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# Observation of quantum entanglement in top-quark pairs using the ATLAS detector

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We report the highest-energy observation of entanglement, in top–antitop quark events produced at the Large Hadron Collider, using a proton–proton collision data set with a center-of-mass energy of  $\sqrt{s} = 13$  TeV and an integrated luminosity of  $140 \text{ fb}^{-1}$  recorded with the ATLAS experiment. Spin entanglement is detected from the measurement of a single observable  $D$ , inferred from the angle between the charged leptons in their parent top- and antitop-quark rest frames. The observable is measured in a narrow interval around the top–antitop quark production threshold, where the entanglement detection is expected to be significant. It is reported in a fiducial phase space defined with stable particles to minimize the uncertainties that stem from limitations of the Monte Carlo event generators and the parton shower model in modelling top-quark pair production. The entanglement marker is measured to be  $D = -0.547 \pm 0.002$  (stat.)  $\pm 0.021$  (syst.) for  $340 < m_{t\bar{t}} < 380$  GeV. The observed result is more than five standard deviations from a scenario without entanglement and hence constitutes both the first observation of entanglement in a pair of quarks and the highest-energy observation of entanglement to date.

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# 1 Main

Entanglement is a striking feature of quantum mechanics [1–3], with applications in fields such as metrology, cryptography, quantum information, and quantum computation [4–8]. If two particles are entangled, the quantum state of one particle cannot be described independently of the other. Entanglement has been observed in a wide variety of systems and length scales, ranging from the microscopic [9–13] to the macroscopic [14–16]. However, entanglement remains largely unexplored at the highest accessible energy scales. Particle colliders, such as the Large Hadron Collider (LHC) at CERN, probe fundamental particles and their interactions at the highest energies accessible in a laboratory, exceeded only by astrophysical sources.

Beyond the fundamental interest of exploring quantum entanglement in a novel setting, this observation demonstrates the potential of using high-energy colliders, such as the LHC, as tools for testing our fundamental understanding of quantum mechanics. Hadron colliders offer a truly relativistic environment and provide a rich menu of fundamental interactions and forces whose interactions are rarely considered for experiments in quantum information. Relativistic effects are expected to play a critical role in quantum information [17] and the measurement described here illustrates the potential for novel approaches to exploring these effects and other foundational problems in quantum mechanics using colliders.

Recently, the heaviest fundamental particle known to exist, the top quark, was proposed as a new laboratory to study quantum entanglement and quantum information [18, 19]. Thanks to its high mass and short lifetime, the quantum numbers of the top quark are not shrouded by strong interactions with other particles before it decays and are therefore accessible via its decay products. In this Article, the spin correlation between the top quark and antitop quark is used to probe the effects of quantum entanglement, in proton–proton ( $pp$ ) collision events recorded with the ATLAS detector at a center-of-mass energy of 13 TeV. Entanglement is observed with a significance of more than five standard deviations for the first time in pairs of quarks.

The simplest example of an entangled system involves a pair of quantum bits (qubits); pieces of quantum information about two particles in the same quantum state which exist in superposition. The spin quantum number of a fermion, a particle whose spin can take values of  $\pm 1/2$ , is one of the simplest and most fundamental examples of a qubit. Among the fundamental fermions of the Standard Model (SM) of particle physics, the top quark is uniquely suited for high-energy spin measurements because of its unique properties: its immense mass gives it a lifetime ( $\sim 10^{-25}$  s) significantly shorter than the timescale needed for a quark’s quantum numbers to be shrouded by hadronization ( $\sim 10^{-24}$  s) and spin decorrelation ( $\sim 10^{-21}$  s) effects [20]. As a result, its spin information is transferred to its decay products. This unique feature provides an opportunity to study a pseudo-bare quark, free of the color-confinement properties of the strong force that shroud other quarks.

Quarks are most commonly produced in hadron collider experiments as matter–antimatter pairs. A pair of top–antitop quarks ( $t\bar{t}$ ) is a two-qubit system whose spin quantum state is described by the spin density matrix  $\rho$ :

$$\rho = \frac{1}{4} [I_4 + \sum_i (B_i^+ \sigma^i \otimes I_2 + B_i^- I_2 \otimes \sigma^i) + \sum_{i,j} C_{ij} \sigma^i \otimes \sigma^j].$$

The first term in the linear sum is a normalization constant, where  $I_n$  is the  $n \times n$  identity matrix. The second term describes the intrinsic polarization of the top and the antitop quarks, where  $\sigma^i$  are the corresponding Pauli matrices and the real number  $B_i^\pm$  characterize the spin polarization of each particle. The third term

describes the spin correlation between the particles, encoded by the spin correlation matrix  $C_{ij}$ . In all expressions, an orthogonal coordinate system is represented by the indices  $i, j = 1, 2, 3$ .

At hadron colliders,  $t\bar{t}$  pairs are produced mainly via the strong interaction and thus have no intrinsic polarization (i.e.  $B_i^\pm \simeq 0$ ) because of parity conservation and time invariance in quantum chromodynamics (QCD) [21]. However, their spins are expected to be correlated and this correlation has already been observed by both the ATLAS and CMS experiments at the LHC [22–26]. Entanglement in top-quark pairs can be observed via an increase in the strength of their spin correlations.

Due to their short lifetime, top quarks cannot be detected directly in experiments. In the SM, they decay almost exclusively into a bottom quark and a  $W$  boson, and the  $W$  boson subsequently decays into either a pair of lighter quarks or a charged lepton and a neutrino. In this measurement, only  $W$  bosons decaying into leptons are considered since charged leptons, especially electrons and muons, are readily detected with high precision at collider experiments. To a good approximation, the degree to which the leptons carry the spin information of their parent top quarks is 100% due to the maximally parity-violating nature of the electro-weak charged current. The angular direction of each of these leptons is correlated with the direction of the spin of their parent top quark or antitop quark in such a way that the normalized differential cross-section ( $\sigma$ ) of the process may be written as [27]:

$$\frac{1}{\sigma} \frac{d\sigma}{d\Omega_+ d\Omega_-} = \frac{1 + \mathbf{B}^+ \cdot \hat{\mathbf{q}}_+ - \mathbf{B}^- \cdot \hat{\mathbf{q}}_- - \hat{\mathbf{q}}_+ \cdot \mathbf{C} \cdot \hat{\mathbf{q}}_-}{(4\pi)^2},$$

where  $\hat{\mathbf{q}}_+$  ( $\hat{\mathbf{q}}_-$ ) is the antilepton (lepton) direction in its parent antitop (top) quark's rest frame and  $\Omega_+$  ( $\Omega_-$ ) is the solid angle associated with the antilepton (lepton). The vectors  $\mathbf{B}^\pm$  determine the top-quark and antitop-quark polarizations, while the matrix  $\mathbf{C}$  contains their spin correlations. These terms are analogous to those that appear in the general form for  $\rho$ . Since the information about the polarizations and spin correlations of the short-lived top quarks is transferred to the decay leptons, their values can be extracted from a measurement of angular observables associated with these leptons, allowing us to reconstruct the  $t\bar{t}$  spin quantum state.

At the LHC,  $t\bar{t}$  pairs are produced mainly via gluon–gluon fusion. When they are produced close to their production threshold, i.e. when their invariant mass  $m_{t\bar{t}}$  is close to twice the mass of the top quark ( $m_{t\bar{t}} \sim 2 \cdot m_t \sim 350$  GeV), approximately 80% of the production cross-section of  $t\bar{t}$  pairs arises from a spin-singlet state [28–30], which is maximally entangled. After averaging over all possible top-quark directions, entanglement only survives at threshold because of the rotational invariance of the spin singlet. This invariance implies that the trace (the sum of all of the diagonal elements) of the correlation matrix  $\mathbf{C}$ , where each diagonal element corresponds to the spin correlation in a particular direction, is a good entanglement witness. It is an observable that can signal the presence of entanglement, with  $\text{tr}[\mathbf{C}] + 1 < 0$  as a sufficient condition for entanglement [18].

