and irreducible background

Modelling uncertainties on the signal arise from the PDF and from the missing higher-order QCD corrections. The former is evaluated following the PDF4LHC recommendations [102], while the latter is estimated by varying the renormalisation and factorisation scales simultaneously by factors of 2.0 and 0.5 relative to the central value.

Several sources of uncertainty are considered for the background coming from  $t\bar{t}t\bar{t}$  production. The uncertainties related to missing higher-order QCD corrections and to the PDF are evaluated in the same way as for the signal. The uncertainty associated to the choice of the parton shower and hadronisation model is estimated by comparing the nominal prediction with the alternative sample generated with MADGRAPH5\_aMC@NLO matched with HERWIG. The uncertainty related to the choice of the generator is obtained by comparing the nominal sample to the one generated with SHERPA 2.2.10. The uncertainty associated to the lack of EW corrections in the nominal sample affects only the shape of the distributions, and it is evaluated by comparing the SHERPA 2.2.11 (QCD-only) and SHERPA 2.2.11 (QCD+EW)<sup>5</sup> simulated samples. A separate 20% uncertainty computed at NLO in QCD including EW corrections [34] is applied on the total cross-section.

Several sources of uncertainty affect the modelling of the  $t\bar{t}W$ +jets,  $t\bar{t}Z$ +jets, and  $t\bar{t}H$ +jets production. Uncertainties associated to the generator are estimated by comparing the prediction from the nominal samples with the alternative samples generated with MADGRAPH5 aMC@NLO described in Section 3. The uncertainties due to missing higher-order QCD corrections are evaluated in the same way as for the signal. An uncertainty of 12% (10%) is applied on the  $t\bar{t}Z$  ( $t\bar{t}H$ ) total cross-section [71]. A 1% uncertainty from PDF, estimated following the PDF4LHC prescription [102], is applied to both  $t\bar{t}Z$  and  $t\bar{t}H$  processes. No uncertainty on the cross-section is assigned to  $t\bar{t}W$  QCD production as its normalisation is estimated in the fit (see Section 5.1). An uncertainty of 20% [103] is applied to the  $t\bar{t}W$  EW cross-section. In order to cover for the difference between data and prediction in the  $t\bar{t}W$  validation region defined in Section 8, where a data excess is observed for high jet multiplicities, an additional 124% (200%) uncertainty is added to  $t\bar{t}W$ QCD production with seven (eight or more) jets. Events arising from  $t\bar{t}W$ +jets,  $t\bar{t}Z$ +jets, and  $t\bar{t}H$ +jets production can enter into the signal region if they have additional heavy-flavour jets. As these processes are difficult to model in the simulation, an uncertainty of 50% is assigned to the events with an additional true *b*-jet and a separate 50% uncertainty to the events with additional two or more true *b*-jets. Those estimates are taken from Ref. [33], and treated as uncorrelated between the three different processes due to the different setups used to simulate the events.

<sup>&</sup>lt;sup>5</sup> EW corrections are included into the Sherpa 2.2.11 sample as additional weights. Thus, when using the QCD-only version the EW weights are not used.

The uncertainty on the  $t\bar{t}t$  production cross-section is set to 100% as done in Ref. [33]. Following the same motivation given earlier about the uncertainties for processes with additional heavy flavour jets for  $t\bar{t}V$ +jets samples, an extra uncertainty of 50% is applied to  $t\bar{t}t$  events with at least one additional true *b*-jet.

An uncertainty of 30% is applied to the cross-section of the tZ and tWZ single-top-quark processes [104, 105]. The uncertainty on the diboson cross-section is set to 40% following studies on the WZ + b production. For the rare top-quark processes, i.e.  $t\bar{t}WW$ ,  $t\bar{t}ZZ$ ,  $t\bar{t}WZ$ ,  $t\bar{t}HH$ , and  $t\bar{t}WH$ , an uncertainty on the cross-section of 50% is applied [29]. For the remaining small backgrounds, an uncertainty of 50% is assigned to the cross-section. An additional uncertainty of 50% is applied to all small backgrounds except  $t\bar{t}t$ . This uncertainty is applied to events with one additional true b-jet, and separately to events with at least two additional true b-jets.

### 6.3 Modelling uncertainties on the reducible background

The uncertainties on the background coming from charge misidentification arise from the uncertainties in the measurement of the electron charge misidentification rates. The following contributions are considered: the statistical uncertainty from the likelihood fit to data, the difference between the rates extracted in simulated events with the likelihood method and the truth rates, and the changes in the measured rates when the size of the side-band regions used to subtract the background from the Z-peak is varied from 8 to 12 GeV.

The uncertainties from the material conversion and virtual photon decay backgrounds only come from the shape of the distributions used in the template fit. No uncertainty on the normalisation of these processes is assigned since the overall normalisations of these backgrounds are estimated in the fit. The shape uncertainty is estimated in a region enriched in  $Z(\rightarrow \mu\mu) + \gamma$  events, by comparing data with the POWHEG+PYTHIA 8 simulation of  $Z(\rightarrow \mu\mu) + \gamma$ /jets production. The uncertainty is supposed to cover for the extrapolation from the "CR Conv", i.e. events with  $m_{ee}^{CV} \in [0, 0.1]$  GeV, to the regions with events with larger  $m_{ee}^{CV}$ . The uncertainty was estimated to be 50% (100%) for the material conversion (virtual photon decay) background, and it is applied to events with  $m_{ee}^{CV} > 0.1$  GeV in all control and signal regions.

Similarly as for the background from material conversion and virtual photon decay, the only uncertainty of the heavy-flavour non-prompt background comes from the shape of the distributions used in the fit. This uncertainty is estimated by a bin-by-bin comparison of the data and the post-fit background prediction in every region used in the analysis, where the contribution of non-prompt leptons has been enhanced. This is done by using a loose lepton selection with the isolation requirements dropped and the identification criteria relaxed. The shape uncertainty is treated as correlated among all regions. It is derived separately for electrons and muons.

The uncertainty assigned to the normalisation of the background coming from light-flavour non-prompt leptons is 100%. This value has been derived from the agreement between data and simulation in a light-flavour non-prompt lepton enriched region. For the remaining sources of fakes/non-prompt leptons, an uncertainty of 30% is applied as done in Ref. [33].

Other uncertainties affecting the shape of the distributions of the background coming from fake/non-prompt leptons arise from the modelling of the heavy-flavour content of the main source of reducible background,  $t\bar{t}$ +jets production. Based on the measurement of  $t\bar{t}$  production with additional heavy-flavour jets [106], an uncertainty of 30% is assigned to events with three true *b*-jets, and a separate 30% uncertainty to events with at least four true *b*-jets.

