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Observation of a pseudoscalar excess at the top quark pair production threshold

The CMS Collaboration*

Abstract

A search for resonances in top quark pair ($t\bar{t}$) production in final states with two charged leptons and multiple jets is presented, based on proton-proton collision data collected by the CMS experiment at the CERN LHC at $\sqrt{s} = 13\,\text{TeV}$, corresponding to $138\,\text{fb}^{-1}$. The analysis explores the invariant mass of the $t\bar{t}$ system and two angular observables that provide direct access to the correlation of top quark and antiquark spins. A significant excess of events is observed near the kinematic $t\bar{t}$ threshold compared to the nonresonant production predicted by fixed-order perturbative quantum chromodynamics (pQCD). The observed enhancement is consistent with the production of a color-singlet pseudoscalar (${}^1\mathrm{S}_0^{[1]}$) quasi-bound toponium state, as predicted by nonrelativistic quantum chromodynamics. Using a simplified model for ${}^1\mathrm{S}_0^{[1]}$ toponium, the cross section of the excess above the pQCD prediction is measured to be $8.8\,^{+1.2}_{-1.4}\,\text{pb}$.

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*See Appendix A for the list of collaboration members

1 Introduction

The discovery of the top quark in 1995 at the Fermilab Tevatron collider was a major milestone in particle physics [1, 2]. Uniquely among quarks, the top quark's lifetime is shorter than the hadronization timescale [3, 4]. This causes the spin of the top quark to be transferred directly to its decay products, enabling precise measurements of spin properties via angular distributions. While the polarization of the top quark and antiquark (t and $\bar{\mathrm{t}}$) in a strongly produced $\mathrm{t\bar{t}}$ system is minimal, their spins are correlated in the standard model (SM) [5, 6], which was experimentally confirmed both at the Tevatron and the LHC [7–12].

While $\mathrm{t\bar{t}}$ pairs do not form stable bound states given the short lifetime of the top quark, calculations in nonrelativistic quantum chromodynamics (NRQCD) predict bound state enhancements at the $\mathrm{t\bar{t}}$ threshold [13–18]. Since this effect is present only when the $\mathrm{t\bar{t}}$ pairs are in the color singlet configuration, the dominant contribution at the LHC is from the gluon-gluon initial state, leading to the production of the ${}^1\mathrm{S}_0^{[1]}$ "toponium" quasi-bound state η_t. Contributions from other spin states are much smaller at the LHC; for instance, the ${}^3\mathrm{P}_0^{[1]}$ state χ_t is suppressed by additional powers of the top quark velocity, which is nearly zero at the threshold. The color octet configuration, on the other hand, is suppressed below the $\mathrm{t\bar{t}}$ threshold because of a repulsive interaction between the top quarks, and has a steeply rising cross section as a function of the $\mathrm{t\bar{t}}$ invariant mass $m_{\mathrm{t\bar{t}}}$ above the threshold [18]. The presence of such an η_t state would therefore manifest itself as an enhancement in the number of events near the production threshold with distinctive patterns in $\mathrm{t\bar{t}}$ spin correlation observables caused by its pseudoscalar nature. However, due to the possibility of initial- and final-state radiation, the color configurations of the $\mathrm{t\bar{t}}$ pairs are not necessarily the same as the partons in the initial state, making theoretical predictions of toponium production challenging.

This Letter reports the observation of a threshold enhancement in $\mathrm{t\bar{t}}$ production consistent with pseudoscalar toponium. The analyzed proton-proton (pp) collision data at $\sqrt{s} = 13\,\mathrm{TeV}$ were recorded by the CMS experiment at the CERN LHC in 2016–2018, corresponding to an integrated luminosity of $138\,\mathrm{fb}^{-1}$. The analysis, whose tabulated results are provided in the HEPData record [19], is conducted within the context of a generic search for neutral spin-0 bosons produced through gluon fusion and decaying to $\mathrm{t\bar{t}}$, covering the full $m_{\mathrm{t\bar{t}}}$ range. Here, we focus on the threshold production of a composite CP-odd pseudoscalar η_t and a CP-even scalar χ_t as signal hypotheses, where CP refers to the charge-parity symmetry. These represent the simplest hypotheses that can explain the observation, since they arise naturally within NRQCD. However, the available experimental data does not exclude alternative explanations like additional pseudoscalar bosons, whose existence is predicted by several theoretical models beyond the SM. This possibility is explored in Ref. [20], the companion paper to this publication, where we present the generic search.

The analysis considers final states with two charged leptons (electrons and/or muons) and at least two jets, referred to as the $\ell\ell$ channel. A similar analysis was previously performed by the CMS experiment using the data sample collected in 2016 and considering the $\ell\mathrm{j}$ channel (i.e., final states with one charged lepton and at least four jets) in addition to the $\ell\ell$ channel [21]. In that analysis, a moderate pseudoscalar-like deviation with a mass at the lowest investigated value of $400\,\mathrm{GeV}$ was found. Compared to that superseded analysis, we consider only the $\ell\ell$ channel here, but use more than three times the data, consider resonances with masses below the $\mathrm{t\bar{t}}$ production threshold, and add a second angular observable that provides direct access to $\mathrm{t\bar{t}}$ spin correlation.

Similar searches have also been conducted by the ATLAS Collaboration using data at $\sqrt{s} =$

8 [22] and 13 TeV [23]. The results presented in Ref. [23] use the data sample collected in 2015–2018 and combine the $\ell\ell$ and ℓj channels, with the latter being predominant. The analysis in the $\ell\ell$ channel differs from our approach in that it investigates the invariant mass $m_{\mathrm{bb}\ell\ell}$ of the $\mathrm{b\overline{b}}\ell^+\ell^-$ system rather than $m_{\mathrm{t\bar{t}}}$ and it utilizes an angular variable whose sensitivity to $\mathrm{t\bar{t}}$ spin correlation is significantly diluted by kinematic effects. We have verified that incorporating these differences into our analysis would not result in a significant enhancement at the threshold. Consequently, the conclusions of Ref. [23] are not directly comparable to the ones reported in this paper, nor do they refute or confirm the findings reported herein.

Moreover, our findings are consistent with enhancements at the threshold in previous $\mathrm{t\bar{t}}$ differential cross section measurements reported by ATLAS [11, 24] and CMS [12, 25]. Similarly, the mild tension between the observed and expected measurement of spin correlation in the $\mathrm{t\bar{t}}$ threshold region, which has been reported by both ATLAS [26] and CMS [27] as part of their studies of quantum entanglement, has been reproduced by this analysis.