It is more convenient to define an entanglement marker by using  $D = \text{tr}[\mathbf{C}]/3$  [18], which can be experimentally measured as:

$$D = -3 \cdot \langle \cos \varphi \rangle,$$

where  $\langle \cos \varphi \rangle$  is the average value of the cosine of the angle (dot product) between the charged-lepton directions after they have been Lorentz boosted into the  $t\bar{t}$  rest frame and then their parent top-quark and antitop-quark's rest frames, which can be measured experimentally in an ensemble data set. The existence of an entangled state is demonstrated if the measurement satisfies  $D < -1/3$ .

The SM is a quantum theory and entanglement is implicitly present in its predictions. Nevertheless, a demonstration of spin entanglement in  $t\bar{t}$  pairs is challenging due to the inability to control the internal

degrees of freedom in the initial state [19]. Currently, entanglement can only be detected with the help of a dedicated analysis in a restricted phase space like the one presented here.

## 1.1 The ATLAS detector and event samples

The ATLAS experiment [31–33] at the LHC is a multipurpose particle detector with a forward–backward symmetric cylindrical geometry and a solid-angle coverage of almost  $4\pi$ .<sup>1</sup> It is used to record particles produced in LHC collisions through a combination of particle position and energy measurements. It consists of an inner-tracking detector surrounded by a thin superconducting solenoid providing a 2 T axial magnetic field, electromagnetic and hadronic calorimeters, and a muon spectrometer. The muon spectrometer surrounds the calorimeters and is based on three large superconducting air-core toroidal magnets with eight coils each providing a field integral of between 2.0 and 6.0 T m across the detector. An extensive software suite [34] is used in data simulation, in the reconstruction and analysis of real and simulated data, in detector operations, and in the trigger and data acquisition systems of the experiment. The complete data set of  $pp$  collision events at a center-of-mass energy of  $\sqrt{s} = 13$  TeV collected with the ATLAS experiment during 2015–2018 is used, corresponding to an integrated luminosity of  $140 \text{ fb}^{-1}$ . This analysis focuses on the data sample recorded using single-electron or single-muon triggers [35].

A unique feature of particle physics is that very precise simulations of the SM can be realized through the use of Monte Carlo (MC) event generators. These simulations replicate real collisions and their resultant particles on an event-by-event basis and these events can be passed through sophisticated simulations of the ATLAS detector to produce simulated data. Comparing these simulated events to those actually recorded by the detector is one way to test the predictions of the SM. Another is to use the simulated data to model how the ATLAS detector responds to a particular physics process, such as the pair production of top quarks, and to use this to create corrections to undo the effect of the detector response on real data and then to compare this corrected data to theoretical predictions. This measurement uses the latter strategy.

Three distinct types of real and simulated data are used, each with associated physics objects. Detector level refers to real data before it has been corrected for detector effects and simulated data after they have been passed through simulation of the ATLAS detector. Parton level refers to simulated MC events where the particles arise from the fundamental interaction being simulated, such as quarks and bosons, or to real collision data that has been corrected to this level. Particle level refers to simulated data with physics objects that are built only from the stable particles that remain after the decay of the particles that exist at parton level, i.e. particles that live long enough to interact with the detector, or to data that has been corrected to this level. This measurement relies on the selection and reconstruction of muons, electrons, quarks and gluons as hadronic jets, neutrinos as missing transverse momentum ( $\vec{p}_T^{\text{miss}}$ ),  $W$  bosons and top quarks. These objects are each reconstructed at detector level, particle level, and parton level. Details of how these objects are reconstructed in ATLAS and in MC simulations are provided in Methods A.1.

MC event simulations are used to model the  $t\bar{t}$  signal and the expected SM background processes. The production of  $t\bar{t}$  events was modeled using the POWHEG Box v2 heavy-quark (hq) [36–39] generator at next-to-leading order (NLO) precision in QCD and the events were interfaced to either PYTHIA 8.230 [40]

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<sup>1</sup> ATLAS uses a right-handed coordinate system with its origin at the nominal interaction point in the center of the detector and the  $z$ -axis along the beam pipe. The  $x$ -axis points from the interaction point to the center of the LHC ring, and the  $y$ -axis points upwards. Cylindrical coordinates  $(r, \phi)$  are used in the transverse plane, where  $\phi$  is the azimuth 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  $\Delta R \equiv \sqrt{(\Delta\eta)^2 + (\Delta\phi)^2}$ .

or HERWIG 7.2.1 [41, 42] to model the parton shower and hadronization. The decays of the top quarks, including their spin correlations, were modeled at leading-order (LO) precision in QCD. An additional sample that generates  $t\bar{t}$  events at full NLO accuracy in production and decay was generated using the POWHEG BOX RES [43, 44] ( $bb4\ell$ ) generator, interfaced to PYTHIA. Further details of the setup and tuning of these generators are provided in Methods A.2. An important difference between PYTHIA and HERWIG is that the former uses a  $p_T$ -ordered shower, while the latter uses an angular-ordered shower (see Methods A.6). Another important consideration is that full information on the spin density matrix is not passed to the parton shower programs and therefore is not fully preserved during the shower.

The SM background processes which contribute to the analysis are the production of a single top quark with a  $W$  boson ( $tW$ ), pair production of top quarks with an additional boson  $t\bar{t} + X$  ( $X = H, W, Z$ ) production, and the production of dileptonic events from either one or two massive gauge bosons ( $W, Z$  bosons). The generators for the hard-scatter processes and the showering are listed in Methods A.2. The procedure for identifying and reconstructing detector-level objects are the same for data and MC events.

## 1.2 Analysis procedure

Only events taken during stable-beam conditions, and for which all relevant components of the detector were operational, are considered. To be selected, events must have exactly one electron and one muon with opposite-sign electric charges. A minimum of two jets is required, and at least one of them must be identified to originate from a  $b$ -hadron ( $b$ -tagged).

The background contribution of events with reconstructed objects that are misidentified as leptons, referred to as the “fake-lepton” background, is estimated using a combination of MC prediction and correction based on data. This data-driven correction is obtained from a control region dominated by fake leptons. It is defined by using the same selection criteria as above, except that the two leptons must have same-sign electric charges. The difference between the numbers of observed events and predicted events in this region is taken as a scale factor and applied to predicted fake-lepton events in the signal region.

Events that pass the event selection are separated into three analysis regions, based on either the detector-level, particle-level, or parton-level  $m_{t\bar{t}}$ , depending on the region. The signal region is constructed to be dominated by events that are as close to the production threshold as the resolution of the reconstruction method will allow, as this is the region where the entanglement of the top quarks is expected to be maximized.

The optimal mass window for the signal region was determined to be  $340 < m_{t\bar{t}} < 380$  GeV. Two additional validation regions are defined in order to validate the method used for the measurement. Firstly, a region is defined close to the limit where entanglement is not expected to be observable, and also with significant dilution from misreconstructed events from non-entangled regions, by requiring  $380 < m_{t\bar{t}} < 500$  GeV. Secondly, a region in which no signal of entanglement is expected is defined with  $m_{t\bar{t}} > 500$  GeV. Each of the regions has a  $t\bar{t}$ -event purity of about 90%. The dominant sources of background processes arise from the production of a single top quark via electroweak interactions and the production of a  $Z$  boson with additional jets, each of which accounts for approximately 40% of the background in the signal region. The remaining 20% of background events arise from events containing misidentified leptons and from the production of two electroweak bosons. The distribution of  $\cos\varphi$  in the signal region and the reconstruction-level  $D$  value after background subtraction are shown in the left and right panels of Figure 1, respectively.

In order to compare the data with calculations and correct for detector effects, we must also define an event selection using the “truth” information in the MC event record. This selection uses particle-level objects to match as closely as possible the selection at detector level and is called a *fiducial* particle-level selection. Particle-level events are required to contain exactly one electron and one muon with opposite-sign electric charges and at least two particle-level jets, one of which must contain a  $b$ -hadron. The  $\cos \varphi$  distribution is then constructed from the particle-level top quarks and charged leptons in the same manner as at detector level.