## 7 Statistical analysis

The presence of the signal is tested by fitting the BSM pBDT score in the BSM SR jointly to the control regions as described in Section 5. The statistical analysis uses a binned likelihood function  $\mathcal{L}(\mu, \lambda, \theta)$  constructed as a product of Poisson probability terms over all bins considered in the search. This function depends on the signal strength parameter  $\mu$ , defined as a factor multiplying the expected yield of  $t\bar{t}H/A(\rightarrow t\bar{t})$  signal events,  $\theta$ , a set of nuisance parameters that encode the effect of systematic uncertainties on the signal and background expectations, and  $\lambda$ , a set of multiplicative factors used to normalise the background expectation. All nuisance parameters are subject to Gaussian constraints in the likelihood. Therefore, the expected total number of events in a given bin depends on  $\mu$ ,  $\theta$  and  $\lambda$ .

For a given value of  $\mu$ , the nuisance parameters  $\theta$  and the normalisation factors  $\lambda$  allow variations of the expectations for signal and background according to the corresponding systematic uncertainties, and their fitted values result in the deviations from the nominal expectations that globally provide the best-fit to the data. This procedure allows a reduction of the impact of systematic uncertainties on the search sensitivity by taking advantage of the highly populated background-dominated bins included in the likelihood fit. Simulation statistical uncertainties in each bin are taken into account by dedicated parameters in the fit modelled with Poisson constraints. The best-fit branching fraction is obtained by performing a binned likelihood fit to the data under the signal-plus-background hypothesis, maximising the likelihood function  $\mathcal{L}(\mu, \theta, \lambda)$  over  $\mu$ ,  $\theta$  and  $\lambda$ .

The test statistic  $q_{\mu}$  is defined as the profile likelihood ratio,  $q_{\mu} = -2 \ln(\mathcal{L}(\mu, \hat{\theta}_{\mu}, \hat{\lambda}_{\mu})/\mathcal{L}(\hat{\mu}, \hat{\theta}_{\hat{\mu}}, \hat{\lambda}_{\hat{\mu}}))$ , where  $\hat{\mu}$ ,  $\hat{\theta}$  and  $\hat{\lambda}$  are the values of the parameters that maximise the likelihood function (subject to the constraint  $0 \le \hat{\mu} \le \mu$ );  $\hat{\theta}_{\mu}$  and  $\hat{\lambda}_{\mu}$  are respectively the values of the nuisance parameters and normalisation factors that maximise the likelihood function for a given value of  $\mu$ . The test statistic  $q_{\mu}$  is evaluated with the RooFit package [107, 108]. A related test statistic is used to determine whether the observed data is compatible with the background-only hypothesis by setting  $\mu = 0$  in the profile likelihood ratio and leaving  $\hat{\mu}$  unconstrained:  $q_0 = -2 \ln(\mathcal{L}(0, \hat{\theta}_0, \hat{\lambda}_0)/\mathcal{L}(\hat{\mu}, \hat{\theta}, \hat{\lambda}))$ . The *p*-value representing the level of agreement between the data and the background-only hypothesis, is estimated by integrating the distribution of  $q_0$ based on the asymptotic formulae in Ref. [109], above the observed value of  $q_0$  in the data. Upper limits on  $\mu$  are derived by using  $q_{\mu}$  in the CL<sub>s</sub> method [110, 111]. For a given signal scenario, values of  $\mu$  yielding CL<sub>s</sub> < 0.05, where CL<sub>s</sub> is computed using the asymptotic approximation [109], are excluded at  $\geq 95\%$ confidence level (CL).

# 8 Results and interpretation

The signal strength for every signal hypothesis and the normalisation factors of the background processes described in Section 5.1.1 are determined via a binned likelihood fit done simultaneously in all signal and control regions defined in Table 1.

For the *BSM SR*, the binning of the BSM pBDT distribution has been optimised for every signal hypothesis to provide the best discrimination between the tested signal and the background, avoiding the presence of bins with no contribution of major backgrounds. The results obtained for the background-only fit shown in this section are the ones obtained when the fitted distribution in the signal region is the BSM pBDT score assigned to the background events when the training is done against the signal assuming

 $m_H = 400$  GeV. Similar results are obtained when the BSM pBDT score for the training done against other signal hypotheses is used.

The normalisation factors from the background-only fit to data for the different background processes are shown in Table 2. The data and post-fit background comparison for the distributions of the discriminant variables fitted in the control regions is shown in Figure 4. A good agreement between data and post-fit background is observed. Pre-fit and post-fit background yields in the *BSM SR* are shown in Table 3. The signal yields corresponding to the pre-fit estimation in the 2HDM for tan  $\beta = 1$ , and for a few signal hypotheses, are also shown. The total background yield is consistent within 1 standard deviation from the SM prediction. For the  $t\bar{t}W$  QCD background, the significant difference between the pre-fit and post-fit yield arises not only from the change in its normalisation factor  $\lambda_{t\bar{t}WQCD}$ , but also from several nuisance parameters associated to the generator, scale variation, and to the systematic uncertainty assigned to events with eight or more jets. The measured normalisation factor  $\lambda_{t\bar{t}WQCD}$  is found to agree with that of [95]. No other nuisance parameters were found to be significantly pulled or constrained in the fit.

The modelling of the  $t\bar{t}W$  QCD background has been validated based on the fact that  $t\bar{t}W$ +jets is charge asymmetric, and by definition, remove all the charge-symmetric processes. The difference between the number of events with a positive sum and the number of events with a negative sum of the charges of the selected leptons is calculated in a region with at least four jets, where at least two are *b*-tagged. The SM BDT distribution for this selection is shown in Figure 5. A good agreement within uncertainties between data and post-fit background is observed.

Table 2: Normalisation factors for the different background processes obtained from the background-only fit. The fit is done simultaneously in all signal and control regions. The fitted distribution in the *BSM SR* is the BSM pBDT score assigned to the background events when the training is done against the signal assuming  $m_H = 400$  GeV. The uncertainties include both statistical and systematic uncertainties.