2 Method

2.1 The CMS detector and event reconstruction

The CMS apparatus [28, 29] is a multipurpose, nearly hermetic detector, designed to trigger on [30, 31] and identify electrons, muons, photons, and charged and neutral hadrons [32–34]. A global reconstruction algorithm [35] combines the information provided by the all-silicon inner tracker and by the crystal electromagnetic (ECAL) and brass-scintillator hadron calorimeters, operating inside a 3.8 T superconducting solenoid, with data from gas-ionization muon detectors interleaved with the solenoid return yoke [36–38].

Electrons are measured in the pseudorapidity range $|\eta| < 2.5$ as energy deposits in the ECAL matched to a track, accounting for their emitted bremsstrahlung energy [32, 39]. Well-identified electron candidates are selected using identification criteria based on boosted decision trees [32]. Muons are measured in the range $|\eta| < 2.4$ as tracks in the inner tracker consistent with a track in the muon system. Well-identified muon candidates are required to pass the “tight” working point of the identification criteria described in Ref. [33]. Both electrons and muons are required to be isolated from other activity in the event.

Hadronic jets are clustered from the reconstructed particles using the anti-k_{T} algorithm [40, 41] with a distance parameter of 0.4. The charged-hadron subtraction algorithm [35] is used to mitigate the effect of additional pp interactions within the same or nearby bunch crossings (pileup). Jet energy corrections are applied to match the average measured energy of jets to that of particle-level jets [36]. Only jets in the range $|\eta| < 2.4$ with transverse momentum $p_{\mathrm{T}} > 20\,\mathrm{GeV}$ are considered in the analysis. Additionally, jets are required to be separated by $\Delta R = \sqrt{(\Delta\eta)^2 + (\Delta\phi)^2} > 0.4$ from any selected lepton, where $\Delta\eta$ and $\Delta\phi$ are the η and azimuthal angle differences between the jet and the lepton. Jets originating from b quarks are identified (“tagged”) with the DeepJet algorithm [42–44], using the working point with an efficiency of 77% and a misidentification rate of 3%. The missing transverse momentum vector $\vec{p}_{\mathrm{T}}^{\,\mathrm{miss}}$ is computed as the negative vector sum of the p_{T} of all the reconstructed particles in an event, and its magnitude is denoted as $p_{\mathrm{T}}^{\mathrm{miss}}$ [37].

2.2 Data and simulated event samples

The data used in this analysis were recorded with triggers that require the presence of one or two isolated electrons and/or muons, with an overall trigger efficiency above 96–98%. To compare the collected data to theoretical predictions, Monte Carlo (MC) event samples are generated for all relevant production processes. Different event generators are used for the calculation of matrix elements (MEs). In all cases, the next-to-next-to-leading order (NNLO) NNPDF3.1 parton distribution functions (PDFs) [45] are used, and the ME calculation is interfaced with PYTHIA 8.240 [46] to simulate parton showers, fragmentation, and hadronization, using the CP5 underlying event tune [47, 48]. The top quark mass m_{t} is set to 172.5 GeV in all samples involving top quarks, as well as in the computation of theoretical corrections that are applied to them. The simulated events are processed through the CMS detector simulation based on the GEANT4 program [49], and pileup interactions generated with PYTHIA are overlaid to match the observed pileup distribution in data. Separate MC samples are generated and dedicated corrections to the simulations ("scale factors") are applied for different data-taking eras to take into account evolving conditions.

Pseudoscalar η_{t} production is modeled as a generic resonance matched to NRQCD calculations [17, 50], implemented in the MADGRAPH5_aMC@NLO 2.6.5 event generator [51] at leading order (LO), with an effective contact interaction for the gluon-η_{t} coupling. Samples of resonant $\eta_{\mathrm{t}} \rightarrow \mathrm{WbWb}$ events are produced, thus including contributions from off-shell top quarks. The η_{t} mass and width are set to 343 and 2.8 GeV, respectively, corresponding to the expectation that the toponium mass is twice m_{t} minus a binding energy of about 2 GeV [17], and its decay width is twice the width of the top quark [13]. The nonrelativistic Hamiltonian reweighting mentioned in Refs. [17, 52] is not applied since its impact on the analysis is expected to be negligible [15]. Scalar χ_{t} production is simulated in the same way with identical mass and width values, but with relevant CP-odd couplings replaced by CP-even ones.

The nonresonant $\mathrm{t\bar{t}}$ production process is simulated at next-to-LO (NLO) in perturbative quantum chromodynamics (pQCD) using the `hvq` model implemented in POWHEG v2 [53–56]. The factorization and renormalization scales (μ_{F} and μ_{R}) are set to $\sqrt{m_{\mathrm{t}}^2 + p_{\mathrm{T,t}}^2}$, where $p_{\mathrm{T,t}}$ is the p_{T} of the top quarks in the underlying Born-level configuration. Decays of the top quarks are performed using the narrow-width approximation [57]. The sample is normalized to the predicted $\mathrm{t\bar{t}}$ production cross section of $833.9\,^{+20.5}_{-30.0}$ pb, as calculated with the TOP++2.0 program at NNLO in pQCD, and including soft-gluon resummation at next-to-next-to-leading-logarithmic (NNLL) accuracy [58]. To improve the theoretical description of the kinematic distributions of the $\mathrm{t\bar{t}}$ production process, the sample is reweighted to account for higher-order corrections. The prediction at NNLO in pQCD is calculated using the MATRIX program [59], and electroweak (EW) corrections at NLO using the HATHOR program [60–65]. Both predictions are computed at the level of stable top quarks with a nominal scale choice of $0.5\big(\sqrt{m_{\mathrm{t}}^2 + p_{\mathrm{T,t}}^2} + \sqrt{m_{\mathrm{t}}^2 + p_{\mathrm{T,\bar{t}}}^2}\big)$, where $p_{\mathrm{T,\bar{t}}}$ is the p_{T} of the top antiquark, and using the same NNPDF3.1 PDF set as the POWHEG $\mathrm{t\bar{t}}$ sample. The POWHEG $\mathrm{t\bar{t}}$ sample is reweighted to the NNLO pQCD and NLO EW predictions using double-differential weights evaluated at the generator level as a function of $m_{\mathrm{t\bar{t}}}$ and of the cosine of the angle between the direction of the top quark in the zero-momentum frame of the $\mathrm{t\bar{t}}$ system and the direction of the $\mathrm{t\bar{t}}$ system in the laboratory frame. The $\mathrm{t\bar{t}}$ production sample obtained in this way is referred to as fixed-order (FO) pQCD sample in the following. In addition, three further samples are generated with different generator setups: (i) the same POWHEG ME calculation matched to HERWIG 7.2.2 [66, 67], using the angular-ordered parton shower model; (ii) MADGRAPH5_aMC@NLO at NLO in pQCD with up to two additional jets in the ME and matched to PYTHIA with the FxFx merging scheme [68]; and (iii) the `bb4l` ME generator in POWHEG vRES [69–71], which simulates the full process $\mathrm{pp} \rightarrow \mathrm{b\bar{b}}\ell^+\ell^-\nu\bar{\nu}$ at NLO in pQCD and thus includes full off-shell contributions beyond the narrow-width approximation, matched to PYTHIA. The same NNLO pQCD and NLO EW corrections as before are also applied to these samples.

