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Letter

Search for a new heavy resonance decaying to a top quark and a neutral scalar boson in proton-proton collisions at $\sqrt{s} = 13$ TeV

The CMS Collaboration [1]

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ABSTRACT

A first search at the LHC for a new heavy resonance decaying to a top quark and a neutral scalar boson ϕ in the fully hadronic final state is presented, where the ϕ boson is identified by its decay into a bottom quark-antiquark pair. The search is focused on final states in which the decay products of the highly Lorentz boosted top quark and ϕ boson are each reconstructed as a single, large-radius jet with distinct substructure. The analysis is performed using proton-proton collision data at a center-of-mass energy of 13 TeV, corresponding to an integrated luminosity of 138 fb^{-1}, recorded with the CMS detector at the LHC in 2016–2018. The single production of a vector-like top quark, T′, is used as a benchmark model for the signal process. The results of this search are combined with those of a previous CMS search in which semileptonic decays of the top quark were used. No significant excess of data is observed with respect to the background prediction. For the case where the neutral scalar is a standard model Higgs boson and the T′ quark width is 5% of its mass, T′ quark masses between 0.85 and 1.3 TeV are excluded at 95% confidence level and the most stringent limits to date are set for masses above 2 TeV. For other ϕ boson masses, upper limits as low as 0.1 fb are set on the product of the T′ quark production cross section and branching fraction for its decay to a top quark and a ϕ boson.

1. Introduction

The standard model (SM) of particle physics has been extensively tested and shown to be consistent with experimental results, yet it does not explain why the Higgs boson mass (m_{H}) lies near the electroweak (EW) scale, given the quadratic corrections arising from quantum loops. Naively, the Higgs boson mass would instead be expected to lie near the Planck scale, many orders of magnitude away from its measured value [1–4]. Of the many beyond-the-SM (BSM) theories attempting to address this hierarchy problem, those of particular interest to the search reported in this Letter introduce new particles called vector-like quarks (VLQs), which are nonchiral, color-charged, spin-1/2 partners of the third-generation SM quarks [5].

The nonchiral nature of VLQs allows for Lagrangian mass terms that do not arise from Yukawa couplings to the Higgs field. Therefore, they are free from the stringent constraints on the existence of sequential fourth-generation quarks set by precision EW measurements at the Fermilab Tevatron and the CERN LHC [6]. At the LHC, VLQs can be produced singly or in pairs via the EW and strong interactions, respectively, with the former typically dominating for VLQ masses greater than 1 TeV. One such VLQ, the hypothetical top quark partner T′, couples to the third-generation bottom (b) and top (t) quarks, and can decay to these quarks in association with a Higgs, W, or Z boson. In the case where the VLQ is a weak-isospin singlet, the branching fractions ($\mathcal{B}$) are 50, 25, and 25% for the $\text{T}' \to \text{bW}$, $\text{T}' \to \text{tH}$, and $\text{T}' \to \text{tZ}$ decays, respectively. For the doublet state, the branching fractions into tH and tZ are both 50% [7]. Comprehensive reviews of searches for single and pair production of VLQs at $\sqrt{s} = 13$ TeV have been published by the ATLAS [8] and CMS [9] Collaborations. These searches have targeted the direct decays of VLQs coupled predominantly to third-generation quarks and decaying through various bosonic channels. In particular, the ATLAS Collaboration has performed a combination of searches for singly produced vector-like top quark partners in the tH and tZ channels [10].

However, the vector-like top quark partner need not couple solely to SM particles and, as a result, decays to new scalar or pseudoscalar particles become possible in nonminimal BSM scenarios [11–15]. One such example is a two-Higgs-doublet model [16] that is modified to include a VLQ [13]. The Higgs sector of such a model is extended to include an additional neutral scalar, neutral pseudoscalar, and two charged scalar bosons. The neutral scalar boson is predicted to decay to similar bosonic and fermionic final states as those of the SM Higgs boson, and the branching fraction of the VLQ decay to this scalar boson increases with the VLQ mass.

Motivated by such models, this Letter presents a search for the EW production of a single top quark partner T′ in association with a bottom quark and decaying to a top quark and a neutral scalar boson ϕ, wherein

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the top quark decays hadronically and the ϕ boson is assumed to decay to a bottom quark-antiquark pair ($b\bar{b}$). To take advantage of the larger VLQ single production cross sections at high mass, we target T′ quark masses ($m_{T'}$) ranging from 0.8 to 3 TeV and consider masses of the new scalar boson (m_ϕ) ranging from 75 to 500 GeV. In this regime, the top quark and ϕ boson are each highly Lorentz boosted, such that their decay products merge, creating a dijet topology with large-radius jets in the final state.