Parameter	$\lambda_{t\bar{t}WQCD}$	$\lambda_{\mathrm{Mat.\ Conv.}}$	$\lambda_{\mathrm{Low}m_{\gamma^*}}$	$\lambda_{\mathrm{HF}e}$	$\lambda_{ m HF\mu}$
Value	$1.3 \pm 0.3$	$1.5 \pm 0.5$	$0.6 \pm 0.5$	$0.9 \pm 0.4$	$1.0 \pm 0.2$

The different post-fit BSM pBDT distributions corresponding to the signal benchmarks  $m_H = 400$  and 1000 GeV in the *BSM SR* for the background-only fit are shown in Figure 6. Under the signal-plusbackground hypothesis the best fit signal cross-section ranges between  $4^{+6}_{-5}$  fb and  $2^{+2}_{-2}$  fb for a heavy Higgs boson mass between 400 GeV and 1000 GeV, respectively. No significant excess of events above the SM prediction is observed. The results are then interpreted in the context of the 2HDM type-II. The observed and expected upper limits on the  $t\bar{t}H/A$  cross-section times branching fraction of  $H/A \rightarrow t\bar{t}$  at 95% CL as a function of  $m_{H/A}$  are shown in Figure 7. The observed upper limits range between 14 fb and 6 fb for the studied mass range. These upper limits on the cross-section can be translated into limits in the tan  $\beta$  versus mass plane. Two different scenarios are considered: one where both the scalar H and pseudo-scalar A have equal masses and both contribute to the BSM  $t\bar{t}t\bar{t}$  production, and another one where only the scalar H contributes. The observed and expected 95% CL exclusion regions for these scenarios are shown in Figure 8. In the case where both particles contributes to the BSM  $t\bar{t}t\bar{t}$  production, the excluded values of tan  $\beta$  range between 1.6 and 0.6 between 400 GeV and 1000 GeV, respectively. When considering only the scalar H, the values of tan  $\beta$  below 1.2 and 0.5 are excluded for the same mass range. In the parameter-space studied, the limits for the pseudo-scalar A alone are similar to those of the scalar H.

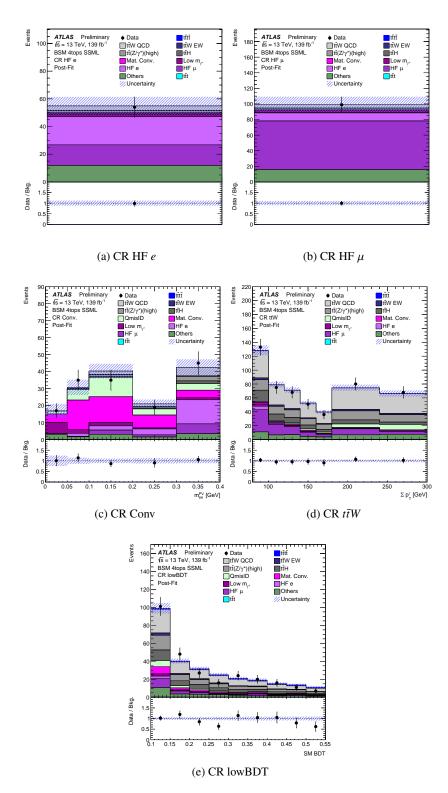


Figure 4: Data and post-fit background comparison for the distributions of the discriminant variables fitted in the control regions obtained with the background-only fit. The fit is done simultaneously in all signal and control regions. The fitted distribution in the *BSM SR* is the BSM pBDT score assigned to the background events when the training is done against the signal assuming  $m_H = 400$  GeV. The band includes the total uncertainty of the post-fit estimation. The lower panel shows the ratio of the data and post-fit background. The first and last bins of (c), (d) and (e) contain underflow and overflow events, respectively.

Table 3: Pre-fit and post-fit background yields in the *BSM SR* obtained with the background-only fit. The fit is done simultaneously in all signal and control regions. The fitted distribution in the *BSM SR* is the BSM pBDT score assigned to the background events when the training is done against the signal assuming  $m_H = 400$  GeV. The signal yields correspond to the pre-fit estimation in the 2HDM type-II for tan  $\beta = 1$  and for  $m_H = 400$  GeV and 1000 GeV, assuming only the production of the new scalar *H*. The number of data events is also shown. The total systematic uncertainty differs from the sum in quadrature of the different uncertainties due to the correlations.

Process	Pre-fit	Post-fit
tīttī	$22.3 \pm 5.4$	$25.9 \pm 5.4$
$t\bar{t}W$ QCD	$9.4 \pm 9.3$	$17.1 \pm 6.9$
$t\bar{t}W$ EW	$1.3 \pm 0.5$	$1.4 \pm 0.6$
tŦWW	$1.8 \pm 1.0$	$1.9 \pm 1.0$
$t\bar{t}(Z/\gamma^*)$ (high mass)	$8.5 \pm 2.2$	$9.2 \pm 2.3$
tīH	$7.2 \pm 1.7$	$7.8 \pm 1.7$
QmisID	$2.1 \pm 0.1$	$2.1 \pm 0.1$
Mat. Conv.	$1.8 \pm 0.6$	$3.0 \pm 1.2$
Low $m_{\gamma^*}$	$1.2 \pm 0.6$	$0.8 \pm 0.8$
HF e	$0.6 \pm 0.5$	$0.6 \pm 0.5$
HF $\mu$	$2.7 \pm 1.0$	$2.9 \pm 1.2$
LF	$1.1 \pm 1.2$	$0.4 \pm 1.0$
Other fake	$1.1 \pm 0.7$	$1.3 \pm 0.7$
tZ, tWZ	$0.9 \pm 0.3$	$0.9 \pm 0.3$
VV, VH, VVV	$0.3 \pm 0.1$	$0.3 \pm 0.1$
tīt	$1.9 \pm 1.9$	$2.3 \pm 2.1$
$t\bar{t}WZ, t\bar{t}ZZ, t\bar{t}WH, t\bar{t}HH$	$1.3 \pm 0.3$	$1.4 \pm 0.3$
Total background	65.6 ± 13.2	$79.5 \pm 6.8$
$t\bar{t}H(\rightarrow t\bar{t}), m_H = 400 \text{ GeV}$	$38.6 \pm 2.4$	
$t\bar{t}H(\rightarrow t\bar{t}), m_H = 1000 \text{ GeV}$	$4.4 \pm 0.2$	_
Data	91	

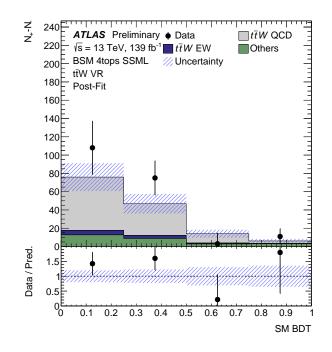


Figure 5: Data and post-fit background comparison obtained with the background-only fit in the validation region defined for  $t\bar{t}W$ +jets events. The fit is done simultaneously in all signal and control regions. The y-axis shows the difference between the number of events with a positive sum and the number of events with a negative sum of the charges of the selected leptons. The band includes the total uncertainty of the post-fit estimation. The lower panel shows the ratio of the data and post-fit background.

The robustness of the results has been checked by reproducing the fit results using data split by data taking periods, or by splitting the *BSM SR* into events in the same-sign dilepton channel and trilepton channel. An additional test was also performed by using same-sign dilepton events only positively or only negatively charged. The tests show stable response of the fit in terms of fitted nuisance parameters and signal strength.

The systematic uncertainties having the highest impact in the results are the ones associated to the dominant backgrounds in the *BSM SR*. Thus, the highest ranked systematics are the ones related to the SM  $t\bar{t}t\bar{t}$  cross-section, the SM  $t\bar{t}t\bar{t}$  generator uncertainty, and the uncertainty assigned to  $t\bar{t}W$  QCD events with eight or more jets.