The η_{t} and χ_{t} samples are added to the FO pQCD $\mathrm{t\bar{t}}$ sample without interference [50, 72, 73]. It has been tested that adding the η_{t} signal to WbWb production simulated in FO NLO pQCD as suggested in Ref. [50] gives similar results to the most recent NRQCD prediction using the NLO QCD potential for Coulomb resummation and performing threshold resummation at next-to-leading-logarithmic (NLL) accuracy [18].

Reducible background (BG) contributions in the analysis originate from single top quark production (tX), Drell–Yan production (Z/γ^*), diboson production (WW, WZ, and ZZ), and $\mathrm{t\bar{t}}$ production in association with a vector boson ($\mathrm{t\bar{t}V}$). The tX processes via the t, tW, and s channels are generated at NLO using POWHEG v2, POWHEG, and MADGRAPH5_aMC@NLO, respectively [51, 74, 75], and normalized to the NLO cross section predictions for the t and s channels [64, 76], and the approximate NNLO prediction for the tW channel [77]. For the Z/γ^* process, samples are generated with POWHEG [54, 55] with multi-scale-improved NNLO accuracy in QCD [78, 79], matched with PYTHIA for initial-state radiation (ISR) and PHOTOS [80, 81] for final-state radiation (FSR). The total yield of the Z/γ^* prediction is corrected using data following a modified version of the procedure described in Ref. [82]. The diboson processes are generated using PYTHIA and normalized to the respective NNLO (WW) [83] or NLO (WZ and ZZ) [84] cross sections. We checked that replacing the WW contribution with the nonresonant $\mathrm{WWb\bar{b}}$ production, which leads to the same final state as $\mathrm{t\bar{t}}$ production, does not change the results of this work. The $\mathrm{t\bar{t}V}$ events are generated at NLO with MADGRAPH5_aMC@NLO. Background contributions due to QCD multijet events with two fake or non-prompt leptons are found to be negligible. Further details on other reducible background predictions are given in Ref. [20].

2.3 Event selection

Candidate events are required to have exactly two well-identified leptons (electrons and/or muons) of opposite charge, with $p_{\mathrm{T}} > 20\,\mathrm{GeV}$ and at least one of them with $p_{\mathrm{T}} > 25\,\mathrm{GeV}$. Events with an additional well-identified electron or muon with $p_{\mathrm{T}} > 20\,\mathrm{GeV}$ are rejected. The invariant mass $m_{\ell\ell}$ of the dilepton pair is required to be larger than 20 GeV to suppress low-mass resonances. To suppress Z/γ^* background contributions, events in the ee and $\mu\mu$ channels are required to have $p_{\mathrm{T}}^{\mathrm{miss}} > 40\,\mathrm{GeV}$ and $|m_{\ell\ell} - 91\,\mathrm{GeV}| > 15\,\mathrm{GeV}$, i.e., to be outside of the Z boson mass window [85]. The presence of at least two jets with $p_{\mathrm{T}} > 30\,\mathrm{GeV}$ and of at least one b-tagged jet with $p_{\mathrm{T}} > 20\,\mathrm{GeV}$ is required, resulting in two or more jets per selected event.

Each event is reconstructed using a kinematic reconstruction algorithm, which assumes that the final state consists of a $\mathrm{t\bar{t}}$ pair that decays into two leptonically decaying W bosons [86]. The algorithm proceeds in two steps, first identifying b and $\mathrm{\bar{b}}$ quark candidates and then reconstructing the momenta of the neutrinos. In the first step, we consider all b-tagged jets in the event as b and $\mathrm{\bar{b}}$ quark candidates. For events with exactly one b-tagged jet, either the b or $\mathrm{\bar{b}}$ quark candidate, but not both, are taken from the non-b-tagged jets. The invariant masses of the visible top quark decay products $m_{\ell^+\mathrm{b}}$ and $m_{\ell^-\mathrm{\bar{b}}}$ are calculated for all possible $\mathrm{b\bar{b}}$ candidate pair assignments, and the pair maximizing the likelihood of being the correct pair is chosen for the second step. The likelihood is constructed using the expected distribution of the invariant mass of the lepton and b-tagged jet system, which has a different shape depending on whether the lepton and b-tagged jet originate from the decay of the same top quark, or not. The second step uses an analytic method [87] to solve a system of equations in the ν_ℓ and $\overline{\nu}_\ell$ momenta formed by requiring that: (i) the invariant masses of the $\ell^+\nu_\ell\mathrm{b}$ and $\ell^-\overline{\nu}_\ell\mathrm{\bar{b}}$ systems are equal to 172.5 GeV, (ii) the invariant masses of the $\ell^+\nu_\ell$ and $\ell^-\overline{\nu}_\ell$ systems are equal to the

W boson mass, and (iii) the $\nu_\ell\overline{\nu}_\ell$ system is the sole source of the measured $\vec{p}_{\mathrm{T}}^{\mathrm{miss}}$. In case of multiple real solutions, the one with the lowest reconstructed value of $m_{\mathrm{t\bar{t}}}$ is used, which has been found to minimize possible biases with respect to the true $m_{\mathrm{t\bar{t}}}$ value [88, 89]. This step is repeated 100 times, with random smearing applied to the momenta of the ℓ^+, ℓ^-, b, and $\overline{\mathrm{b}}$ candidates, by sampling from the distributions of the relative energy difference and angular distance between reconstructed and truth-level particles. The effect of the smearing is propagated to the measured $\vec{p}_{\mathrm{T}}^{\mathrm{miss}}$. This smearing procedure incorporates the detector resolution into the reconstruction and, in particular, recovers solutions in cases where the nominal configuration would lead to a system of equations without real solution. The final result of the reconstruction is taken as the weighted averages of the t and $\bar{\mathrm{t}}$ quark four-momenta, computed over all repetitions that result in a real solution with weight evaluated via the same likelihood based on $m_{\ell^+\mathrm{b}}$ and $m_{\ell^-\overline{\mathrm{b}}}$ used for the $\mathrm{b\overline{b}}$ quark candidate assignment. Events yielding no real solution in any iteration are rejected. The resolution of the reconstructed $m_{\mathrm{t\bar{t}}}$ is around 15% at the $\mathrm{t\bar{t}}$ threshold and increases up to 25% for higher $m_{\mathrm{t\bar{t}}}$ values.