Potential signal jet candidates are distinguished from background using neural network identification algorithms, referred to as "taggers", which discriminate the jets originating from top quark or Higgs boson decays from those produced via quantum chromodynamics (QCD), referred to henceforth as the QCD multijet background. Since the final state includes one jet from the hadronic decay of a top quark and one $\phi \to b\bar{b}$ candidate jet, which could be a misidentified hadronic top quark decay, events involving top quark pair production ($t\bar{t}$) form the dominant background in this search. Although the selection on the tagging algorithm's outputs is efficient at removing QCD multijet events, these events nonetheless remain the next most dominant background, followed by minor contributions from W and Z boson production in association with jets, henceforth collectively termed V + jets.

We construct a binned likelihood model composed of QCD multijet, $t\bar{t}$, V + jets, and signal components in the plane spanned by the reconstructed mass of the scalar boson, m_ϕ^{rec}, and the invariant mass of the system composed of the reconstructed scalar boson and top quark, $m_{T'}^{rec}$. This analysis targets a localized excess of events in the two-dimensional (2D) plane of ($m_{T'}^{rec}, m_\phi^{rec}$) that would correspond to the presence of a T′ quark resonance, decaying to a top quark and a ϕ boson. The QCD multijet background in the signal region (SR) of this analysis is modeled using the prediction from a signal-depleted control region (CR) in data defined by inverting the tagger selection on the ϕ candidate jet. All other background sources and the signal are modeled using Monte Carlo (MC) simulation. To avoid bias in the prediction of the QCD multijet background in the SR, the data there are initially kept blind and the background estimation procedure is first validated using pseudo-data generated from the sum of the MC backgrounds and the QCD multijet background prediction obtained from multijet-enriched CR, as described in Section 5.

The results from a combination of the fully hadronic channel with the channel wherein the top quark decays semileptonically, described in detail in Ref. [17], are presented. A charged-lepton veto in the fully hadronic channel ensures the orthogonality with the semileptonic channel by construction, and sources of systematic uncertainty that are common between the two channels are treated as correlated in the likelihood. Both analyses are performed using proton-proton (pp) collision data collected with the CMS detector in 2016–2018 at $\sqrt{s} = 13$ TeV, corresponding to an integrated luminosity of 138 fb^{-1} [18,19]. These are the first searches for the decay of a VLQ to a BSM particle.

This Letter is organized as follows. Section 2 provides an introduction to the CMS detector and event reconstruction. Section 3 describes the simulated signal and background samples used in this analysis. The event selection and object identification criteria are outlined in Section 4, followed by a description of the background estimation strategy in Section 5. Having thus introduced the search in the fully hadronic channel, a brief overview of the search performed in the semileptonic channel is provided in Section 6. Section 7 summarizes the sources of systematic uncertainty in the analysis, as well as the treatment of the combination of the fully hadronic and semileptonic channels. Finally, the results are presented in Section 8 and this Letter is summarized in Section 9. Tabulated results can be found in the HEPData record for this analysis [20].

2. The CMS detector and event reconstruction

The central feature of the CMS apparatus is a superconducting solenoid of 6 m internal diameter, providing a magnetic field of 3.8 T. Within the solenoid volume are a silicon pixel and strip tracker, a lead tungstate crystal electromagnetic calorimeter (ECAL), and a brass and scintillator hadron calorimeter, each composed of a barrel and two endcap sections. Forward calorimeters extend the pseudorapidity (η) coverage provided by the barrel and endcap detectors. Muons are measured in gas-ionization detectors embedded in the steel flux-return yoke outside the solenoid. A more detailed description of the CMS detector, together with a definition of the coordinate system used and the relevant kinematic variables, can be found in Ref. [21,22].

Events of interest are initially selected using a two-tiered trigger system. The first level (L1), composed of custom hardware processors, uses information from the calorimeters and muon detectors to select events at a rate of around 100 kHz within a fixed latency of about 4μs [23]. The second level, known as the high-level trigger, consists of a farm of processors running a version of the full event reconstruction software optimized for fast processing, and reduces the event rate to around 1 kHz before data storage [24,25].