The response of the detector, the event selections, and the top-quark reconstruction distort the shape of the  $\cos \varphi$  distribution. The observed distribution is corrected for these effects with a simple method: a simulation-based calibration curve which connects any value at the detector level to the corresponding particle-level value. We correct the data for detector effects by using a unique calibration curve built for each signal and validation region based on the expected signal model, after subtracting the expected contribution from background processes. Due to limited resolution of the reconstructed mass of the  $t\bar{t}$  system, some events that truly belong to the validation regions can enter the signal region at detector level. These events are treated as detector effects.

To build these curves, MC event samples are created with alternative values of  $D$  by reweighting the events, following the procedure described in Methods A.3. The calibration curve corrects the value  $D_{\text{detector}}$  measured at the detector level to a corresponding value  $D_{\text{particle}}$  at particle level. To construct the calibration curve, several hypotheses for different values of  $D$ , denoted by  $D'_{\text{particle}}$  with a corresponding  $D'_{\text{detector}}$  value, are created corresponding to changes in the expected value of entanglement.

The pairs of  $D'_{\text{detector}}$  and  $D'_{\text{particle}}$  are plotted in Figure 2(a). A straight line interpolates between the points. With this calibration curve, any value for  $D_{\text{detector}}$  can be calibrated to the particle level.

Three categories of uncertainties are included in the calibration curves: uncertainties in modeling  $t\bar{t}$  production and decay, uncertainties in modeling the backgrounds, and detector-related uncertainties for both the  $t\bar{t}$  signal and the SM background processes. Each source of systematic uncertainty can result in a different calibration curve because it changes the shape of the  $\cos \varphi$  distribution at particle level and/or detector level. For each source of systematic uncertainty, the data are corrected using this new calibration curve and the resultant deviation from the data corrected by the nominal curve is taken as the systematic uncertainty of the data due to that source. Systematic uncertainties from all sources are summed in quadrature to determine the final uncertainty in the result.

For all of the detector-related uncertainties, the particle-level quantity is not affected and only detector-level values change. For signal modeling uncertainties, the effects at particle level propagate to detector level, resulting in shifts in both. Uncertainties in modeling the background processes affect how much background is subtracted from the expected or observed data and can therefore cause changes in the calibration curve. These uncertainties are treated as fully correlated between the signal and background (i.e. if a source of systematic uncertainty is expected affect both the signal and background processes, this is estimated simultaneously and not separately).

A summary of the different sources of systematic uncertainty and their impact on the result is given in Table 1. The size of each systematic uncertainty depends on the value of  $D$  and is given in Table 1 for the SM prediction, calculated with POWHEG+PYTHIA. The systematic uncertainties considered in the analysis are described in detail in Method A.5.

To compare the particle-level result with the parton-level entanglement limit  $D < -1/3$ , the limit must be folded to the particle level. A second calibration curve is constructed to relate the value of  $D_{\text{parton}}$  to



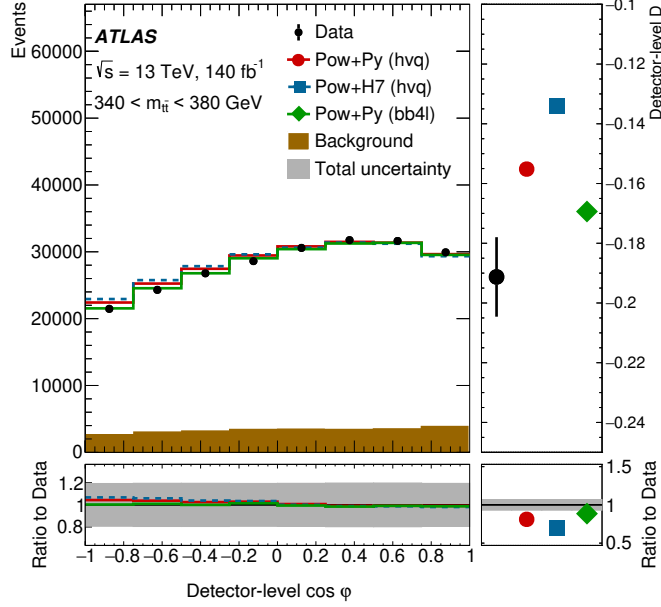


Figure 1: The left panel shows the  $\cos \varphi$  observable in the signal region at detector level and the right panel shows the entanglement marker  $D$ , calculated from the detector-level distributions, from three different MC generators; the POWHEG+PYTHIA and POWHEG+HERWIG heavy-quark models, labelled “Pow+Py (hvq)” and “Pow+H7 (hvq)”, respectively, and the POWHEG+PYTHIA  $bb4\ell$  model, labelled “Pow+Py ( $bb4\ell$ )”, are shown after background processes are subtracted. The uncertainty band shows the uncertainties from all sources added in quadrature. The ratios of the predictions to the data are shown at the bottom of the figure. The quoted value for  $D$  for the  $bb4\ell$  model also includes a subtraction of the single-top-quark background.

the corresponding  $D_{\text{particle}}$ . The definitions of parton-level top quarks and leptons in the MC generator follow Ref. [24] and correspond approximately to those of stable top quarks and leptons in a fixed-order calculation. Only systematic uncertainties related to the modeling of the  $t\bar{t}$  production and decay process are considered when building this calibration curve. The migration of parton level events from the signal region into the validation regions at particle level and vice versa is very small.

### 1.3 Results

The calibration procedure is performed in the signal region and the two validation regions to correct the data to a *fiducial* phase space at particle level, as described in Section 1.2. All systematic uncertainties are included in the three regions. The observed (expected) results are:

$$D = -0.547 \pm 0.002 [\text{stat.}] \pm 0.021 [\text{syst.}] \quad (-0.470 \pm 0.002 [\text{stat.}] \pm 0.018 [\text{syst.}]) ,$$

in the signal region of  $340 < m_{t\bar{t}} < 380$  GeV and:

$$D = -0.222 \pm 0.001 [\text{stat.}] \pm 0.027 [\text{syst.}] \quad (-0.258 \pm 0.001 [\text{stat.}] \pm 0.026 [\text{syst.}]) ,$$

$$D = -0.098 \pm 0.001 [\text{stat.}] \pm 0.021 [\text{syst.}] \quad (-0.103 \pm 0.001 [\text{stat.}] \pm 0.021 [\text{syst.}]) ,$$



Source of uncertainty	$\Delta D_{\text{observed}}(D = -0.547)$	$\Delta D$ [%]	$\Delta D_{\text{expected}}(D = -0.470)$	$\Delta D$ [%]
Signal modeling	0.017	3.2	0.015	3.2
Electrons	0.002	0.4	0.002	0.4
Muons	0.001	0.1	0.001	0.1
Jets	0.004	0.7	0.004	0.8
$b$ -tagging	0.002	0.4	0.002	0.4
Pile-up	$< 0.001$	$< 0.1$	$< 0.001$	$< 0.1$
$E_{\text{T}}^{\text{miss}}$	0.002	0.3	0.002	0.4
Backgrounds	0.010	1.8	0.009	1.8
Total statistical uncertainty	0.002	0.3	0.002	0.4
Total systematic uncertainty	0.021	3.8	0.018	3.9
Total uncertainty	0.021	3.8	0.018	3.9

Table 1: A summary of the effect of the groups of uncertainties at the expected SM value of  $D_{\text{expected}} = -0.470$ , corresponding to the POWHEG+PYTHIA modeling, and the observed value  $D_{\text{observed}} = -0.547$ , both in the signal region.  $E_{\text{T}}^{\text{miss}}$  denotes the magnitude of the missing transverse momentum. The total systematic uncertainty is calculated as the sum in quadrature of the individual groups of systematic uncertainties.

in the validation regions of  $380 < m_{t\bar{t}} < 500$  GeV and  $m_{t\bar{t}} > 500$  GeV, respectively. The expected values are those predicted by POWHEG+PYTHIA. The calibration curve for the signal region and a summary of the results in all regions are presented in Figure 2.

The observed values of the entanglement marker  $D$  are compared with the entanglement limit in Figure 2(b). The parton-level bound  $D = -1/3$  is converted to a particle-level bound by folding the limit to particle level to better highlight the differences between predictions using different parton shower orderings. For POWHEG+PYTHIA, this yields  $-0.322 \pm 0.009$ , where the uncertainty includes all uncertainties in the POWHEG+PYTHIA model except the parton shower uncertainty (for more details of these uncertainties, see Methods A.5). Similarly, for POWHEG+HERWIG, with an angular-ordered parton shower, a value of  $-0.27$  is obtained. No uncertainties are assigned in this case since it is merely used as an alternative model.