All results above are done with the  $t\bar{t}t\bar{t}$  contribution constrained to the SM prediction. The binned likelihood fit has also been performed with the goal of measuring the normalisation factor of  $t\bar{t}t\bar{t}$  events assuming no contribution from the BSM  $t\bar{t}t\bar{t}$  signal, and by fitting the SM BDT distribution in the *baseline SR*. The best fitted value is found to be compatible with the observation from the previous ATLAS  $t\bar{t}t\bar{t}$  cross-section measurement [33].

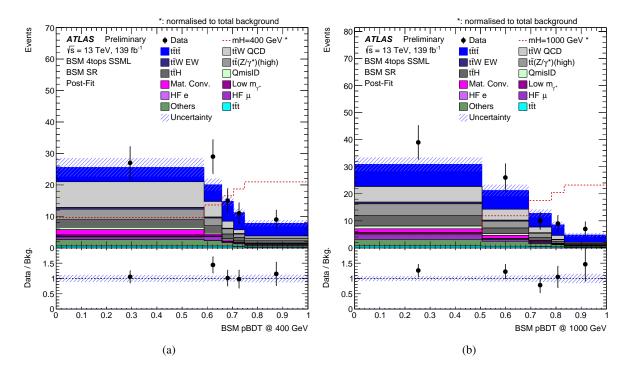


Figure 6: Data and post-fit background comparison obtained with the background-only fit in the *BSM SR* for the BSM pBDT distribution used for  $m_H = 400$  GeV (a) and 1000 GeV (b). The fit is done simultaneously in all signal and control regions. The band includes the total uncertainty of the post-fit estimation. The respective signal hypothesis is also shown. The signal has been normalised to the total background for better visibility. The lower panel shows the ratio of the data and post-fit background.

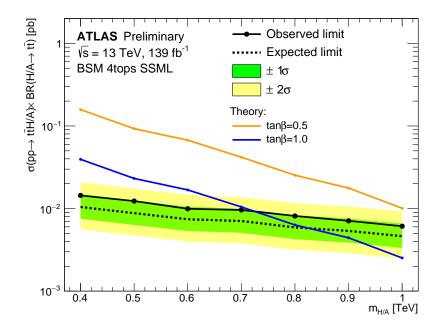


Figure 7: Observed (black solid line) and expected (black dashed line) 95% CL upper limits on the  $t\bar{t}H/A$  cross-section times branching fraction of  $H/A \rightarrow t\bar{t}$  as a function of  $m_{H/A}$ . The limits are estimated assuming that both, a heavy scalar H and pseudo-scalar A, contribute to the  $t\bar{t}t\bar{t}$  final state and have the same mass  $m_H = m_A$ . The green (yellow) band shows the  $\pm 1\sigma$  ( $\pm 2\sigma$ ) variation on the expected limits. Theoretical predictions for two values of tan  $\beta$  are shown.

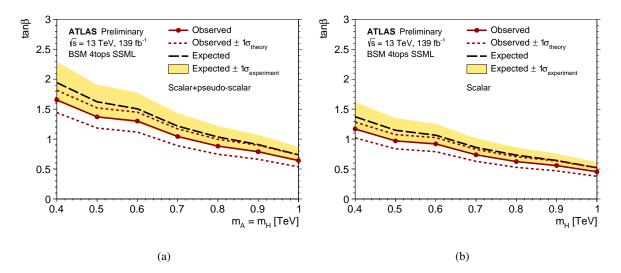


Figure 8: Observed (red line) and expected (black dashed line) exclusion regions at 95% CL in the tan  $\beta$  versus mass plane assuming that both, a heavy scalar *H* and pseudo-scalar *A*, contribute to the  $t\bar{t}t\bar{t}$  final state and have the same mass  $m_H = m_A$  (a) or assuming that only the scalar *H* contributes (b). The limits for the pseudo-scalar *A* alone are similar to those of (b). The yellow band shows the  $\pm 1\sigma$  variation on the expected exclusion region. The region below the red solid line is excluded at 95% CL. The exclusion regions are derived in the context of 2HDM type-II. Variations on the theory cross-section are also shown as dashed red lines.

# 9 Conclusion

A search for a new heavy Higgs boson in the process  $t\bar{t}H/A \rightarrow t\bar{t}t\bar{t}$  in the same-sign dilepton and multilepton channel has been presented. The search makes use of 139 fb<sup>-1</sup> of proton-proton collision data collected by the ATLAS detector at the LHC at a centre-of-mass energy of 13 TeV.

No significant excess of events over the Standard Model expectation is observed. The results are then interpreted in the context of the 2HDM type-II. The observed (expected) upper limits at 95% CL on the  $t\bar{t}H/A$  cross-section times branching ratio of  $H/A \rightarrow t\bar{t}$  range between 14 (10) fb and 6 (5) fb for a heavy Higgs boson mass between 400 GeV and 1000 GeV, respectively. These upper limits on the cross-section are translated into limits in the tan  $\beta$  versus mass plane. Assuming that only one particle, either the scalar H or the pseudo-scalar A, contributes to the  $t\bar{t}t\bar{t}$  final state, the values of tan  $\beta$  below 1.2 and 0.5 are excluded for the studied mass range. This exclusion range increases up to tan  $\beta$  between 1.6 and 0.6 when both particles are considered.