The particle-flow (PF) algorithm [26] aims to reconstruct and identify each individual particle in an event with an optimized combination of information from the various elements of the CMS detector. For each event, hadronic jets are clustered from these reconstructed particles (PF candidates) using the infrared- and collinear-safe anti-k_T algorithm [27,28]. Two different jet collections, referred to as AK4 and AK8 jets, are clustered using distance parameter values of 0.4 and 0.8, respectively. Jet momentum is determined as the vectorial sum of all particle momenta in the jet, and is found from simulation to be, on average, within 5–10% of the true momentum over the whole transverse momentum (p_T) spectrum and detector acceptance. Additional pp interactions within the same or nearby bunch crossings (pileup) can contribute additional tracks and calorimetric energy depositions to the jet momentum. The pileup per particle identification algorithm [29,30] is used to mitigate the effect of pileup at the reconstructed particle level, making use of local shape information, event pileup properties, and tracking information.

Jet energy corrections are derived from simulation to bring the measured response of jets to that of particle level jets on average. In situ measurements of the momentum balance in dijet, photon + jet, Z + jet, and multijet events are used to account for any residual differences in the jet energy scale between data and simulation [31]. The jet energy resolution amounts typically to 15–20% at 30 GeV, 10% at 100 GeV, and 5% at 1 TeV [31]. Additional selection criteria are applied to each jet to remove jets potentially dominated by anomalous contributions from various subdetector components or reconstruction failures [30]. In the case of AK8 jets, masses are calculated after applying a modified mass-drop algorithm [32,33], known as the "soft-drop" algorithm [34], to remove wide-angle soft and collinear radiation from the jets.

3. Signal and background simulation

The signal process pp → T′ → tϕ is generated at leading order for T′ quarks in a mass range of 0.8–3 TeV, in steps of 100 GeV, using the MC generatorMadGraph5_aMC@NLO [35] (version 2.6.5). The T′ quark is treated as a weak-isospin singlet produced in association with a bottom quark, with a width of 1% of its mass. Because the reconstructed mass of the T′ quark is insensitive to small variations in the generated width, the results can be compared with theoretical predictions for singlet T′ quarks with the decay widths of both 1% and 5% of their mass. We assume $\mathcal{B}(\phi \to b\bar{b}) = 100\%$ in the interpretation of the resulting cross sections in Section 8, except for the special case where the scalar is the Higgs boson, $m_\phi = m_H = 125$ GeV, in which case the results are scaled by the SM branching fraction for the decay $H \to b\bar{b}$. When interpreting the results in the context of the T′ → tH decay, the cross sections are evaluated at next-to-leading order in the narrow-width approximation [36–38] for singlet T′ VLQs with a fixed branching fraction of 25% to tH.

The ϕ boson is generated with masses ranging from 75 to 500 GeV in varying steps, with a minimum step size of 25 GeV for lower-mass signals, but increasing to 100 GeV at higher masses. In order to decrease these gaps in the signal MC sample coverage, we perform interpolation between generated signal mass points in the region where $m_{T'} \gtrsim 1$ TeV and $m_\phi < 350$ GeV to produce signal shapes with 25 GeV spacing in m_ϕ. To accomplish the interpolation, each generated signal mass point is first modeled by fitting a double-sided Crystal Ball function [39,40] to its reconstructed m_ϕ^{rec} and $m_{T'}^{rec}$ spectra, which is then normalized to obtain a continuous probability distribution function representing the shape of the signal along each reconstructed mass axis. The shape of an interpolated signal of mass M, situated between two existing signals of masses M_1 and M_2, such that $M_1 < M < M_2$, is then calculated along both axes following the method described in Ref. [41]. The final shape of the interpolated signal is derived as the product of these two distributions, yielding a 2D distribution as a function of $(m_{T'}^{rec}, m_\phi^{rec})$. The normalization of the signal is obtained by linear interpolation between the expected yields of the existing signals of masses M_1 and M_2. The procedure is validated by running the algorithm on the generated signal mass points and comparing the resulting distributions to the original. For all these signal mass points, the differences are negligible and the algorithm successfully reconstructs the original signal shape. We use the same interpolation strategy to produce the shape and normalization of the systematic uncertainty templates for each interpolated signal.