Two angular observables c_{hel} and c_{han} are defined to probe the spin correlation of the $\mathrm{t\bar{t}}$ system as follows. We define $\widehat{\ell}_{\mathrm{t}}^{+}$ and $\widehat{\ell}_{\bar{\mathrm{t}}}^{-}$ as the unit vectors of the momenta of the two leptons in the rest frames of their parent t and $\bar{\mathrm{t}}$, respectively [20]. The variable c_{hel} is then defined as the scalar product of $\widehat{\ell}_{\mathrm{t}}^{+}$ and $\widehat{\ell}_{\bar{\mathrm{t}}}^{-}$, and c_{han} similarly but with a sign flip in the component parallel to the t direction (i.e., the $\widehat{k}$ direction in Ref. [90]) of either $\widehat{\ell}_{\mathrm{t}}^{+}$ or $\widehat{\ell}_{\bar{\mathrm{t}}}^{-}$. The slopes of both distributions are related to the degree of alignment between the t and $\bar{\mathrm{t}}$ spins. The production of η_{t} results in a $\mathrm{t\bar{t}}$ system in the ${}^1\mathrm{S}_0^{[1]}$ state with anticorrelated t and $\bar{\mathrm{t}}$ spins, resulting in a normalized c_{hel} distribution with a maximal slope of $+1$, steeper than the one of the FO pQCD prediction. In contrast, χ_{t} production of a $\mathrm{t\bar{t}}$ system in the ${}^3\mathrm{P}_0^{[1]}$ state results in a c_{hel} slope of $-1/3$. Concerning c_{han}, the normalized distribution predicted by FO pQCD is almost flat, whereas η_{t} and χ_{t} production result in slopes of $+1/3$ and -1, respectively [20].

2.4 Statistical analysis

A binned profile maximum likelihood fit [91–94], implemented in COMBINE [95], is performed to evaluate the compatibility of the observed data with the predictions and to obtain a best fit estimate of the cross section of the η_{t} and/or χ_{t} contributions. A three-dimensional (3D) template built from $m_{\mathrm{t\bar{t}}}$, c_{hel}, and c_{han} is used as the fitted distribution. Various sources of uncertainty affect the 3D template and are implemented as nuisance parameters in the fit, capable of changing both the rate and the shape of the templates. Experimental uncertainties related to trigger, electron identification [32], muon identification [33], and b tagging (separately for b/c and u/d/s/g jets) [42] efficiencies, as well as to pileup reweighting, are evaluated by varying the corresponding corrections to the simulation by their uncertainties. Uncertainties in the jet p_{T} scale and resolution [36], as well as an additional uncertainty in the $p_{\mathrm{T}}^{\mathrm{miss}}$ contribution from detector deposits not clustered into jets [37], are evaluated by varying the jet p_{T} and $p_{\mathrm{T}}^{\mathrm{miss}}$ directly. Additional nuisance parameters are assigned for an inefficiency caused by the gradual shift in the timing of the ECAL trigger inputs [31], and for the uncertainty of 1.6% in the integrated luminosity measurement [96–98] that affects the normalization of all simulated processes. Besides experimental effects, several theoretical uncertainties related to the modeling of the signal and background processes are considered, as described below.

First, we consider theoretical uncertainties in the FO pQCD prediction of $\mathrm{t\bar{t}}$ production. The NLO EW correction depends on the value of the top quark Yukawa coupling, entering through interference with diagrams containing a virtual Higgs boson, and an uncertainty of $+11/-12$%

around the SM prediction is evaluated, conservatively using the uncertainty from the measurement reported in Ref. [99]. Following Ref. [65], the difference between the multiplicative and additive application schemes when combining the NLO EW corrections with the NNLO pQCD corrections of about 1–2% is taken as an additional uncertainty. The uncertainty in m_{t} is considered by shifting its value in simulation by $\pm 1\,\mathrm{GeV}$ [100]. We have checked that the exact value of the m_{t} uncertainty does not influence the conclusions of this work. The values of μ_{R} and μ_{F} in the ME calculation are varied independently up and down by a factor of 2. The effects of the m_{t}, μ_{R}, and μ_{F} variations on the shape of the 3D template are considered at NLO accuracy, whereas the effects on the overall normalization are taken from the NNLO+NNLL calculation [58, 101]. The scales used to evaluate the strong coupling constant α_{S} in the PS simulation of ISR and FSR are varied independently by a factor of 2 in each direction. Uncertainties in the underlying event tune are estimated by varying the CP5 parameters [48]. Two uncertainties are considered for the color reconnection model, with one based on the "QCD-inspired" model [102], and the other by switching on the early resonance decay option in PYTHIA [103]. The uncertainty in the ME-PS matching scale is evaluated by varying the POWHEG parameter h_{damp}, which controls the radiation of additional high-p_{T} jets. The nominal value of h_{damp} and the considered variations are $1.58\,^{+0.66}_{-0.59}\,m_{\mathrm{t}}$ [104]. The uncertainty from the PDF choice is evaluated by reweighting the simulated $\mathrm{t\bar{t}}$ events using 100 replicas of the NNPDF3.1 PDF set, and taking the base variation with the largest eigenvalue as obtained from a principal component analysis in the space of the final 3D templates. The uncertainty in the value of α_{S} in the PDF set is used as a second independent PDF uncertainty.

The choice of ME event generator for the $\mathrm{t\bar{t}}$ FO pQCD prediction is validated through a comparison of the nominal $\mathrm{t\bar{t}}$+tW FO pQCD prediction with the alternative prediction obtained with `bb4l`, which includes off-shell contributions to the $\mathrm{b\bar{b}}\ell^{+}\ell^{-}\nu\bar{\nu}$ final state. The difference between the two predictions is assigned as an additional uncertainty. Similarly, the comparison of the nominal $\mathrm{t\bar{t}}$ FO pQCD prediction with the alternative generator setup using HERWIG is used to assign an additional uncertainty for the choice of the parton shower program.