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## References

- [1] ATLAS Collaboration, Observation of a new particle in the search for the Standard Model Higgs boson with the ATLAS detector at the LHC, Phys. Lett. B 716 (2012) 1, arXiv: 1207.7214 [hep-ex] (cit. on p. 2).
- [2] CMS Collaboration,
   Observation of a new boson at a mass of 125 GeV with the CMS experiment at the LHC,
   Phys. Lett. B 716 (2012) 30, arXiv: 1207.7235 [hep-ex] (cit. on p. 2).
- [3] ATLAS Collaboration, *Combined measurements of Higgs boson production and decay using up to*  $80 fb^{-1}$  of proton–proton collision data at  $\sqrt{s} = 13$  TeV collected with the ATLAS experiment, Phys. Rev. D **101** (2020) 012002, arXiv: 1909.02845 [hep-ex] (cit. on p. 2).
- [4] CMS Collaboration, Combined measurements of Higgs boson couplings in proton–proton collisions at  $\sqrt{s} = 13 \text{ TeV}$ , Eur. Phys. J. C **79** (2019) 421, arXiv: 1809.10733 [hep-ex] (cit. on p. 2).
- [5] F. Englert and R. Brout, Broken Symmetry and the Mass of Gauge Vector Mesons, Phys. Rev. Lett. 13 (1964) 321, ed. by J. C. Taylor (cit. on p. 2).
- [6] P. W. Higgs, *Broken symmetries, massless particles and gauge fields*, Phys. Lett. **12** (1964) 132 (cit. on p. 2).
- [7] P. W. Higgs, *Broken Symmetries and the Masses of Gauge Bosons*, Phys. Rev. Lett. **13** (1964) 508, ed. by J. C. Taylor (cit. on p. 2).
- [8] G. S. Guralnik, C. R. Hagen and T. W. B. Kibble, *Global Conservation Laws and Massless Particles*, Phys. Rev. Lett. 13 (1964) 585, ed. by J. C. Taylor (cit. on p. 2).
- P. W. Higgs, Spontaneous Symmetry Breakdown without Massless Bosons, Phys. Rev. 145 (1966) 1156 (cit. on p. 2).
- [10] T. W. B. Kibble, Symmetry breaking in nonAbelian gauge theories, Phys. Rev. 155 (1967) 1554, ed. by J. C. Taylor (cit. on p. 2).
- G. C. Branco et al., *Theory and phenomenology of two-Higgs-doublet models*, Phys. Rept. **516** (2012) 1, arXiv: 1106.0034 [hep-ph] (cit. on p. 2).
- [12] P. Fayet, Supersymmetry and Weak, Electromagnetic and Strong Interactions, Phys. Lett. B 64 (1976) 159 (cit. on p. 2).
- P. Fayet,
   Spontaneously Broken Supersymmetric Theories of Weak, Electromagnetic and Strong Interactions,
   Phys. Lett. B 69 (1977) 489 (cit. on p. 2).
- [14] J. E. Kim, *Light Pseudoscalars, Particle Physics and Cosmology*, Phys. Rept. 150 (1987) 1 (cit. on p. 2).
- [15] ATLAS Collaboration,
  Search for a heavy Higgs boson decaying into a Z boson and another heavy Higgs boson in the *llbb* and *llWW* final states in pp collisions at √s = 13 TeV with the ATLAS detector,
  Eur. Phys. J. C 81 (2020) 396, arXiv: 2011.05639 [hep-ex] (cit. on p. 2).
- [16] ATLAS Collaboration, Search for Higgs boson pair production in the two bottom quarks plus two photons final state in pp collisions at  $\sqrt{s} = 13$  TeV with the ATLAS detector, (2021), arXiv: 2112.11876 [hep-ex] (cit. on p. 2).

- [17] ATLAS Collaboration, Search for resonances decaying into photon pairs in 139 fb<sup>-1</sup> of pp collisions at  $\sqrt{s} = 13$  TeV with the ATLAS detector, Phys. Lett. B 822 (2021) 136651, arXiv: 2102.13405 [hep-ex] (cit. on p. 2).
- [18] ATLAS Collaboration, Search for heavy resonances decaying into a pair of Z bosons in the  $\ell^+\ell^-\ell'^+\ell'^-$  and  $\ell^+\ell^-\nu\bar{\nu}$  final states using 139 fb<sup>-1</sup> of proton–proton collisions at  $\sqrt{s} = 13$ , TeV with the ATLAS detector, Eur. Phys. J. C **81** (2020) 332, arXiv: 2009.14791 [hep-ex] (cit. on p. 2).
- [19] ATLAS Collaboration, Search for Heavy Higgs Bosons Decaying into Two Tau Leptons with the ATLAS Detector Using pp Collisions at  $\sqrt{s} = 13$  TeV, Phys. Rev. Lett. **125** (2020) 051801, arXiv: 2002.12223 [hep-ex] (cit. on p. 2).
- [20] ATLAS Collaboration, Search for heavy neutral Higgs bosons produced in association with *b*-quarks and decaying into *b*-quarks at  $\sqrt{s} = 13$  TeV with the ATLAS detector, Phys. Rev. D **102** (2020) 032004, arXiv: 1907.02749 [hep-ex] (cit. on p. 2).
- [21] CMS Collaboration, Search for a heavy Higgs boson decaying to a pair of W bosons in proton–proton collisions at  $\sqrt{s} = 13$  TeV, JHEP **03** (2020) 034, arXiv: 1912.01594 [hep-ex] (cit. on p. 2).
- [22] CMS Collaboration, Search for new neutral Higgs bosons through the  $H \rightarrow ZA \rightarrow \ell^+ \ell^- b\bar{b}$ process in pp collisions at  $\sqrt{s} = 13$  TeV, JHEP **03** (2020) 055, arXiv: 1911.03781 [hep-ex] (cit. on p. 2).
- [23] CMS Collaboration, Search for a heavy pseudoscalar Higgs boson decaying into a 125 GeV Higgs boson and a Z boson in final states with two tau and two light leptons at  $\sqrt{s} = 13$  TeV, JHEP **03** (2020) 065, arXiv: 1910.11634 [hep-ex] (cit. on p. 2).
- [24] CMS Collaboration, Search for MSSM Higgs bosons decaying to  $\mu^+\mu^-$  in proton–proton collisions at  $\sqrt{s} = 13$  TeV, Phys. Lett. B **798** (2019) 134992, arXiv: 1907.03152 [hep-ex] (cit. on p. 2).
- [25] CMS Collaboration, Search for a heavy pseudoscalar boson decaying to a Z and a Higgs boson at  $\sqrt{s} = 13$  TeV, Eur. Phys. J. C **79** (2019) 564, arXiv: 1903.00941 [hep-ex] (cit. on p. 2).
- [26] ATLAS Collaboration, Search for heavy Higgs bosons A/H decaying to a top quark pair in pp collisions at  $\sqrt{s} = 8$  TeV with the ATLAS detector, Phys. Rev. Lett. **119** (2017) 191803, arXiv: 1707.06025 [hep-ex] (cit. on p. 2).
- [27] CMS Collaboration, Search for heavy Higgs bosons decaying to a top quark pair in proton–proton collisions at  $\sqrt{s} = 13$  TeV, JHEP 04 (2020) 171, arXiv: 1908.01115 [hep-ex] (cit. on p. 2).
- [28] N. Craig, J. Hajer, Y.-Y. Li, T. Liu and H. Zhang,
   *Heavy Higgs bosons at low* tan β: from the LHC to 100 TeV, JHEP 01 (2017) 018,
   arXiv: 1605.08744 [hep-ph] (cit. on p. 2).
- [29] ATLAS Collaboration, Search for new phenomena in events with same-charge leptons and b-jets in pp collisions at  $\sqrt{s} = 13$  TeV with the ATLAS detector, JHEP **12** (2018) 039, arXiv: **1807.11883** [hep-ex] (cit. on pp. 2, 3, 15).
- [30] CMS Collaboration, Search for production of four top quarks in final states with same-sign or multiple leptons in proton–proton collisions at  $\sqrt{s} = 13$  TeV, Eur. Phys. J. C 80 (2020) 75, arXiv: 1908.06463 [hep-ex] (cit. on p. 2).