The two main backgrounds in this search arise from $t\bar{t}$ production in which the top quarks decay hadronically and from QCD multijet events. Other sources of background, such as V + jets production, are found to have minimal contributions. To simulate SM $t\bar{t}$ production, the next-to-leading-order POWHEG v2 [42–46] matrix element event generator is used, and for QCD multijet and V + jets simulation, MADGRAPH5_aMC@NLO [35] (versions 2.6.1 and 2.6.5, respectively) is used at leading order accuracy. The simulated QCD multijet samples are only used for checks of self-consistency of the background estimate and do not enter in the final likelihood model used to extract results.

Hadronization and parton showering are simulated using the PYTHIA (version 8.240) software package [47]. The NNPDF3.1 [48] parton distribution functions (PDFs) at next-to-next-to-leading order accuracy are used with the CP5 [49] underlying event tune for all simulations. The CMS detector simulation is performed with GEANT4 [50].

To simulate the effect of pileup, additional simulated inelastic pp collisions are superimposed on the hard scattering process using PYTHIA. Simulated samples are reweighted to correct the pileup simulation by using the total inelastic cross section of 69.2 mb [51,52] to approximate the distribution of the number of pileup interactions in data, after which the simulated events are reconstructed in the same manner as the collision data.

4. Event selection

Different sets of triggers based on jet properties are used for event selection across the three data-taking years. The first trigger criterion is based on the scalar p_T sum of all AK8 jets in the event (H_T), requiring an H_T of at least 900 (1050) GeV for the 2016 (2017–2018) data set. An additional trigger used in the 2017 (2018) data set requires an event to possess $H_T > 750$ (850) GeV as well as an AK8 jet with a trimmed jet mass of at least 50 GeV. For these triggers, the jet mass is calculated by a trimming algorithm [53] similar to the soft-drop algorithm described in Section 2.

The second trigger criterion requires a single AK8 jet above a given p_T threshold in the event. In both 2017 and 2018 a trigger requiring a single AK8 jet with $p_T > 500$ GeV was used. An additional trigger required an AK8 jet with $p_T > 400$ GeV together with a trimmed jet mass of at least 30 GeV. Such triggers with only a p_T criterion were not used in 2016. All these triggers are combined with a logical OR in order to maximize the trigger efficiency in each year. The trigger reaches full efficiency for a dijet invariant mass of approximately 1 TeV for the two leading AK8 jets, and simulated events with dijet invariant masses below this threshold are weighted according to trigger efficiency correction factors measured in an orthogonal data set.

The initial event selection focuses on exploiting the kinematic properties of the decays of very heavy resonances, which are produced nearly at rest, causing their decay products to be highly Lorentz boosted and reconstructed roughly opposite to one another in the transverse plane. Therefore, events are required to have at least two AK8 jets, each with $p_T > 350$ GeV, $|\eta| < 2.4$, and a soft-drop jet mass of at least 50 GeV. The top quark and ϕ boson candidates are then chosen from the remaining jets as the two leading-p_T jets that have an azimuthal angular separation $\Delta\phi > \pi/2$. Additionally, all events must pass a set of standard data quality filters designed to remove events affected by noise in the various subdetectors [54]. Finally, all events containing reconstructed leptons satisfying loose identification criteria [55,56] are vetoed in order to remain orthogonal to the selections imposed by the semileptonic channel [17].

After this initial selection, the two leading-p_T jets are then subject to identification as the $\phi \to b\bar{b}$ ("ϕ jet") and $t \to bW(q\bar{q}')$ ("t jet") candidates. Identification of the ϕ jet is performed using a discriminant formed by the output of the PARTICLENET [57] algorithm, referred to here as T_{Xbb}. Identification of the t jet is achieved using either the PARTICLENET discriminant, T_{bqq}^{PNet}, or the output of the DEEPAK8 [58] algorithm, T_{bqq}^{DAK8}, depending on whether the event belongs to the SR or the $t\bar{t}$-enriched CR($t\bar{t}$), respectively. A description of these algorithms and the selection criteria for the different analysis regions follows.