The uncertainties due to μ_{F}, ISR, and FSR scales in the η_{t} and χ_{t} simulations are evaluated by independently varying them up and down by a factor of 2. Since the employed model uses effective η_{t} and χ_{t} production via a contact interaction with no dependence on α_{S}, variations of μ_{R} have no effect. The uncertainty in m_{t} is considered by varying its value in simulation by $\pm 1\,\mathrm{GeV}$, and is treated as fully correlated with the m_{t} variation in the FO pQCD $\mathrm{t\bar{t}}$ prediction. Other theoretical uncertainties in the η_{t} and χ_{t} simulations, such as the PDF variations, are found to be small compared to the already considered effects and are thus neglected.

The μ_{R}, μ_{F}, ISR, and FSR scale uncertainties are also independently considered for the Z/γ^{*} and tX processes. Normalization uncertainties for the non-$\mathrm{t\bar{t}}$ background processes are assigned based on the precision of relevant cross section measurements [105–110], resulting in larger uncertainties than those of the corresponding theoretical computations.

3 Results

We observe an excess of events in the data with respect to the FO pQCD prediction. This excess occurs mainly at low $m_{\mathrm{t\bar{t}}}$, and its strength depends on c_{hel} and c_{han}. We analyze the $m_{\mathrm{t\bar{t}}}$ distribution in 3×3 equal-sized c_{hel} and c_{han} bins, and show three of these bins in Fig. 1: the bin ($-1 < c_{\mathrm{hel}} < -1/3$, $-1 < c_{\mathrm{han}} < -1/3$) where the η_{t} contribution is expected to be small (left), the intermediate bin ($-1/3 < c_{\mathrm{hel}} < 1/3$, $-1/3 < c_{\mathrm{han}} < 1/3$) (middle), and the bin ($1/3 < c_{\mathrm{hel}} < 1$, $1/3 < c_{\mathrm{han}} < 1$) where the η_{t} contribution is expected to be

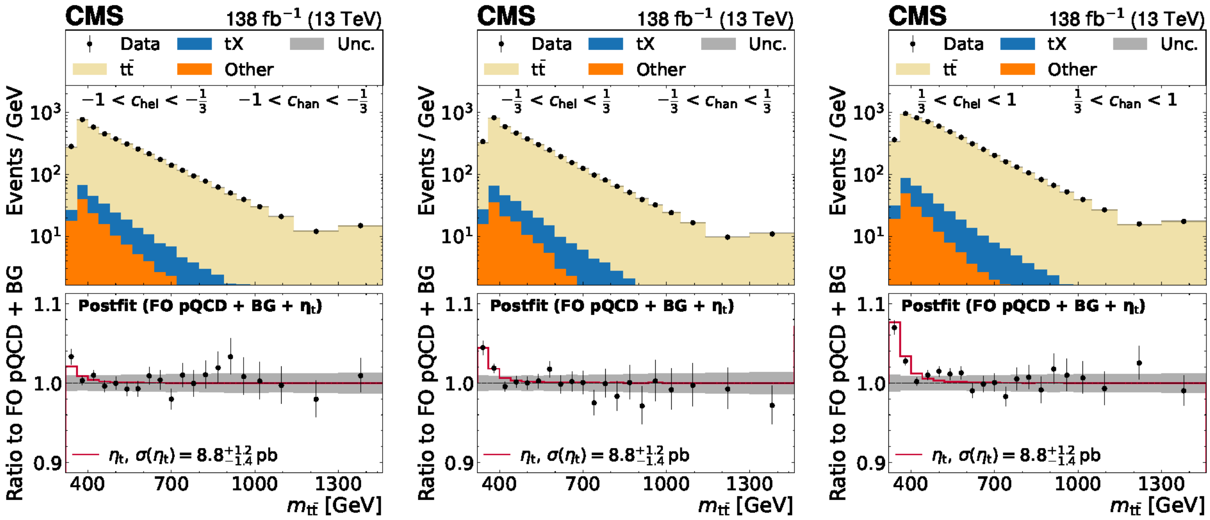

Figure 1: Observed (points with statistical error bars) and predicted (stacked colored histograms) $m_{t\bar{t}}$ distribution in three out of nine (c_{hel}, c_{han}) bins. In the upper panels, the $t\bar{t}$ histogram shows the FO pQCD prediction after the fit to the data that includes the η_t signal model (whose contribution is not drawn), and the shown event rates are divided by the bin width. The lower panels display the ratio of the data to the FO pQCD + background prediction, with η_t signal overlaid at its best fit η_t cross section (red line). The gray band indicates the postfit uncertainty. The first and last $m_{t\bar{t}}$ bins include all events with reconstructed $m_{t\bar{t}}$ below 360 and above 1300 GeV, respectively, and the drawn bin width is used for the normalization in these bins.

enhanced (right). In Fig. 2 (left), the c_{hel} distribution is shown for $m_{t\bar{t}} < 360$ GeV and integrated over c_{han}. The data show a steeper slope than the FO pQCD prediction, as expected from an additional pseudoscalar contribution. As can be seen in both figures, the η_t model can accommodate the excess.

We measure an η_t production cross section of

$$\sigma(\eta_t) = 8.8 \pm 0.5\,(\text{stat})\,^{+1.1}_{-1.3}\,(\text{syst})\,\text{pb} = 8.8\,^{+1.2}_{-1.4}\,\text{pb}.$$

Here, the statistical component of the uncertainty is estimated by fixing all nuisance parameters to their postfit values, while the systematic component is obtained as the quadratic difference between the total and the statistical uncertainty. Our result is comparable to the magnitude of the theory estimate of 6.43 pb, which is obtained by fitting the results of an NRQCD calculation from Ref. [15] and subtracting the NLO+NLL pQCD prediction [17], within the range of $338 < m_{t\bar{t}} < 350$ GeV. This is compatible with the recent NRQCD calculation in Ref. [18]. The cross section measured in this work is without any explicit restrictions on the $m_{t\bar{t}}$ range. The significance of the excess over the hypothesis with no η_t production exceeds five standard deviations (SDs).

To explore the spin and CP structure of the resonant excess, we perform an alternative fit that simultaneously includes contributions from pseudoscalar η_t and scalar χ_t production. The results are shown in Fig. 3. While the data is compatible with zero contribution from the χ_t state within one SD, zero contribution from the η_t state is excluded with a significance exceeding five SDs. This establishes the presence of a pseudoscalar excess.