- [31] CMS Collaboration, Search for the production of four top quarks in the single-lepton and opposite-sign dilepton final states in proton–proton collisions at  $\sqrt{s} = 13$  TeV, JHEP **11** (2019) 082, arXiv: **1906.02805** [hep-ex] (cit. on p. 2).
- [32] ATLAS Collaboration, Measurement of the  $t\bar{t}t\bar{t}$  production cross section in pp collisions at  $\sqrt{s} = 13$  TeV with the ATLAS detector, JHEP **11** (2021) 118, arXiv: **2106.11683** [hep-ex] (cit. on p. 2).
- [33] ATLAS Collaboration, Evidence for  $t\bar{t}t\bar{t}$  production in the multilepton final state in proton–proton collisions at  $\sqrt{s} = 13$ TeV with the ATLAS detector, Eur. Phys. J. C **80** (2020) 1085, arXiv: 2007.14858 [hep-ex] (cit. on pp. 2, 8, 10, 11, 14, 15, 20).
- [34] R. Frederix, D. Pagani and M. Zaro, Large NLO corrections in tīW<sup>±</sup> and tītī hadroproduction from supposedly subleading EW contributions, JHEP 02 (2018) 031, arXiv: 1711.02116 [hep-ph] (cit. on pp. 3, 5, 14).
- [35] ATLAS Collaboration, The ATLAS Experiment at the CERN Large Hadron Collider, JINST 3 (2008) S08003 (cit. on p. 3).
- [36] ATLAS Collaboration, ATLAS Insertable B-Layer: Technical Design Report, ATLAS-TDR-19; CERN-LHCC-2010-013, 2010, URL: https://cds.cern.ch/record/1291633 (cit. on p. 4).
- [37] B. Abbott et al., *Production and integration of the ATLAS Insertable B-Layer*, JINST **13** (2018) T05008, arXiv: **1803.00844** [physics.ins-det] (cit. on p. 4).
- [38] ATLAS Collaboration, *Performance of the ATLAS trigger system in 2015*, Eur. Phys. J. C **77** (2017) 317, arXiv: 1611.09661 [hep-ex] (cit. on p. 4).
- [39] ATLAS Collaboration, The ATLAS Collaboration Software and Firmware, ATL-SOFT-PUB-2021-001, 2021, URL: https://cds.cern.ch/record/2767187 (cit. on p. 4).
- [40] ATLAS Collaboration,
   ATLAS data quality operations and performance for 2015–2018 data-taking,
   JINST 15 (2020) P04003, arXiv: 1911.04632 [physics.ins-det] (cit. on p. 4).
- [41] ATLAS Collaboration, Performance of electron and photon triggers in ATLAS during LHC Run 2, Eur. Phys. J. C 80 (2020) 47, arXiv: 1909.00761 [hep-ex] (cit. on pp. 4, 13).
- [42] ATLAS Collaboration, Performance of the ATLAS muon triggers in Run 2, JINST 15 (2020) P09015, arXiv: 2004.13447 [hep-ex] (cit. on pp. 4, 13).
- [43] ATLAS Collaboration, *The ATLAS Simulation Infrastructure*, Eur. Phys. J. C 70 (2010) 823, arXiv: 1005.4568 [physics.ins-det] (cit. on p. 4).
- [44] GEANT4 Collaboration, S. Agostinelli et al., *GEANT4 a simulation toolkit*, Nucl. Instrum. Meth. A 506 (2003) 250 (cit. on p. 4).
- [45] J. Alwall et al., The automated computation of tree-level and next-to-leading order differential cross sections, and their matching to parton shower simulations, JHEP 07 (2014) 079, arXiv: 1405.0301 [hep-ph] (cit. on p. 4).
- [46] S. Frixione, P. Nason and G. Ridolfi,
   A positive-weight next-to-leading-order Monte Carlo for heavy flavour hadroproduction,
   JHEP 09 (2007) 126, arXiv: 0707.3088 [hep-ph] (cit. on p. 4).

- [47] P. Nason, *A new method for combining NLO QCD with shower Monte Carlo algorithms*, JHEP **11** (2004) 040, arXiv: hep-ph/0409146 (cit. on p. 4).
- [48] S. Frixione, P. Nason and C. Oleari, Matching NLO QCD computations with parton shower simulations: the POWHEG method, JHEP 11 (2007) 070, arXiv: 0709.2092 [hep-ph] (cit. on p. 4).
- [49] S. Alioli, P. Nason, C. Oleari and E. Re, A general framework for implementing NLO calculations in shower Monte Carlo programs: the POWHEG BOX, JHEP 06 (2010) 043, arXiv: 1002.2581 [hep-ph] (cit. on p. 4).
- [50] E. Re,
   Single-top Wt-channel production matched with parton showers using the POWHEG method,
   Eur. Phys. J. C 71 (2011) 1547, arXiv: 1009.2450 [hep-ph] (cit. on p. 4).
- [51] R. Frederix, E. Re and P. Torrielli, Single-top t-channel hadroproduction in the four-flavour scheme with POWHEG and aMC@NLO, JHEP 09 (2012) 130, arXiv: 1207.5391 [hep-ph] (cit. on p. 4).
- [52] S. Alioli, P. Nason, C. Oleari and E. Re, *NLO single-top production matched with shower in POWHEG: s- and t-channel contributions*, JHEP 09 (2009) 111, arXiv: 0907.4076 [hep-ph] (cit. on p. 4).
- [53] T. Sjöstrand et al., An introduction to PYTHIA 8.2, Comput. Phys. Commun. 191 (2015) 159, arXiv: 1410.3012 [hep-ph] (cit. on p. 4).
- [54] ATLAS Collaboration, ATLAS Pythia 8 tunes to 7 TeV data, ATL-PHYS-PUB-2014-021, 2014, URL: https://cds.cern.ch/record/1966419 (cit. on p. 4).
- [55] R. D. Ball et al., *Parton distributions for the LHC run II*, JHEP 04 (2015) 040, arXiv: 1410.8849 [hep-ph] (cit. on pp. 4, 5).
- [56] D. J. Lange, *The EvtGen particle decay simulation package*, Nucl. Instrum. Meth. A 462 (2001) 152 (cit. on p. 4).
- [57] S. Frixione, E. Laenen, P. Motylinski and B. R. Webber, Angular correlations of lepton pairs from vector boson and top quark decays in Monte Carlo simulations, JHEP 04 (2007) 081, arXiv: hep-ph/0702198 (cit. on p. 5).
- [58] P. Artoisenet, R. Frederix, O. Mattelaer and R. Rietkerk, *Automatic spin-entangled decays of heavy resonances in Monte Carlo simulations*, JHEP 03 (2013) 015, arXiv: 1212.3460 [hep-ph] (cit. on p. 5).
- [59] M. Bähr et al., *Herwig++ physics and manual*, Eur. Phys. J. C 58 (2008) 639, arXiv: 0803.0883 [hep-ph] (cit. on p. 5).
- [60] J. Bellm et al., *Herwig 7.0/Herwig++ 3.0 release note*, Eur. Phys. J. C 76 (2016) 196, arXiv: 1512.01178 [hep-ph] (cit. on p. 5).
- [61] L. Harland-Lang, A. Martin, P. Motylinski and R. Thorne, Parton distributions in the LHC era: MMHT 2014 PDFs, Eur. Phys. J. C 75 (2015) 204, arXiv: 1412.3989 [hep-ph] (cit. on p. 5).
- [62] E. Bothmann et al., *Event generation with Sherpa 2.2*, SciPost Phys. 7 (2019) 034, arXiv: 1905.09127 [hep-ph] (cit. on p. 5).