Classification of the two jets as signal jet candidates is performed using the dynamic graph convolutional neural network PARTICLENET [57]. For every jet in an event, the PARTICLENET algorithm returns probability-like scores for the jet to have originated from the hadronic decay of some massive particle or from the hadronization of light quarks or gluons. In this search, the PARTICLENET "top quark score" is given by the algorithm's default output for discrimination between jets originating from the hadronic decay of a top quark and from the hadronization of lighter quarks or gluons, referred to here as T_{bqq}^{PNet}. The PARTICLENET "ϕ score" is given by a discriminant termed T_{Xbb}, defined by $P(X_{MD} \to b\bar{b})/(P(X_{MD} \to b\bar{b}) + P(\text{QCD}))$, where $P(\text{QCD})$ is the score corresponding to the QCD multijet background and $P(X_{MD} \to b\bar{b})$ is the probability-like score corresponding to a jet arising from the decay of some massive resonance to $b\bar{b}$. The subscript of the ϕ score indicates that it is mass decorrelated (MD), meaning that the tagger response does not significantly change as a function of the jet mass, making this score criterion suitable to identify $\phi \to b\bar{b}$ decays without biasing the background mass distributions. Mass decorrelation is achieved by enforcing a uniform distribution in the jet mass and p_T of the simulated signal and background samples used in the training of the network. Because the network is only trained on scalar resonances with masses ranging from 15 to 250 GeV, the selection efficiency for jets with m_ϕ in this range is greater than those with masses above 250 GeV by a factor of four.

Using these tagger scores, the dijet events are separated into one of three different analysis regions: a QCD multijet-enriched CR(QCD), a $t\bar{t}$-enriched CR($t\bar{t}$), and the SR in which the search is performed. Because only two jets are considered in each event, selecting one jet as the t jet candidate naturally selects the other as the ϕ jet candidate. To belong in the SR, events must contain at least one jet passing the high-purity (HP) working point (WP) of the PARTICLENET top quark tagger corresponding to a 0.1% mistagging rate, $T_{bqq}^{PNet} >$ HP WP. If neither jet meets this criterion, the event is discarded. If only one jet passes the HP WP it is assigned as the t jet candidate. If both jets pass, then the jet with the higher T_{bqq}^{PNet} score is assigned as the t jet candidate.

The CR(QCD) is defined by inverting the tagging requirement on the t jet, selecting only events in which the t jet candidate has a score passing only a very loose tagger selection on T_{bqq}^{PNet} such that $0.2 < T_{bqq}^{PNet} <$ HP WP. An additional ϕ tagging veto is placed on the t jet candidate in this region, requiring that it has $T_{Xbb} < 0.2$ to reduce possible signal contamination in the CR(QCD) introduced by the T_{bqq}^{PNet} score inversion.

Following the identification of the t jet candidate, additional ϕ tagging selection is imposed on the ϕ candidate jet in all events in both the SR and CR(QCD), dividing both regions into "Fail" and "Pass" regions. These regions are defined identically in the SR and CR(QCD), with the Fail region defined by ϕ candidate jets with $0.8 < T_{Xbb} < 0.98$ and the Pass region by ϕ candidate jets with $T_{Xbb} > 0.98$.

A dedicated CR($t\bar{t}$) is used to constrain the systematic uncertainties affecting the dominant $t\bar{t}$ background. The CR($t\bar{t}$) is defined similarly to the SR at first, with one jet having T_{bqq}^{PNet} > HP WP. The second jet is then subject to a requirement of $T_{Xbb} < 0.8$ to avoid overlap with events in the SR. The Pass and Fail regions of the CR($t\bar{t}$) are then populated by events where this second jet passes or fails the HP WP of the mass-decorrelated DEEPAK8 [58] top quark tagger, T_{bqq}^{DAK8}, corresponding to a 0.1% mistagging rate.

5. Background estimation

A binned 2D likelihood model is constructed in the $(m_{T'}^{rec}, m_{\phi}^{rec})$ plane from QCD multijet, $t\bar{t}$, V + jets, and signal components. The V + jets component appears mainly in the CR(QCD) because of the inversion of the top quark tagging requirements. The $t\bar{t}$ and V + jets backgrounds are estimated from MC simulation, for which the effects of systematic uncertainties are incorporated in the fit by altered distributions obtained from the simulated samples, corresponding to variations in a given uncertainty source. The QCD multijet component is instead estimated using a method in which the distribution of multijet events taken from data in the T_{Xbb} Fail region is multiplied by a smooth, parametric transfer function (TF) to estimate the distribution in the T_{Xbb} Pass region. Because the T_{Xbb} tagger response is not correlated with the jet mass, the shape of the QCD multijet background in the Pass region can be obtained directly from the shape in the Fail region. The discussion in the following paragraph is intended to be generic for both the SR and CR($t\bar{t}$), each of which has its own Pass and Fail tagging regions.