## 1.4 Discussion

In both of the validation regions, with no entanglement signal, the measurements are found to agree with the predictions from different MC setups within the uncertainties. This serves as a consistency check to validate the method used for the measurement.

Even though the different models yield different predictions, the current precision of the measurements in the validation regions does not allow us to rule out any of the MC setups that were used. It is important to note that close to the threshold, non-relativistic QCD processes, such as Coulomb bound state effects, affect the production of  $t\bar{t}$  events [28] and are not accounted for in the MC generators. However, other effects that result in similar changes to  $\cos \varphi$  and  $m_{t\bar{t}}$  are included in the systematic uncertainties. These systematic uncertainties are, at their largest, only a 1% effect on the final measurement and therefore the

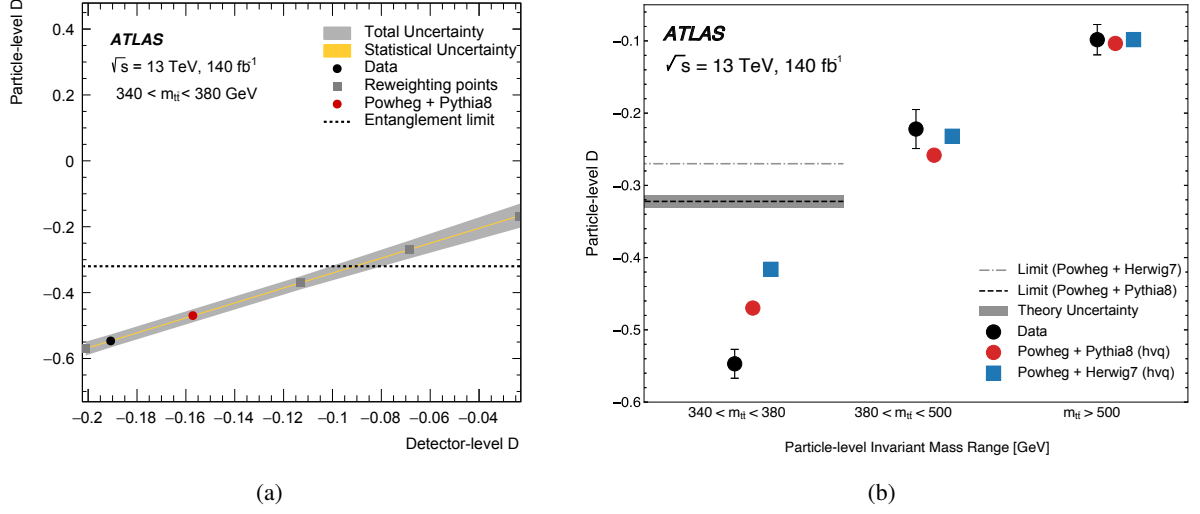


Figure 2: (a): Calibration curve for the dependence between the particle-level value of  $D$  and the detector-level value of  $D$ , in the signal region. The yellow band represents the statistical uncertainty, while the grey band represents the total uncertainty obtained by adding the statistical and systematic uncertainties in quadrature. The measured values and expected values from Powheg + Pythia8 (hqv) are marked with black and red circles, respectively, and the entanglement limit is shown as a dashed line. (b): The particle-level  $D$  results in the signal and validation regions compared with various MC models. The entanglement limit shown is a conversion from its parton-level value of  $D = -1/3$  to the corresponding value at particle level, and the uncertainties which are considered for the band are described in the text.

absence of these effects in the MC simulation used to derive the calibration curve is expected to be minimal. Additionally, the impact of the enhancement of the cross-section due to pseudo-bound-state effects on the calibration curve and particle-level measurement has been assessed in a stress test, and found to be small compared to the modelling uncertainties already included in the measurement.

In the signal region the POWHEG+PYTHIA and POWHEG+HERWIG generators yield different predictions. The size of the observed difference is consistent with changing the method of shower ordering and is discussed in detail in Methods A.6.

In the signal region, the observed and expected significances with respect to the entanglement limit are well beyond five standard deviations, independently of the MC model used to correct the entanglement limit to account for the *fiducial* phase space of the measurement. This is illustrated in Figure 2(b), where the hypothesis of no entanglement is shown. The observed result in the region with  $340 < m_{t\bar{t}} < 380$  GeV establishes the formation of entangled  $t\bar{t}$  states. This constitutes the first observation of entanglement in a quark–antiquark pair.

Apart from the fundamental interest in testing quantum entanglement in a new environment, this measurement in top quarks paves the way to use high-energy colliders, such as the LHC, as a laboratory to study quantum information and foundational problems in quantum mechanics. From a quantum information perspective, high energy colliders are particularly interesting due to their relativistic nature, and the richness of the interactions and symmetries that can be probed there. Furthermore, highly demanding measurements, such as measuring quantum discord and reconstructing the steering ellipsoid, can be naturally implemented at the LHC due to the vast number of available  $t\bar{t}$  events [45]. From a high-energy physics perspective,

borrowing concepts from quantum information theory inspires new approaches and observables that can be used to search for physics beyond the SM [46–49].

## A Methods

### A.1 Object Identification in the ATLAS detector

Reconstructed (detector level) objects are defined as follows. Electron candidates are required to satisfy the “tight” likelihood-based identification requirement as well as calorimeter- and track- based isolation criteria [50], and have pseudorapidity  $|\eta| < 1.37$  or  $1.52 < |\eta| < 2.47$ . Muon candidates are required to satisfy the “medium” identification requirement as well as track-based isolation criteria [51–53], and have  $|\eta| < 2.5$ . Electrons and muons must have a minimum transverse momentum ( $p_T$ ) of 25–28 GeV, depending on the data-taking period. Showers of particles (jets) that arise from the hadronization of quarks and gluons [54] are reconstructed from particle-flow objects [55], using the anti- $k_t$  algorithm [56, 57] with a radius parameter  $R = 0.4$ , a  $p_T$  threshold of 25 GeV, and a  $|\eta| < 2.5$  requirement. A Jet-Vertex-Tagger requirement is applied to jets with  $p_T < 60$  GeV and  $|\eta| < 2.4$  to suppress jets originating from additional interactions in the same or neighbouring bunch crossings (pile-up) [58]. Jets are tagged as containing  $b$ -hadrons using the DL1r tagger [59] with a  $b$ -tagging efficiency of 85%. Missing transverse momentum ( $\vec{p}_T^{\text{miss}}$ ) [60, 61] is determined from the imbalance in the transverse momenta of all reconstructed objects. In order to measure  $D$ , the top quarks must be reconstructed from their measured decay products. In the  $t\bar{t}$  dileptonic decay, in addition to charged leptons and jets, there are two neutrinos which are not measured by the detector. Several methods are available to reconstruct the top quarks from the detector-level charged leptons, jets and  $\vec{p}_T^{\text{miss}}$ . The main method used in this work is the Ellipse method [62], which is a geometric approach to analytically calculate the neutrino momenta. This method yields at least one real solution in 85% of events. If this method fails (e.g. the resultant solutions are all complex), the Neutrino Weighting method [63] is used; it assigns a weight to each possible solution by assessing the compatibility of the neutrino momenta and the  $\vec{p}_T^{\text{miss}}$  in the event, after scanning possible values of the pseudorapidities of the neutrinos. If both methods fail, a simple pairing of each lepton with its closest  $b$ -tagged jet is used. If a second  $b$ -tagged jet is not present in the event, the leading (highest)  $p_T$  untagged jet is used instead. In all cases, a  $W$  boson mass of 80.4 GeV and a top-quark mass of 172.5 GeV are used as input parameters.