- [63] S. Schumann and F. Krauss,
   *A parton shower algorithm based on Catani–Seymour dipole factorisation*, JHEP 03 (2008) 038, arXiv: 0709.1027 [hep-ph] (cit. on p. 5).
- [64] S. Höche, F. Krauss, M. Schönherr and F. Siegert, *A critical appraisal of NLO+PS matching methods*, JHEP 09 (2012) 049, arXiv: 1111.1220 [hep-ph] (cit. on p. 5).
- [65] S. Höche, F. Krauss, M. Schönherr and F. Siegert, QCD matrix elements + parton showers. The NLO case, JHEP 04 (2013) 027, arXiv: 1207.5030 [hep-ph] (cit. on p. 5).
- [66] S. Catani, F. Krauss, R. Kuhn and B. R. Webber, *QCD Matrix Elements + Parton Showers*, JHEP **11** (2001) 063, arXiv: hep-ph/0109231 (cit. on p. 5).
- [67] S. Höche, F. Krauss, S. Schumann and F. Siegert, *QCD matrix elements and truncated showers*, JHEP **05** (2009) 053, arXiv: **0903.1219** [hep-ph] (cit. on p. 5).
- [68] F. Cascioli, P. Maierhöfer and S. Pozzorini, *Scattering Amplitudes with Open Loops*, Phys. Rev. Lett. **108** (2012) 111601, arXiv: **1111.5206** [hep-ph] (cit. on p. 5).
- [69] A. Denner, S. Dittmaier and L. Hofer,
   *Collier: A fortran-based complex one-loop library in extended regularizations*,
   Comput. Phys. Commun. 212 (2017) 220, arXiv: 1604.06792 [hep-ph] (cit. on p. 5).
- [70] F. Buccioni et al., OpenLoops 2, Eur. Phys. J. C 79 (2019) 866, arXiv: 1907.13071 [hep-ph] (cit. on p. 5).
- [71] D. de Florian et al.,
   Handbook of LHC Higgs Cross Sections: 4. Deciphering the Nature of the Higgs Sector, (2016),
   arXiv: 1610.07922 [hep-ph] (cit. on pp. 6, 14).
- [72] ATLAS Collaboration, Studies on top-quark Monte Carlo modelling for Top2016, ATL-PHYS-PUB-2016-020, 2016, URL: https://cds.cern.ch/record/2216168 (cit. on p. 6).
- [73] S. Frixione, E. Laenen, P. Motylinski, C. White and B. R. Webber, Single-top hadroproduction in association with a W boson, JHEP 07 (2008) 029, arXiv: 0805.3067 [hep-ph] (cit. on p. 6).
- [74] M. L. Ciccolini, S. Dittmaier and M. Krämer, *Electroweak radiative corrections to associated WH and ZH production at hadron colliders*, Phys. Rev. D 68 (2003) 073003, arXiv: hep-ph/0306234 [hep-ph] (cit. on p. 6).
- [75] O. Brein, A. Djouadi and R. Harlander, *NNLO QCD corrections to the Higgs-strahlung processes at hadron colliders*, Phys. Lett. B 579 (2004) 149, arXiv: hep-ph/0307206 (cit. on p. 6).
- [76] O. Brein, R. Harlander, M. Wiesemann and T. Zirke, *Top-Quark Mediated Effects in Hadronic Higgs-Strahlung*, Eur. Phys. J. C 72 (2012) 1868, arXiv: 1111.0761 [hep-ph] (cit. on p. 6).
- [77] L. Altenkamp, S. Dittmaier, R. V. Harlander, H. Rzehak and T. J. E. Zirke, *Gluon-induced Higgs-strahlung at next-to-leading order QCD*, JHEP **02** (2013) 078, arXiv: 1211.5015 [hep-ph] (cit. on p. 6).

- [78] A. Denner, S. Dittmaier, S. Kallweit and A. Mück, *HAWK 2.0: A Monte Carlo program for Higgs production in vector-boson fusion and Higgs strahlung at hadron colliders*, Comput. Phys. Commun. **195** (2015) 161, arXiv: 1412.5390 [hep-ph] (cit. on p. 6).
- [79] O. Brein, R. V. Harlander and T. J. E. Zirke, vh@nnlo Higgs Strahlung at hadron colliders, Comput. Phys. Commun. 184 (2013) 998, arXiv: 1210.5347 [hep-ph] (cit. on p. 6).
- [80] R. V. Harlander, A. Kulesza, V. Theeuwes and T. Zirke, Soft gluon resummation for gluon-induced Higgs Strahlung, JHEP 11 (2014) 082, arXiv: 1410.0217 [hep-ph] (cit. on p. 6).
- [81] T. Sjöstrand, S. Mrenna and P. Skands, A brief introduction to PYTHIA 8.1, Comput. Phys. Commun. 178 (2008) 852, arXiv: 0710.3820 [hep-ph] (cit. on p. 6).
- [82] ATLAS Collaboration, The Pythia 8 A3 tune description of ATLAS minimum bias and inelastic measurements incorporating the Donnachie–Landshoff diffractive model, ATL-PHYS-PUB-2016-017, 2016, URL: https://cds.cern.ch/record/2206965 (cit. on p. 6).
- [83] ATLAS Collaboration, Vertex Reconstruction Performance of the ATLAS Detector at  $\sqrt{s} = 13$  TeV, ATL-PHYS-PUB-2015-026, 2015, URL: https://cds.cern.ch/record/2037717 (cit. on p. 6).
- [84] ATLAS Collaboration, Electron and photon performance measurements with the ATLAS detector using the 2015–2017 LHC proton–proton collision data, JINST 14 (2019) P12006, arXiv: 1908.00005 [hep-ex] (cit. on pp. 6, 7, 13).
- [85] ATLAS Collaboration, *Muon reconstruction and identification efficiency in ATLAS using the full Run 2 pp collision data set at*  $\sqrt{s} = 13$  *TeV*, Eur. Phys. J. C **81** (2021) 578, arXiv: 2012.00578 [hep-ex] (cit. on pp. 7, 13).
- [86] ATLAS Collaboration,
   Jet reconstruction and performance using particle flow with the ATLAS Detector,
   Eur. Phys. J. C 77 (2017) 466, arXiv: 1703.10485 [hep-ex] (cit. on p. 7).
- [87] M. Cacciari, G. P. Salam and G. Soyez, *The anti-k<sub>t</sub> jet clustering algorithm*, JHEP **04** (2008) 063, arXiv: **0802.1189** [hep-ph] (cit. on p. 7).
- [88] ATLAS Collaboration, Jet energy scale and resolution measured in proton–proton collisions at  $\sqrt{s} = 13$  TeV with the ATLAS detector, Eur. Phys. J. C **81** (2020) 689, arXiv: 2007.02645 [hep-ex] (cit. on pp. 7, 14).
- [89] ATLAS Collaboration, *Tagging and suppression of pileup jets with the ATLAS detector*, ATLAS-CONF-2014-018, 2014, URL: https://cds.cern.ch/record/1700870 (cit. on p. 7).
- [90] ATLAS Collaboration,
   Selection of jets produced in 13 TeV proton-proton collisions with the ATLAS detector,
   ATLAS-CONF-2015-029, 2015, URL: https://cds.cern.ch/record/2037702 (cit. on p. 7).
- [91] ATLAS Collaboration, Optimisation and performance studies of the ATLAS b-tagging algorithms for the 2017-18 LHC run, ATL-PHYS-PUB-2017-013, 2017, URL: https://cds.cern.ch/record/2273281 (cit. on pp. 7, 14).
- [92] ATLAS Collaboration, Identification of Jets Containing b-Hadrons with Recurrent Neural Networks at the ATLAS Experiment, ATL-PHYS-PUB-2017-003, 2017, URL: https://cds.cern.ch/record/2255226 (cit. on p. 7).