The TF is defined as the ratio of events passing to those failing the tagging requirement. For the SR and CR(QCD) this is the requirement on the second jet's T_{Xbb} score, and for the CR($t\bar{t}$) this is the requirement on the second jet's T_{bqq}^{DAK8} score. To estimate the QCD multijet background in the Pass tagging region, the QCD multijet event yield in every bin of the $(m_{T'}, m_{\phi})$ plane of the Fail region ($n_F^{QCD}(i)$) is represented by an unconstrained parameter in the likelihood, whose initial value is given by the difference between the observed data ($n_F^{Data}(i)$) and the total background from MC simulation ($n_F^{MC\ bkgs}(i)$) in that bin, prior to the fit. Thus, the number of QCD multijet events in a given bin i of any Pass tagging region, $n_P^{QCD}(i)$, is given by

$$n_P^{QCD}(i) = n_F^{QCD}(i)\,\mathrm{TF}(m_{T'}, m_{\phi}), \quad (1)$$

where

$$n_F^{QCD}(i) = n_F^{Data}(i) - n_F^{MC\ bkgs}(i). \quad (2)$$

A simultaneous maximum likelihood fit of the Pass and Fail regions is performed to determine the optimal parameters for $n_F^{QCD}(i)$ and $\mathrm{TF}(m_{T'}, m_{\phi})$, which also ensures that the QCD multijet estimates in the Fail regions are not strictly equal to the difference between the data and simulated background yields.

The CR(QCD) is used in the analysis only to validate the QCD multijet background estimation procedure described above, and to obtain an initial estimate for the TF in the SR before the SR data are unblinded. The choice of parameterization for the TF was determined by Fisher tests [59,60] and found to be constant along both reconstructed mass axes in the CR(QCD). The postfit value of the constant TF, found to be 0.14 ± 0.03, was then used to generate pseudo-data in the SR before unblinding to help further validate the QCD multijet estimation procedure. The pseudo-data generated by the application of the TF measured in the CR(QCD) is found to be consistent with the expected QCD multijet background in the T_{Xbb} Pass region of the SR, as the fitted value of the TF in the SR is 0.11 ± 0.02. A separate TF was measured in the CR($t\bar{t}$) whose best fit polynomial representation was also found to be constant along both reconstructed mass axes, with a fitted value of 0.010 ± 0.001.

The total background in the SR and CR($t\bar{t}$) is then estimated by constructing a likelihood composed of the QCD multijet prediction and the $t\bar{t}$ and V + jets contributions, which are represented by 2D histograms obtained from MC simulation and modified by the systematic uncertainties described in Section 7. The total background model, constructed as the sum of the individual background contributions using a Poisson model for each bin of the $(m_{T'}^{rec}, m_{\phi}^{rec})$ distribution, is then used to test the signal hypothesis by comparing the number of events from the background-only and signal-plus-background models, where the various signal mass hypotheses enter the likelihood as 2D histograms obtained from MC simulation.

In order to constrain the systematic uncertainties affecting the dominant $t\bar{t}$ backgrounds, the SR and CR($t\bar{t}$) are fit simultaneously. The QCD multijet background yields in both regions are estimated in parallel, but uncorrelated with one another, by using a separate TF for each region. The final TFs are determined to be constant factors for both the SR and CR($t\bar{t}$).

6. Summary of the semileptonic result used in the combination

A brief summary of the search strategy for the semileptonic top quark decay channel is presented in this Section, together with a description of the procedure for its combination with the fully hadronic channel. A complete description of the semileptonic analysis can be found in Ref. [17].

The semileptonic analysis targets single production of a vector-like top quark partner decaying to a top quark and a new scalar boson where the top quark decays to a bottom quark, charged lepton (ℓ), and neutrino (ν) via the $t \to bW \to b\ell\nu$ channel and the scalar boson decays to $b\bar{b}$. The analysis targets events with an AK4 jet and an AK8 jet containing the hadronization products of the b quark and ϕ boson, one electron or muon, and the presence of missing transverse momentum, $\vec{p}_T^{miss}$, defined as the negative vector p_T sum of all PF candidates in the event.