In simulated events, parton-level objects are taken directly from the MC history information and are required to have status code of 1, indicating that they are the fundamental particles (partons) of the interaction. Top quarks are required to be partons that decay to a  $W$  boson and a  $b$  quark, whereas charged leptons are required to be the immediate decay parton from the  $W$  boson from the top quark. Particle-level objects are reconstructed using simulated stable particles in the MC simulation before their reconstruction in the detector, but after hadronization. A particle is defined as stable if it has a mean lifetime greater than 30 ps, within the pseudorapidity acceptance of the detector. The selection criteria for the particle-level objects are chosen to correspond as closely as possible to the criteria applied to the detector-level objects. Electrons, muons and neutrinos are required to come from the electroweak decay of a top quark, and are discarded if they arise from the decay of a hadron or a  $\tau$ -lepton. Electrons and muons are then “dressed” by summing their four-momenta with any prompt photons within  $\Delta R = 0.1$ ; they must then lie within  $\Delta R > 0.4$  from a jet to avoid being removed from the event. Leptons are also required to have  $p_T > 10$  GeV and  $|\eta| < 2.5$ , and at least one lepton must have  $p_T > 25$  GeV. Jets are built by clustering all stable particles, using the anti- $k_t$  algorithm with a radius parameter of  $R = 0.4$ , and are tagged as containing  $b$ -hadrons if they have at least one ghost-matched  $b$ -hadron [64, 65] with  $p_T > 5$  GeV. Jets are also required to have  $p_T > 25$  GeV

and  $|\eta| < 2.5$ . Each  $W$  boson is reconstructed by combining an available electron and electron neutrino or muon and muon neutrino. The top quark and antitop quark are reconstructed by pairing the two leading  $b$ -tagged jets, or the  $b$ -tagged jet and the highest- $p_T$  untagged jet in events with only one  $b$ -tag, with the reconstructed  $W$  bosons. Both potential jet–lepton combinations are formed and the one which minimizes  $|m_t - m(W_1 + b_{1/2})| + |m_t - m(W_2 + b_{2/1})|$  is taken as the correct pairing, where  $m_t$  denotes the mass of the top quark,  $b_{1/2}$  denotes the two jets selected for the reconstruction,  $W_{1/2}$  refers to the reconstructed  $W$  bosons, and  $m$  is the invariant mass of the objects in brackets.

## A.2 Monte Carlo Simulation

The production of  $t\bar{t}$  events was modeled using the POWHEG Box v2 heavy-quark (hvw) [36–39] event generator. This generator uses matrix elements calculated at next-to-leading-order (NLO) precision in a strong coupling constant power expansion in QCD with the NNPDF3.0<sub>NLO</sub> [66] parton distribution function (PDF) set and the  $h_{\text{damp}}$  parameter<sup>2</sup> set to  $1.5 m_t$  [67]. The decays of the top quarks, including their spin correlations, were modeled at leading-order (LO) precision in QCD. As an alternative, the POWHEG Box RES [43, 44] event generator, developed to treat decaying resonances within the POWHEG Box framework and including off-shell and non-resonant effects in the matrix element calculation, was used to produce an additional event sample, labelled as  $bb4\ell$  in the following.<sup>3</sup>

In the  $bb4\ell$  event sample, spin correlations are calculated at NLO, and full NLO accuracy in  $t\bar{t}$  production and decays is attained. To model the parton shower, hadronization, and underlying event, the events from both POWHEG Box v2 and POWHEG Box RES were interfaced to PYTHIA 8.230 [40], with parameters set according to the A14 set of tuned parameters [68] and using the NNPDF2.3<sub>LO</sub> set of PDFs [69]. Similarly, the events from POWHEG Box v2 (hvw) were also interfaced to HERWIG 7.2.1 [41, 42], using the HERWIG 7.2.1 default set of tuned parameters. The decays of bottom and charm hadrons were performed by EVTGEN 1.6.0 [70]. The spin information from the matrix element calculation is not passed to the parton shower programs and therefore is not fully preserved during the shower.

All simulated event samples include pile-up interactions, and the events are reweighted to reproduce the observed distribution of the average number of collisions per bunch crossing.

## A.3 Reweighting the $\cos \varphi$ distribution

In order to construct the calibration curve, templates for alternative scenarios with different degrees of entanglement, and therefore with different values of  $D$ , must be extracted. The degree of entanglement is intrinsic in the calculations of the MC event generators and cannot be changed. However, the effects of entanglement can be directly accessed via  $D$ , measured from the average of the  $\cos \varphi$  distribution in the event. Therefore, an event-by-event reweighting based on  $D$  is used to vary the degree of entanglement. Although the measurement uses detector-level and particle-level objects, the observable  $D$  is changed at parton level, where it is directly related to the entanglement in the entanglement between the top and

<sup>2</sup> The  $h_{\text{damp}}$  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.

<sup>3</sup> Although  $bb4\ell$  is the higher-precision MC sample, it cannot be compared directly with the data after they are corrected for detector effects as it is not possible to remove its off-shell component in a formally correct way. However, the effect of using this model was tested in an approximate way and was found to not significantly change the conclusions of the measurement.

antitop spins. Therefore, each event is reweighted according to its parton-level values of  $m_{t\bar{t}}$  and  $\cos \varphi$ , as described below.

The entanglement variable  $D$  is extracted at parton level from the  $\cos \varphi$  distribution by using either the mean of the distribution  $D = -3 \cdot \langle \cos \varphi \rangle$  or the slope of the normalized differential cross-section  $(1/\sigma) d\sigma/d\cos \varphi = (1/2)(1 - D \cos \varphi)$ .

For simplicity, the analysis always uses the mean of the distribution, although the two methods are equivalent. Thus for the purpose of reweighting, one must change the slope of the  $\cos \varphi$  distribution at parton level. Each event is reweighted according to this slope, which in turn changes the distributions at particle level and detector level.

The observable  $D$  depends on the invariant mass of the  $t\bar{t}$  system,  $m_{t\bar{t}}$ . To perform the reweighting, the differential value of  $D$  per mass unit as a function of  $m_{t\bar{t}}$ ,  $D_\Omega(m_{t\bar{t}})$ , has to be calculated. This is achieved by fitting a third-order polynomial of the form:

$$D_\Omega(m_{t\bar{t}}) = x_0 + x_1 \cdot m_{t\bar{t}}^{-1} + x_2 \cdot m_{t\bar{t}}^{-2} + x_3 \cdot m_{t\bar{t}}^{-3},$$

where  $x_0, x_1, x_2, x_3$  are constants. The values of the parameters of  $D_\Omega(m_{t\bar{t}})$  depend on the MC event generator and have to be calculated for the nominal sample and for the effect of each of the  $t\bar{t}$  theory systematic uncertainties, since they change the parton-level  $\cos \varphi$  values and thus  $D_\Omega(m_{t\bar{t}})$ .

The reweighting method is a simple scaling of the  $\cos \varphi$  distribution according to the desired new value of  $D$ . This is done by assigning a weight  $w$  to each event at parton level as:

$$w = \frac{1 - D_\Omega(m_{t\bar{t}}) \cdot X \cdot \cos \varphi}{1 - D_\Omega(m_{t\bar{t}}) \cdot \cos \varphi},$$

with  $X$  as the scaling hypothesis of  $D$ . If, for example,  $X = 1.2$ , it means that  $D$  is scaled up by 20% relative to its nominal value. In order to build the calibration curve, four alternative values of  $D$  are considered, with  $X = 0.4, 0.6, 0.8, 1.2$ , in addition to the nominal value without reweighting ( $X = 1.0$ ). It is important to note that these  $X$  values change  $D$  across the entire  $m_{t\bar{t}}$  spectrum. In Figure 3 the parton-level distribution of  $D$  is shown in the signal region before and after reweighting.

## A.4 Background modeling

Simulated data in the form of MC samples were produced using either the full ATLAS detector simulation [71] based on the GEANT4 framework [72] or, for the estimation of some of the systematic uncertainties, a faster simulation with parameterized showers in the calorimeters [73]. The effect of pile-up was modeled by overlaying each hard-scattering event with inelastic  $pp$  collisions generated with PYTHIA 8.186 [74] using the NNPDF2.3LO set of PDFs [69] and the A3 set of tuned parameters [75]. Except for the events simulated with SHERPA, the EVTGEN program was used to simulate bottom and charm hadron decays. If not mentioned otherwise, the top-quark mass was set to  $m_t = 172.5$  GeV. All event samples that were interfaced with PYTHIA used the A14 set of tuned parameters [68] and the NNPDF2.3LO PDF set.