- [93] ATLAS Collaboration, ATLAS *b-jet identification performance and efficiency measurement with t* $\bar{t}$  *events in pp collisions at*  $\sqrt{s} = 13$  TeV, Eur. Phys. J. C **79** (2019) 970, arXiv: 1907.05120 [hep-ex] (cit. on p. 7).
- [94] ATLAS Collaboration, *Performance of missing transverse momentum reconstruction with the ATLAS detector using proton–proton collisions at*  $\sqrt{s} = 13$  *TeV*, Eur. Phys. J. C **78** (2018) 903, arXiv: 1802.08168 [hep-ex] (cit. on pp. 8, 14).
- [95] ATLAS Collaboration, Measurement of the  $t\bar{t}Z$  and  $t\bar{t}W$  cross sections in proton–proton collisions at  $\sqrt{s} = 13 \text{ TeV}$  with the ATLAS detector, Phys. Rev. D **99** (2019) 072009, arXiv: **1901.03584** [hep-ex] (cit. on pp. 9, 17).
- [96] P. Baldi, K. Cranmer, T. Faucett, P. Sadowski and D. Whiteson, Parameterized neural networks for high-energy physics, Eur. Phys. J. C76 (2016) 235, arXiv: 1601.07913 [hep-ex] (cit. on p. 11).
- [97] T. Chen and C. Guestrin, XGBoost, Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (2016), URL: http://dx.doi.org/10.1145/2939672.2939785 (cit. on p. 11).
- [98] J. D. Bjorken and S. J. Brodsky, Statistical Model for Electron-Positron Annihilation into Hadrons, Phys. Rev. D 1 (5 1970) 1416, URL: https://link.aps.org/doi/10.1103/PhysRevD.1.1416 (cit. on p. 12).
- [99] ATLAS Collaboration, *Luminosity determination in pp collisions at*  $\sqrt{s} = 13$  *TeV using the ATLAS detector at the LHC*, ATLAS-CONF-2019-021, 2019, URL: https://cds.cern.ch/record/2677054 (cit. on p. 13).
- [100] G. Avoni et al., *The new LUCID-2 detector for luminosity measurement and monitoring in ATLAS*, JINST **13** (2018) P07017 (cit. on p. 13).
- [101] ATLAS Collaboration, *Performance of pile-up mitigation techniques for jets in pp collisions at*  $\sqrt{s} = 8 \text{ TeV using the ATLAS detector, Eur. Phys. J. C$ **76**(2016) 581, arXiv: 1510.03823 [hep-ex] (cit. on p. 14).
- [102] J. Butterworth et al., PDF4LHC recommendations for LHC Run II, J. Phys. G 43 (2016) 023001, arXiv: 1510.03865 [hep-ph] (cit. on p. 14).
- [103] F. F. Cordero, M. Kraus and L. Reina, *Top-quark pair production in association with a W<sup>±</sup> gauge boson in the POWHEG-BOX*, Phys. Rev. D 103 (9 2021) 094014, URL: https://link.aps.org/doi/10.1103/PhysRevD.103.094014 (cit. on p. 14).
- [104] ATLAS Collaboration, Measurement of the production cross-section of a single top quark in association with a Z boson in proton–proton collisions at 13 TeV with the ATLAS detector, Phys. Lett. B 780 (2018) 557, arXiv: 1710.03659 [hep-ex] (cit. on p. 15).
- [105] F. Demartin, B. Maier, F. Maltoni, K. Mawatari and M. Zaro, tWH associated production at the LHC, Eur. Phys. J. C 77 (2017) 34, arXiv: 1607.05862 [hep-ph] (cit. on p. 15).
- [106] ATLAS Collaboration, *Measurements of inclusive and differential fiducial cross-sections of tī production with additional heavy-flavour jets in proton–proton collisions at*  $\sqrt{s} = 13$  *TeV with the ATLAS detector*, JHEP **04** (2019) 046, arXiv: 1811.12113 [hep-ex] (cit. on p. 15).

- [107] W. Verkerke and D. P. Kirkby, *The RooFit toolkit for data modeling*, eConf C0303241 (2003) MOLT007, arXiv: physics/0306116 [physics.data-an] (cit. on p. 16).
- [108] W. Verkerke and D. Kirkby, *RooFit Users Manual*, URL: http://roofit.sourceforge.net (cit. on p. 16).
- [109] G. Cowan, K. Cranmer, E. Gross and O. Vitells, *Asymptotic formulae for likelihood-based tests of new physics*, Eur. Phys. J. C 71 (2011) 1554, Erratum: Eur. Phys. J. C 73 (2013) 2501, arXiv: 1007.1727 [physics.data-an] (cit. on p. 16).
- T. Junk, Confidence level computation for combining searches with small statistics, Nucl. Instrum. Meth. A 434 (1999) 435, arXiv: hep-ex/9902006 (cit. on p. 16).
- [111] A. L. Read, *Presentation of search results: the CL<sub>S</sub> technique*, J. Phys. G **28** (2002) 2693 (cit. on p. 16).
- [112] ATLAS Collaboration, *ATLAS Computing Acknowledgements*, ATL-SOFT-PUB-2021-003, URL: https://cds.cern.ch/record/2776662 (cit. on p. 23).