Similarly to the hadronic channel, the semileptonic analysis uses the mass-decorrelated PARTICLENET T_{Xbb} discriminant to identify boosted ϕ or Higgs boson candidates reconstructed as AK8 jets. Top quark candidates are reconstructed using the information from the charged-lepton candidate, one AK4 jet, and the $\vec{p}_T^{miss}$, which is assumed to represent the neutrino p_T. A multiclass BDT algorithm is trained to distinguish genuine top quark candidates from the misidentified ones in QCD multijet events and all other types of background. The BDT output is used to define a top quark tagging discriminant used to distinguish the genuine from the misreconstructed top quark candidates.

Events are then categorized based on the loose and tight WP thresholds of the T_{Xbb} and BDT top quark tagger scores. The loose and tight T_{Xbb} tagger WP thresholds are identical to those used in the hadronic analysis and serve to separate events into the CR and SR, respectively, with the former used to check the closure of the background estimation procedure and to constrain the background uncertainties in the final maximum likelihood fit. Events are further categorized based on the lepton flavor and the presence or absence of at least one forward jet ($2.4 < |\eta| < 4$), a proxy for the light quark produced in association with the T′ quark signal. A selection on m_{ϕ}^{rec} of the ϕ boson candidate is made separately for each ϕ boson mass hypothesis, ensuring 95% signal efficiency in each case. The signal strength is then extracted from a simultaneous maximum likelihood fit to the invariant mass spectrum of the top quark and ϕ boson candidates in all signal and control regions formed by this event categorization.

7. Systematic uncertainties

The fully hadronic analysis takes into account several systematic uncertainties that can affect both the shape and normalization of the reconstructed mass distributions ($m_{\mathrm{T}'}^{\mathrm{rec}}, m_{\phi}^{\mathrm{rec}}$) in simulation, which are treated as nuisance parameters in the maximum likelihood fit used for signal extraction. The uncertainty in the integrated luminosity, which affects only the overall normalization of the simulated processes, is implemented as a nuisance parameter with a log-normal probability distribution. All other uncertainties also affect the shape of the mass distributions, and they are constructed such that the ± 1 standard deviation of each distribution is mapped to the ± 1 standard deviation of the corresponding unit Gaussian constraint. Unless mentioned otherwise, all sources of uncertainty described here are applied to both the histograms obtained from the generated MC signal samples, as well as the interpolated signal histograms obtained by the procedure described in Section 3.

The relative impacts of the different sources of systematic uncertainty on the best fit signal strength are reported here for a signal with $m_{\mathrm{T}'} = 1100\,\mathrm{GeV}$ and $m_{\phi} = 175\,\mathrm{GeV}$, corresponding to the mass hypothesis with the largest local significance of 1.4 standard deviations. The dominant source of uncertainty in this search is the uncertainty in the TF used to derive the QCD multijet background estimate in the SR, which represents a 12% relative impact on the best fit signal strength. The next most dominant sources of uncertainty arise from the signal efficiency of the $\mathrm{T_{Xbb}}$ and $\mathrm{T_{bqq}^{PNet}}$ taggers applied to the signal simulation, with relative impacts of 8% each, as well as the misidentification efficiency of the $\mathrm{T_{Xbb}}$ tagger applied to the $\mathrm{t\bar{t}}$ simulation in the SR, with a relative impact of 10%.

We consider several sources of theoretical uncertainties related to the modeling of the simulated signal and background processes. The uncertainty in the PDFs used to generate the simulated samples is derived from the PDF variations provided by the NNPDF3.1 set [48]. Uncertainties in the QCD renormalization and factorization scales are obtained by varying these scales independently by factors of 0.5 and 2 with respect to their default values, excluding the two extreme variations.

Experimental uncertainties related to the detector conditions are also considered and applied to MC simulated samples for both signal and background processes. The uncertainty in the integrated luminosity of the data set, taken to be 1.6% [18,19], has a sub-percent impact on the results. The uncertainties in the jet energy scale and resolution are estimated as functions of p_{T} and η of the jets [31] and correspond to a relative impact of 3–5%. The uncertainty in the pileup description is evaluated by varying the total inelastic cross section by $\pm 4.6\%$ [51].