Single-top quark  $tW$  associated production was modeled using the POWHEG BOX v2 [37–39, 76] event generator, which provides matrix elements at NLO in the strong coupling constant  $\alpha_s$  in the five-flavor scheme with the NNPDF3.0NLO [66] PDF set. The functional form of the renormalization and factorization scales was set to the default scale, which is equal to the top-quark mass. The diagram-removal scheme [77] was employed to handle the interference with  $t\bar{t}$  production [67]. The inclusive cross-section was corrected

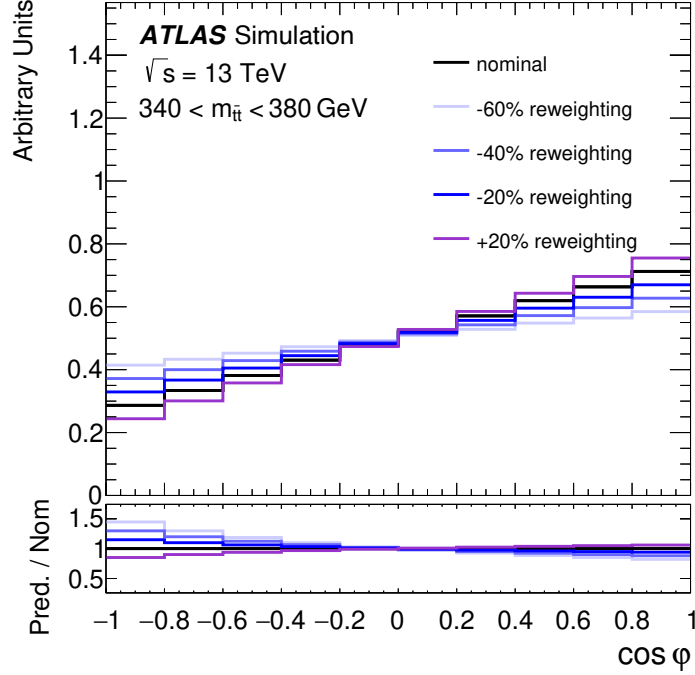


Figure 3: Example of the nominal  $\cos \phi$  distribution and the results of applying the reweighting technique with  $X = 0.4, 0.6, 0.8, 1.2$  in the signal region at parton level. The lower panel shows the ratio of each  $D$  value after reweighting (“Pred.”) to the nominal  $D$  value (“Nom.”).

to the theory prediction calculated at NLO in QCD with next-to-next-leading-logarithm (NNLL) soft-gluon corrections [78, 79]. For  $pp$  collisions at a center-of-mass energy of  $\sqrt{s} = 13$  TeV, this cross-section corresponds to  $\sigma(tW)_{\text{NLO+NNLL}} = 71.7 \pm 3.8$  pb. The uncertainty in the cross-section due to the PDF was estimated using the MSTW2008<sub>NNLO</sub> 90% CL [80, 81] PDF set, and was added in quadrature to the effect of the scale uncertainty.

Samples of diboson final states ( $VV$ ), where  $V$  denotes a  $W$  or  $Z$  boson, were simulated with the SHERPA 2.2.2 [82] event generator, including off-shell effects and Higgs boson contributions, where appropriate. Fully leptonic final states and semileptonic final states, where one boson decays leptonically and the other hadronically, were generated using matrix elements at NLO accuracy in QCD for up to one additional parton and at LO accuracy for up to three additional parton emissions. Samples for the loop-induced processes  $gg \rightarrow VV$  were generated using LO-accurate matrix elements for up to one additional parton emission for both the cases of fully leptonic and semileptonic final states. The matrix element calculations were matched and merged with the SHERPA parton shower based on Catani–Seymour dipole factorization [83, 84] using the MEPS@NLO prescription [85–88]. The virtual QCD corrections were provided by the OPENLOOPS library [89–91]. The NNPDF3.0<sub>NNLO</sub> set of PDFs was used [66], along with the dedicated set of tuned parton-shower parameters developed by the SHERPA authors.

The production of  $V$ +jets events was simulated with the SHERPA 2.2.11 [82] event generator using NLO matrix elements for up to two partons, and LO matrix elements for up to five partons, calculated with the Comix [83] and OPENLOOPS 2 [89–92] libraries. They were matched with the SHERPA parton shower [84] using the MEPS@NLO prescription [85–88]. The set of tuned parameters developed by the SHERPA authors was used, along with the NNPDF3.0<sub>NNLO</sub> set of PDFs [66].



The production of  $t\bar{t}V$  events was modeled using the MADGRAPH5\_AMC@NLO 2.3.3 [93] event generator, which provides matrix elements at NLO in the strong coupling constant  $\alpha_s$  with the NNPDF3.0<sub>NLO</sub> [66] PDFs. The functional form of the renormalization and factorization scales was set to  $0.5 \times \sum_i \sqrt{m_i^2 + p_{T,i}^2}$ , where the sum runs over all the particles generated from the matrix element calculation. Top quarks were decayed at LO using MADSPIN [94, 95] to preserve spin correlations. The events were interfaced with PYTHIA 8.210 [40] for the simulation of parton showering and hadronization. The cross-sections were calculated at NLO QCD and NLO EW accuracy using MADGRAPH5\_AMC@NLO as reported in Ref. [96]. For  $t\bar{t}\ell\ell$  events, the cross-section was scaled by an off-shell correction estimated at one-loop level in  $\alpha_s$ .

The production of  $t\bar{t}H$  events was modeled using the POWHEG BOX v2 [36–39, 97] event generator, which provides matrix elements at NLO in the strong coupling constant  $\alpha_s$  in the five-flavor scheme with the NNPDF3.0<sub>NLO</sub> [66] PDF set. The functional form of the renormalization and factorization scales was set to  $\sqrt[3]{m_T(t) \cdot m_T(\bar{t}) \cdot m_T(H)}$ . The events were interfaced with PYTHIA 8.230. The cross-section was calculated at NLO QCD and NLO EW accuracy using MADGRAPH5\_AMC@NLO as reported in Ref. [96]. The predicted value at  $\sqrt{s} = 13$  TeV is  $507^{+35}_{-50}$  fb, where the uncertainties were estimated from variations of both  $\alpha_s$  and the renormalization and factorization scales.

The background from non-prompt or fake leptons was modeled using simulated MC events to describe the shape of the kinematic distributions. MC event generator information is used to distinguish events with prompt leptons from events with non-prompt or fake leptons. The normalization of this background was obtained from data by using a dedicated control region. This control region uses the same basic event selection as the signal and validation regions, the only difference being that the electric charges of the electron and muon must have the same sign. Within this control region, the number of simulated prompt-lepton events is subtracted from the observed number of data events. The number of events remaining is then divided by the number of simulated fake-lepton events, resulting in a normalization factor of 1.4. This scale factor is then applied to the simulated fake-lepton events in the signal and validation regions.

## A.5 Systematic uncertainties

The systematic uncertainties can be divided into three separate categories: signal modeling uncertainties, which stem from the theory prediction of  $t\bar{t}$  production; object systematic uncertainties, which arise from the uncertainty in the detector response to objects used in the analysis; and background modeling systematic uncertainties, which are related to the theory prediction of the SM backgrounds. All systematic uncertainties, grouped according to their sources, are described in the following sections. The signal modeling uncertainties were found to dominate the overall uncertainty of this measurement.

For each source of systematic uncertainty, a new calibration curve is created and the simulated (or observed) data are corrected, resulting in a shifted corrected result. In most cases the systematic uncertainty is taken to be the difference between the nominal expected/observed result and the systematically shifted result. In cases where a systematic shift only effects the background model (e.g. background cross-section uncertainties), the systematically shifted background sample is subtracted from the data instead before the calibration is performed. In cases where the systematic uncertainty is one-sided, the uncertainty is symmetrized. In cases where uncertainties are asymmetric, the larger of the two variations is symmetrized. The signal modeling uncertainties dominate the measurement and their estimated sizes are presented in Table 2.