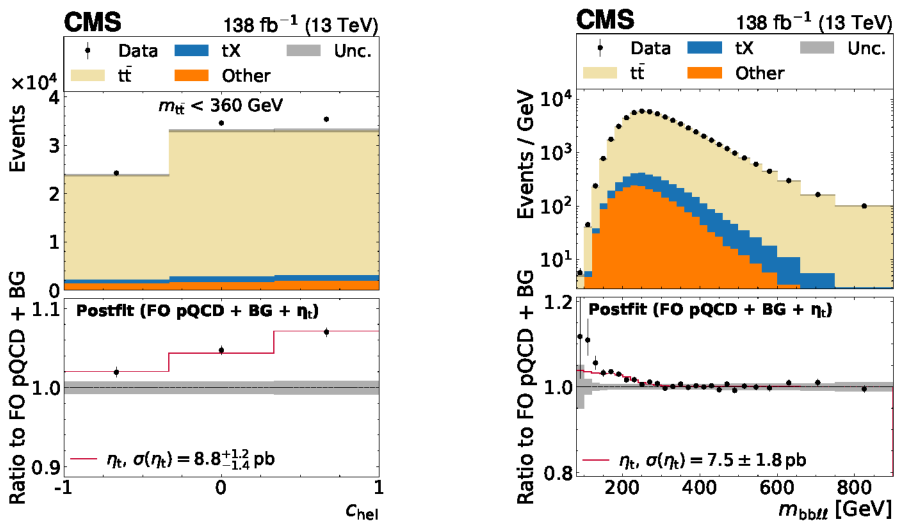

Figure 2: Observed (points with statistical error bars) and predicted (stacked colored histograms) distributions. Left: c_{hel} for $m_{t\bar{t}} < 360\,\text{GeV}$ and integrated over c_{han}, from the nominal fit using $m_{t\bar{t}}$. Right: $m_{bb\ell\ell}$ integrated over c_{hel} and c_{han}, from the alternative fit using $m_{bb\ell\ell}$ instead of $m_{t\bar{t}}$, which is discussed in Section 4.1. In the upper panels, the $t\bar{t}$ histogram shows the FO pQCD prediction after the fit to the data that includes the η_t signal model (whose contribution is not drawn). On the right, the shown event rates are divided by the bin width. The lower panels display the ratio of the data to the FO pQCD + background prediction, with η_t signal overlaid at its best fit η_t cross section (red line). The gray band indicates the postfit uncertainty. The first and last $m_{bb\ell\ell}$ bins include all events with reconstructed $m_{bb\ell\ell}$ below 100 and above 750 GeV, respectively, and the drawn bin width is used for the normalization in these bins.

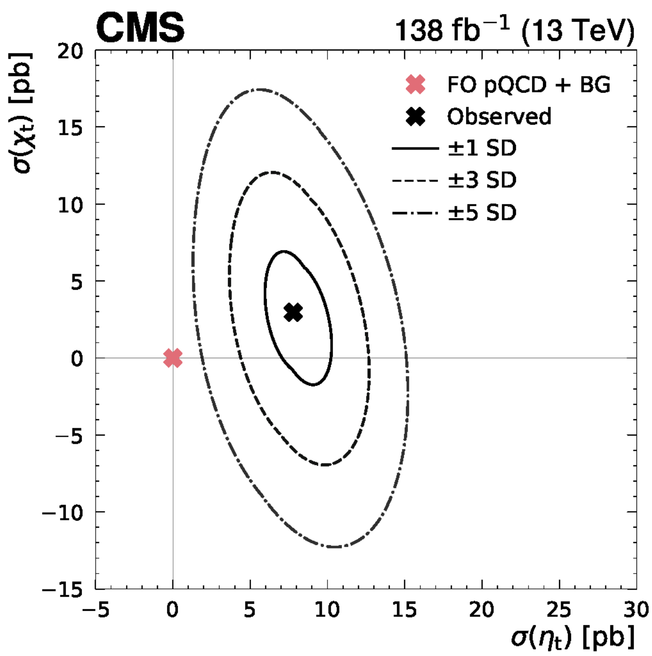

Figure 3: Best fit value (cross) and allowed regions at one (solid line), three (dashed line), and five (dotted-dashed line) SDs for the cross section of η_t and χ_t production, as observed in data (black). The FO pQCD + background expectation of zero η_t and χ_t contributions is denoted by a pink star. Negative cross section values refer to a reduction of the $t\bar{t}$ production cross sections with respect to the FO pQCD + background prediction around the threshold.

4 Discussion

4.1 Robustness of the experimental analysis methods

To ensure that the on-shell assumption used in the kinematic reconstruction algorithm does not sculpt the $m_{t\bar{t}}$ distribution to be signal-like through an unaccounted systematic effect, we repeat the analysis with a similar strategy but changing the fit distribution from $m_{t\bar{t}}$ to $m_{bb\ell\ell}$. This observable is defined without any assumption on the value of m_t, and is shown in Fig. 2 (right). Nuisance parameters encoding the difference between the generators were not included in this check. A cross section of $\sigma(\eta_t) = 7.5 \pm 1.8\,\mathrm{pb}$ is obtained in the $m_{bb\ell\ell}$ fit. This is compatible with the nominal strategy, but with less sensitivity, which is expected. We conclude that the kinematic reconstruction algorithm does not introduce spurious effects in our analysis.

As an additional check, we investigate the impact of possible jet p_T scale mismodeling on $m_{t\bar{t}}$ by fitting pseudodata obtained from the FO pQCD prediction with the jet p_T scale shifted up or down by its prefit uncertainty. We find the resulting shift in the η_t cross section to be less than one SD of the nominal result.

4.2 Comparison between fits with and without η_t contribution

The $m_{t\bar{t}}$ and c_{hel} distributions obtained with a "background-only" fit, i.e., considering only the FO pQCD prediction plus background contributions without the η_t signal (labeled FO pQCD + background) and including all nuisance parameters, are shown in Fig. 4. The fit is able to absorb parts of the low-$m_{t\bar{t}}$ excess of data over prediction. Nevertheless, a c_{hel} distribution with a higher slope than the FO pQCD expectation remains visible, as expected for an η_t contribution, cf. Fig. 2 (left).