### A.5.1 Signal modeling uncertainties

Signal modeling uncertainties are those related to the choice of POWHEG BOX + PYTHIA as the nominal MC setup as well as those affecting the theoretical calculation itself. These systematic uncertainties are considered in two forms: alternative event generators, and weights. For the alternative-generator uncertainties, the difference between the calibrated values of  $D$  is taken as the systematic uncertainty. For the systematic uncertainties involving weights, the difference between the calibrated  $D$  values for the nominal sample and the weight-shifted sample is taken as the uncertainty. These uncertainties are enumerated as follows:

- **pThard setting:** The region of phase space that is vetoed in the showering when matched to a parton shower is varied by changing the internal pThard parameter of POWHEG BOX from 0 to 1, following the prescription described in Ref. [98].
- **Top-quark decay:** The uncertainty in the decay of the top quarks is estimated by comparing the nominal decay in POWHEG BOX with the decays modeled with MADSPIN [94, 95].
- **NNLO reweighting:** The uncertainty due to missing higher-order corrections is estimated by reweighting the  $p_T$  of the top quarks, the  $p_T$  of the  $t\bar{t}$  system, and the  $m_{t\bar{t}}$  spectra at parton level to match the predicted NNLO differential cross-sections [99].
- **Parton shower and hadronization:** This uncertainty is estimated by comparing two different parton-shower and hadronization algorithms, PYTHIA and HERWIG, interfaced to the same matrix element event generator (POWHEG BOX).
- **Recoil scheme:** The nominal sample uses a recoil scheme where partons recoil against  $b$ -quarks. This recoil scheme changes the modeling of second and subsequent gluon emissions from quarks produced by colored resonance decays, such as the  $b$ -quark in a top-quark decay, and therefore affects how the momentum is rearranged between the  $W$  boson and the  $b$ -quark. An alternative sample is produced in which the recoil is set to be against the top quark itself for the second and subsequent emissions [100].
- **Scale uncertainties:** The renormalization and factorization scales are raised and lowered by a factor of 2 in the nominal POWHEG setup, including simultaneous variations in the same direction. The envelope of results from all of these variations is taken as the final uncertainty.
- **Initial-state radiation:** The uncertainty due to initial-state radiation is estimated by choosing the Var3c up/down variations of the A14 tune as described in Ref. [101].
- **Final-state radiation:** The impact of final-state radiation is evaluated by doubling or halving the renormalization scale for emissions from the parton shower.
- **Parton distribution function (PDF):** The systematic uncertainty due to the choice of PDF is assessed using the PDF4LHC15 eigenvector decomposition [102]. The full difference between the results from the nominal PDF and the varied PDF is taken and symmetrised for each of the 30 eigenvectors. The quadrature sum of all result variations is quoted in Table 2.
- **$h_{\text{damp}}$  setting:** The  $h_{\text{damp}}$  parameter is a resummation damping factor and one of the parameters that controls the matching of POWHEG BOX matrix elements to the parton shower and thus effectively regulates the high- $p_T$  radiation against which the  $t\bar{t}$  system recoils. The systematic uncertainty due

to the chosen value of the  $h_{\text{damp}}$  parameter is assessed by comparing the nominal POWHEG+PYTHIA result with one where the  $h_{\text{damp}}$  parameter is increased by a factor of two.

- **Top-quark mass:** The effect of the top-quark mass uncertainty is examined by comparing the nominal sample with alternative samples that use  $m_t = 172$  or  $173$  GeV in the simulation.

Systematic uncertainty source	Relative size (for SM $D$ value)
Top-quark decay	1.6%
Parton distribution function	1.2%
Recoil scheme	1.1%
Final-state radiation	1.1%
Scale uncertainties	1.1%
NNLO reweighting	1.1%
pT <sub>hard</sub> setting	0.8%
Top-quark mass	0.7%
Initial-state radiation	0.2%
Parton shower and hadronization	0.2%
$h_{\text{damp}}$ setting	0.1%

Table 2: Relative sizes of the signal modeling uncertainties at the SM expectation point  $D_{\text{particle}} = -0.47$  for the nominal POWHEG BOX sample.

### A.5.2 Object systematic uncertainties

Systematic uncertainties which originate from the uncertainty in the detector response to the objects used in the analysis are estimated.

- **Electrons:** The systematic uncertainties considered for electrons arise mainly from uncertainties in their trigger, reconstruction, identification, and isolation efficiencies, and are estimated using tag-and-probe measurements in  $Z$  and  $J/\psi$  decays [50, 103]. Electron-related systematic uncertainties have a negligible impact on the final measurement, with a total contribution of about 0.2%.
- **Muons:** The systematic uncertainties considered for muons arise from uncertainties in their trigger, identification, and isolation efficiencies, and their energy scale and resolution, and are estimated using tag-and-probe measurements in  $Z$  and  $J/\psi$  decays [51–53]. Muon-related systematic uncertainties have a negligible impact on the final measurement, with a total contribution of about 0.3%.
- **Jets:** The systematic uncertainties associated with jets are separated into those related to the jet-energy scale and resolution (JES and JER) [54] and those related to the jet-vertex tagger (JVT) algorithm [58]. The JES (JER) uncertainty consists of 31 (13) individual components that are added in quadrature with the JVT uncertainty to obtain the total jet uncertainty. The largest contribution from a single source is 0.2%.
- **$b$ -tagging:** The estimation of these uncertainties is described in Ref. [104]. A total of 17 independent systematic variations are considered: 9 related to  $b$ -hadrons, 4 related to  $c$ -hadrons, and 4 related to light-jet misidentification. In addition, two high- $p_T$  extrapolation uncertainties are taken into account. The largest contribution from a single systematic variation is 0.4%.

- **$E_T^{\text{miss}}$ :** All object-based uncertainties are fully correlated with the reconstruction of the event's  $E_T^{\text{miss}}$  object, the magnitude of the  $\vec{p}_T^{\text{miss}}$  vector. However, there are some uncertainties specific to the reconstruction of  $E_T^{\text{miss}}$  which concern soft tracks not matched to leptons or jets. These uncertainties are divided into parallel and perpendicular response components as well as a scale uncertainty [60]. These have a negligible effect on the measurement.
- **Pile-up:** The effect of pile-up was modeled by overlaying the simulated hard-scattering events with inelastic  $pp$  events. In order to assess the systematic uncertainty due to pile-up, the reweighing performed to match simulation to data is varied within its uncertainty [58]. The resulting uncertainty has an effect of less than 0.1%.
- **Luminosity:** The luminosity uncertainty only changes the normalization of the signal and background samples. The value of  $D$  is calculated from the normalized  $\cos \varphi$  distribution and therefore is not affected by varying the sample normalization. However, the total expected statistical uncertainty can be affected by the luminosity uncertainty. This analysis uses the latest integrated luminosity estimate of  $140.1 \pm 1.2 \text{ fb}^{-1}$  [105]. Its uncertainty affects the measurement by less than 0.1%.

### A.5.3 Background modeling systematic uncertainties

Background events are a relatively small source of uncertainty in this measurement since the event selection and top-quark reconstruction, especially the  $m_{t\bar{t}}$  constraint, tend to suppress them. The uncertainties and their sources are listed in the following.