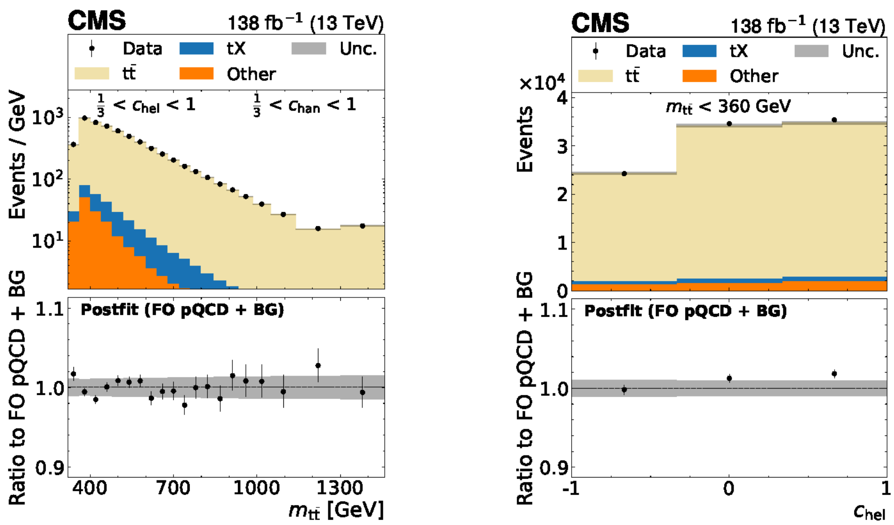

Figure 4: Observed (points with statistical error bars) and predicted (stacked colored histograms) $m_{t\bar{t}}$ distribution in the (c_{hel}, c_{han}) bin with the highest expected η_t contribution (left) and c_{hel} distribution for $m_{t\bar{t}} < 360\,\mathrm{GeV}$ and integrated over c_{han} (right). In the upper panels, the histograms account only for the FO pQCD + background prediction, and are shown after the background-only fit to the data. On the left, the shown event rates are divided by the bin width. The lower panels display the ratio of the data to the FO pQCD + background prediction. The gray band indicates the postfit uncertainty. The binning is the same as in Figs. 1 and 2 (left).

The quality of both the FO pQCD + background + η_t and FO pQCD + background fits is compared in Fig. 5 through the postfit deviations of nuisance parameters from their prefit values

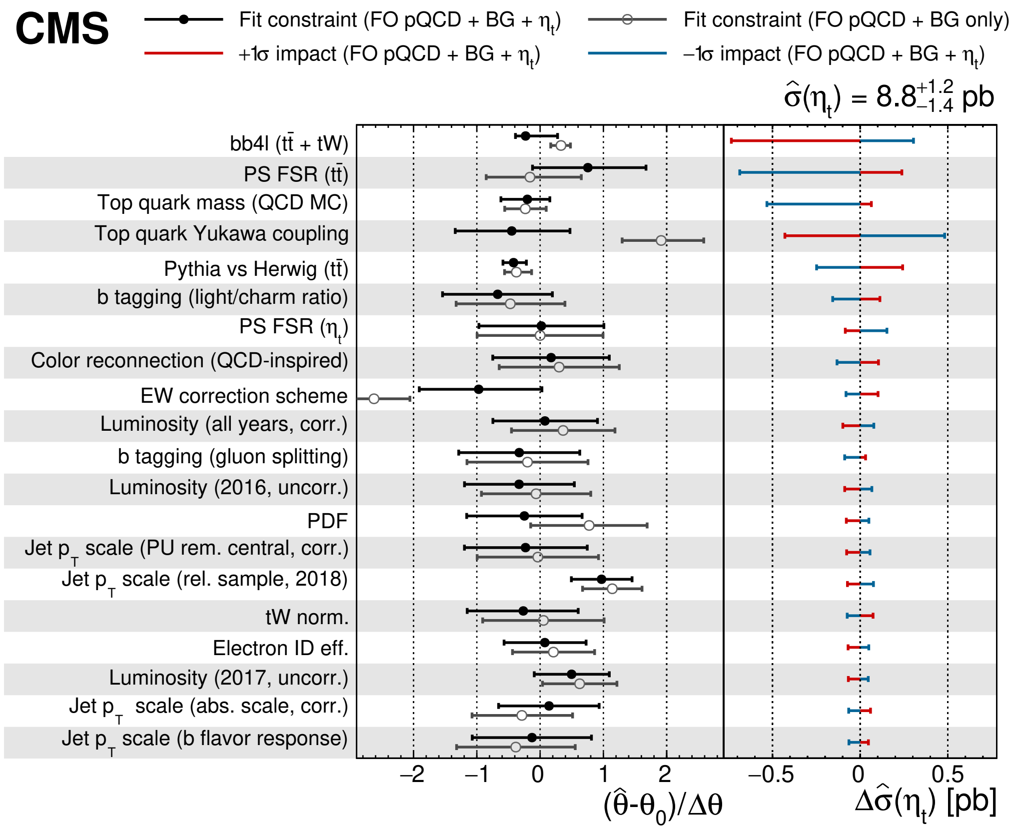

Figure 5: For the nuisance parameters listed in the left column, the pulls $(\hat{\theta} - \theta_0)/\Delta\theta$ (middle column), where $\hat{\theta}$ and θ_0 are the postfit and prefit values of the nuisance parameters and $\Delta\theta$ is the prefit uncertainty, are shown for the FO pQCD + background + η_t (black filled circles) and FO pQCD + background (gray empty circles) fit, as well as the impacts $\Delta\hat{\sigma}(\eta_t)$ (right column) for the FO pQCD + background + η_t fit. The impact $\Delta\hat{\sigma}(\eta_t)$ for a nuisance parameter θ is calculated by varying θ by ±1 SD and evaluating the shift in $\sigma(\eta_t)$. The nuisance parameters are ordered by the maximum of their ±1 SD impacts in the FO pQCD + background + η_t fit.

("pulls") as well as their postfit reduction in uncertainty ("constraints") in both cases. In the FO pQCD + background + η_t fit (black filled circles), no nuisance parameter is pulled from its prefit value by more than one SD. In contrast, in the FO pQCD + background fit (gray empty circles), the two nuisance parameters associated with the EW corrections (the top quark Yukawa coupling and the correction scheme) are pulled strongly away from their expected values, in order to compensate the observed excess of events and slope in c_{hel} [65]. This, together with the fact that there is still a residual positive slope near the $t\bar{t}$ threshold in Fig. 4, corroborates the conclusion of the statistical analysis that a nonzero η_t contribution is the more physically sensible interpretation of the data.

4.3 Comparison between different baseline FO pQCD predictions

Here, we present and discuss the comparison between different setups to generate the FO pQCD + background predictions. Fit results obtained with the nominal FO pQCD $t\bar{t}$ prediction and the three alternative generator setups introduced in Section 2.2 are compared in Table 1. The setup "POWHEG v2 `hvq` + PYTHIA" refers to the sample used in the nominal result. The fit results shown here do not include the two systematic uncertainties for the choice of the ME event generator and the parton shower program, which are evaluated from comparisons between the different generator setups. The setup "POWHEG vRES bb4l + PYTHIA" does not use the nominal FO pQCD tW prediction and has dedicated samples to derive systematic uncertainty templates, whereas the other three setups use the same nominal FO pQCD tW prediction and share the samples used to derive systematic uncertainty templates with the nominal result. The largest difference in $\sigma(\eta_t)$ with respect to the nominal result is found for POWHEG vRES bb4l + PYTHIA, which is lower by $\sim$1.5 SDs.

Table 1: Results for $\sigma(\eta_t)$ obtained with different simulated event samples for the FO pQCD $t\bar{t}$(+tW) prediction. Nuisance parameters encoding the difference between different generators are not included in these results. The nominal result, i.e., POWHEG v2 hvq + PYTHIA including these nuisance parameters, is shown for comparison.

FO pQCD generator setup	$\sigma(\eta_t)$ [pb]
POWHEG v2 hvq + PYTHIA	8.7 ± 1.1
POWHEG v2 hvq + HERWIG	8.6 ± 1.1
MADGRAPH5_aMC@NLO FxFx + PYTHIA	9.8 ± 1.3
POWHEG vRES bb4l + PYTHIA	6.6 ± 1.4
Nominal result	$8.8\,^{+1.2}_{-1.4}$

To illustrate the differences between the generator setups, the ratios to the nominal POWHEG v2 hvq + PYTHIA prediction are shown in Fig. 6 for the $m_{t\bar{t}}$ distribution, as well as the c_{hel} distribution at the $t\bar{t}$ threshold and in the $t\bar{t}$ continuum. It can be seen that HERWIG, compared to PYTHIA, predicts a lower $t\bar{t}$ acceptance, an increase of events at low $m_{t\bar{t}}$ (similar to η_t), and a reduced slope in c_{hel} for low $m_{t\bar{t}}$ (opposite to η_t). Since these effects are contradicting the prediction from η_t production, the observed $\sigma(\eta_t)$ value remains basically unchanged. In contrast, the bb4l prediction predicts a stronger slope in c_{hel} for low $m_{t\bar{t}}$, which is similar to η_t and thus explains the smaller observed $\sigma(\eta_t)$ value when this setup is used as the background prediction. Fig. 6 (right) shows, however, that above the threshold the considered generators predict the same slope in c_{hel}.

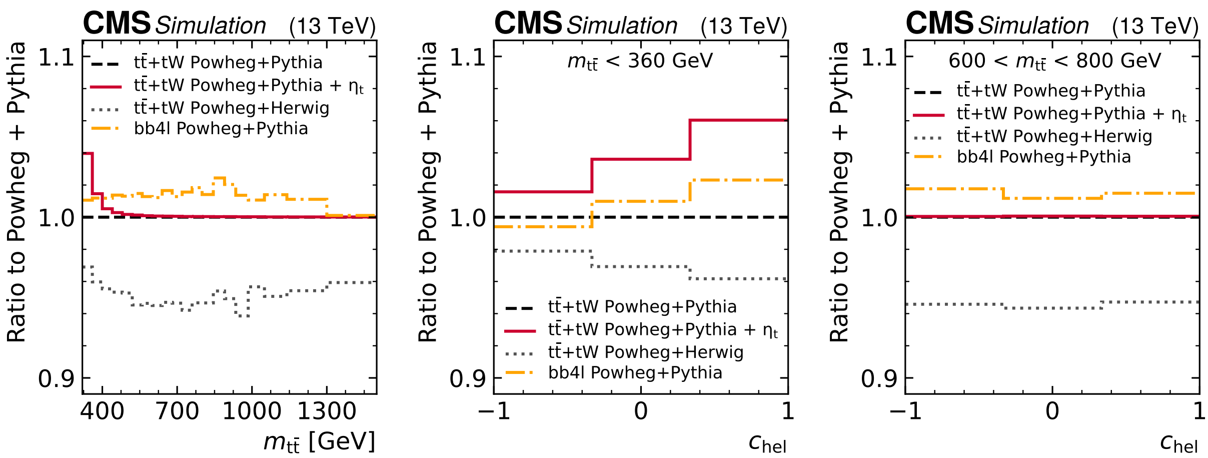

Figure 6: Ratios of the predictions for POWHEG v2 hvq + HERWIG (gray) as well as POWHEG vRES bb4l + PYTHIA (orange) to POWHEG v2 hvq + PYTHIA (black) for $m_{t\bar{t}}$ (left), c_{hel} at the $t\bar{t}$ threshold ($m_{t\bar{t}} < 360\,\text{GeV}$, center), and c_{hel} in the $t\bar{t}$ continuum ($600 < m_{t\bar{t}} < 800\,\text{GeV}$, right), both integrated over c_{han}. The effect of adding η_t to POWHEG v2 hvq + PYTHIA is shown in red for comparison. The binning is the same as in Figs. 1 and 2 (left).

5 Summary

We report the observation of resonant top quark-antiquark ($\mathrm{t\bar{t}}$) production near the kinematic production threshold, with spin properties consistent with contributions from a pseudoscalar state, using proton-proton collision data recorded by the CMS experiment at $\sqrt{s} = 13\,\mathrm{TeV}$ in 2016–2018 and corresponding to an integrated luminosity of $138\,\mathrm{fb}^{-1}$. The data is compared to the standard model prediction including only nonresonant $\mathrm{t\bar{t}}$ production obtained with fixed-order calculations in perturbative quantum chromodynamics. An excess is observed with respect to this model, with a statistical significance exceeding five standard deviations. We emphasize, however, that the modeling of the $\mathrm{t\bar{t}}$ threshold region is challenging and requires further theoretical investigation. It is worth noting that alternative explanations of the excess are also plausible, given the current experimental resolution of the $\mathrm{t\bar{t}}$ invariant mass; we explore this direction further in Ref. [20]. The result is compatible with the formation of a ${}^1\mathrm{S}_0^{[1]}$ toponium quasi-bound state η_t with a measured cross section of $\sigma(\eta_\mathrm{t}) = 8.8\,^{+1.2}_{-1.4}\,\mathrm{pb}$, based on a simplified model inspired by nonrelativistic quantum chromodynamics.

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