- **Single top quark:** Two uncertainties are considered for the single-top quark background: a cross-section uncertainty of 5.3% based on the NNLO cross-section uncertainty [79], and an uncertainty for the choice of scheme used to remove higher-order diagrams that overlap with the  $t\bar{t}$  process. For the latter, the nominal POWHEG+PYTHIA sample, generated with the diagram-removal scheme [77], was compared with an alternative sample generated using the diagram-subtraction scheme [67, 77]. The cross-section uncertainty has a 0.4% effect on the measurement, whereas the choice of diagram scheme has less than a 0.1% effect on the measurement.
- **$t\bar{t} + X$ :** A normalization uncertainty is considered for each of the  $t\bar{t} + X$  backgrounds: a cross-section uncertainty of  $^{+10\%}_{-12\%}$  for  $t\bar{t} + Z$ , and  $^{+13\%}_{-12\%}$  for  $t\bar{t} + W$ . Both are based on the NLO cross-section uncertainty derived from renormalization and factorization scale variations and PDF uncertainties in the matrix element calculation. These uncertainties have a negligible effect on the measurement, since the  $t\bar{t} + X$  processes make a very small contribution in the signal region.
- **Diboson:** A normalization uncertainty of  $\pm 10\%$  is considered for the diboson process to account for the difference between the NLO precision of the SHERPA event generator and precision of the theoretical cross-sections calculated to NNLO in QCD with NLO EW corrections. This simple  $K$ -factor approach is taken, rather than a more elaborate prescription, because the diboson background is small and the phase space selected by the analysis ( $m_{t\bar{t}} < 380 \text{ GeV}$ ) is unlikely to be sensitive to shape effects in the EW corrections, typically observed in high- $p_T$  tails. This uncertainty has less than a 0.1% effect on the measurement.
- **$Z \rightarrow \tau\tau$ :** A conservative cross-section uncertainty of  $\pm 20\%$  is applied to the  $Z \rightarrow \tau\tau$  background in order to account for the uncertainty in the cross-section prediction (which is significantly smaller than this variation) as well as to account for some mismodeling of the rate of associated heavy-flavor production, which is typically seen in  $ee$  and  $\mu\mu$  dileptonic  $t\bar{t}$  analyses and was estimated to be

a 5% (3%) effect in previous iterations of this analysis that included the  $ee$  ( $\mu\mu$ ) channel. This assumption is conservative as it is not possible to isolate a pure  $Z \rightarrow \tau\tau$  control region in which to estimate this effect, and therefore additional lepton-flavor-related effects present in the  $ee$  and  $\mu\mu$  channels are also being included. This uncertainty has a noticeable impact on the final measurement, becoming the largest background-related uncertainty. It becomes large, despite this background being relatively small, because the reconstruction-level  $Z \rightarrow \tau\tau \cos \varphi$  distribution is quite flat and therefore subtracting even a relatively small amount of  $Z \rightarrow \tau\tau$  background can noticeably affect the mean of the overall  $\cos \varphi$  distribution and therefore the  $D$  observable. This uncertainty has an impact of 1.5% on the measurement.

- **Fake and non-prompt leptons:** A normalization uncertainty of  $\pm 50\%$  is assigned to account for the uncertainty in the total yield of fake or non-prompt leptons in the signal region compared to the same-sign control region in order to ensure adequate coverage for our understanding of the rates of these types of events. It is a conservative uncertainty based on the observed level of data–MC agreement in the same-sign region. The uncertainty has only a 0.1% effect on the final measurement.

The majority of systematic uncertainties that are considered are inconsequential to the measurement, and the dominant systematic uncertainties arise mostly from the signal modeling and the  $Z \rightarrow \tau\tau$  cross-section uncertainty. These findings are true for the validation regions as well.

## A.6 Parton shower and hadronization effects

The studies described in the following were performed to gain a more detailed understanding of why the different parton-shower and hadronization algorithms yield different values for the entanglement- and spin-correlation-related observables. The nominal MC sample was produced with the NLO matrix element implemented in POWHEG BOX (hvh). The four-momenta produced with POWHEG BOX were interfaced with either PYTHIA or HERWIG for the parton shower, hadronization and underlying-event model.

At parton level, the two predictions are nearly identical, while at the stable-particle and detector levels the two predictions show larger differences in the shape of the  $\cos \varphi$  distributions. A parton-level measurement would therefore suffer from the ambiguity in  $\cos \varphi$ , while the particle-level measurement presented in this paper does not. An extensive suite of studies was performed to understand the origin of this difference.

Apart from using different parameter-tuning strategies, there are two main differences between the two parton-shower algorithms: their hadronization model and the shower ordering. While PYTHIA is based on the Lund string model and uses a  $p_T$ -ordered dipole shower [106–108], HERWIG is based on a cluster model and uses an angular-ordered shower as the default [109].

A comparison between MC simulations with different hadronization models has shown that these have a negligible effect on the  $\cos \varphi$  distribution, both when not placing a cut on  $m_{t\bar{t}}$  and when using a smaller part of phase space close to the signal region of the analysis, with  $m_{t\bar{t}} < 380$  GeV. Instead, most of the differences seem to originate from the different orderings in the parton shower. To illustrate this, different event generator setups were used for simulation and the corresponding  $\cos \varphi$  distributions were compared at particle level. The  $\cos \varphi$  distributions for the POWHEG+PYTHIA and POWHEG+HERWIG samples used in the analysis are shown in Figure 4(a), together with distributions for two different setups of HERWIG 7 in Figure 4(b). In these setups, HERWIG 7 was used both for the production of the  $t\bar{t}$  events and for the parton shower, hadronization and underlying event. The samples were produced at LO, using either a dipole shower or an angular-ordered shower. All distributions are normalized to unity. A difference of up to 6%

is observed when examining the ratio of POWHEG+HERWIG to POWHEG+PYTHIA distributions. The same behavior is observed when comparing the two different showering orders for HERWIG.

The similarities between the samples used in this analysis and the HERWIG samples with different showering orders implies that the ordering of the shower is the main cause of the observed differences. It has to be noted, however, that POWHEG does not pass the spin correlation information to the parton shower algorithms, while this is done in the LO HERWIG setup used to study these hadronisation effects.

These findings lead to the conclusion that performing the measurement at particle level is more attractive, since the overall uncertainties are smaller. In the validation regions, the level of agreement between either POWHEG+PYTHIA or POWHEG+HERWIG and the data is similar. Since the measurement is performed at the stable-particle level, the parton-level prediction for the entanglement limit was folded to the particle level as well, using a special calibration curve for this step. The prediction for the entanglement limit with POWHEG+HERWIG is further away from the data measurement than the one for POWHEG+PYTHIA. This difference is not symmetrized. All uncertainties in the POWHEG+PYTHIA prediction itself are folded to particle level as well and are included in the grey uncertainty band in Figure 2.

The procedure used in MC event generators to combine the matrix element with a parton-shower algorithm requires special attention in future higher-precision quantum information studies at the LHC.

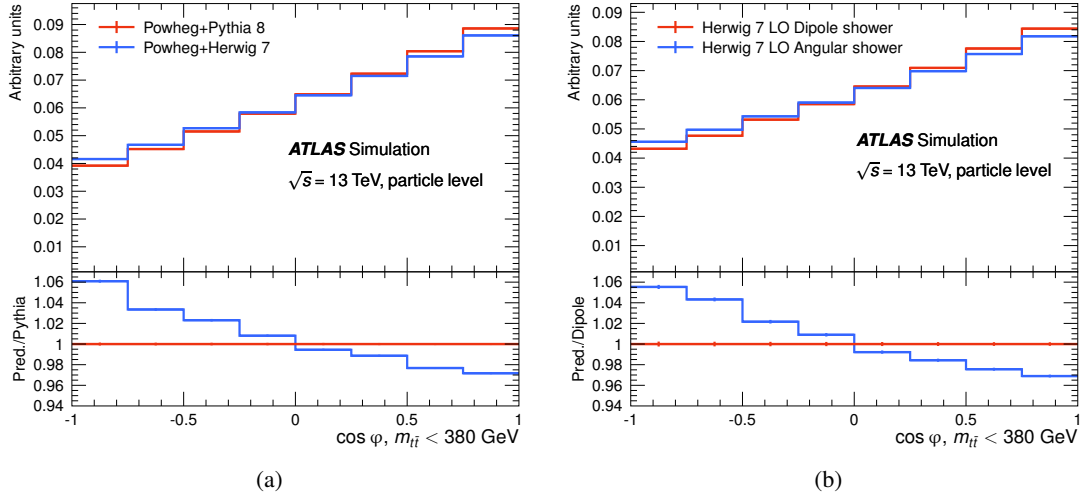


Figure 4: Comparison between  $\cos \varphi$  distributions in the signal region with  $m_{t\bar{t}} < 380$  GeV for different MC event generator setups at stable-particle level. Figure (a) compares events simulated with POWHEG Box which are interfaced with either PYTHIA (red line,  $p_T$ -ordered dipole shower) or HERWIG (blue line, angular-ordered shower) while figure (b) compares events simulated with HERWIG using either a dipole-ordered shower (red line) or an angular-ordered shower (blue line).

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