During the 2016–2017 data-taking period, a gradual shift in the timing of the L1 trigger inputs from the ECAL in the $|\eta| > 2.0$ region caused a trigger inefficiency, denoted as "prefiring" [23]. The trigger missed between 10% and 20% of the events containing an electron (of $p_{\mathrm{T}} \gtrsim 50\,\mathrm{GeV}$) or a jet (of $p_{\mathrm{T}} \gtrsim 100\,\mathrm{GeV}$) in the $2.5 < |\eta| < 3.0$ range, the exact loss depending on the p_{T} and η of the trigger object. Correction factors were computed from data and applied to the acceptance evaluated by simulation. The uncertainties in these corrections are implemented as templates affecting the shape of the p_{T} and η distributions for 2016 and 2017 simulated samples.

The trigger efficiency is measured in an orthogonal data set as a 2D function of ($m_{\mathrm{T}'}^{\mathrm{rec}}, m_{\phi}^{\mathrm{rec}}$). A parametric function is fit to the 2D efficiency curve, which serves to model the efficiency turn-on while simultaneously reducing statistical fluctuations in the measurement. The MC simulation based distributions are then corrected by evaluating the fitted efficiency function at each event's reconstructed ($m_{\mathrm{T}'}^{\mathrm{rec}}, m_{\phi}^{\mathrm{rec}}$) invariant mass, and distributions corresponding to ± 1 standard deviations in the trigger efficiency are derived from the fit uncertainties.

A specific uncertainty in the $\mathrm{t\bar{t}}$ simulation arises from the top quark p_{T} reweighting procedure [61], which is extrapolated to high p_{T}. This uncertainty accounts for the observed discrepancy between the p_{T} spectrum of $\mathrm{t\bar{t}}$ pairs in data and simulation, as measured by the ratio of the distributions of the top quark p_{T} in data and simulation as predicted by POWHEG + PYTHIA [62,63]. A data-to-simulation correction factor $w_t(p_{\mathrm{T}})$ is applied to simulated $\mathrm{t\bar{t}}$ events as a function of their p_{T}, which takes the form $w_t(p_{\mathrm{T}}) = e^{c_1 0.0615 - c_2 (0.0005/\,\mathrm{GeV}) p_{\mathrm{T}}}$, as obtained from Refs. [62,63]. The uncertainty is implemented as uncorrelated variations of $\pm 50\%$ in the c_1 and c_2 parameters of the correction factor and has a 2–3% relative impact on the best fit signal strength.

Additionally, uncertainties in the jet tagging and mistagging efficiencies of the various taggers used in this analysis are treated as shape effects on the signal and dominant $\mathrm{t\bar{t}}$ background. The efficiency of the $\mathrm{T_{Xbb}}$ tagger is calibrated in a data set enriched in jets arising from gluon splitting to $\mathrm{b\bar{b}}$ pairs, $\mathrm{g} \to \mathrm{b\bar{b}}$, the characteristics of which have been sculpted to resemble those of a scalar using a boosted decision tree (BDT) [64], with p_{T}-dependent correction factors and their uncertainties applied to signal simulation as shape templates. To select a subset of the $\mathrm{g} \to \mathrm{b\bar{b}}$ jets in a phase space that most closely resembles that of the signal, the BDT takes as input six variables related to the jet substructure, including information about secondary vertices (SVs) within the jet. An SV is a point in the detector where particle tracks converge that is displaced from the vertex corresponding to the hardest scattering in the event, called the primary vertex. Charged-particle tracks associated with an SV are used to calculate its kinematic properties, such as its invariant mass, p_{T}, and its transverse displacement relative to the primary vertex, d_{xy}.

The six inputs to the BDT are the N-subjettiness ratio τ_{21} [65], the soft-drop masses of the two subjets, the p_{T} of the two SVs matched to each subjet, and the number of tracks associated with each SV. Proxy jets are then selected using nine thresholds of the BDT score that vary as functions of the PARTICLENET tagger discriminant score, such that the shape of the tagger discriminant is similar for both the proxy and signal jets. A fit to the mass of the SV with the maximum d_{xy} significance, defined as d_{xy} normalized by its uncertainty, is performed simultaneously for events with jets failing and passing the given $\mathrm{T_{Xbb}}$ tagger WP. The tagging efficiency ratios between data and simulation obtained from the fit are then used to scale the MC sample yields to data. The calibration procedure yields data-to-simulation correction factors ranging from 0.9 to 1.3 for the $\mathrm{T_{Xbb}}$ tagger efficiency, depending on the jet p_{T} and data-taking year. A comprehensive description of the calibration of the mass-decorrelated PARTICLENET algorithm is provided in Ref. [64].

The mistagging efficiency for the $\mathrm{T_{Xbb}}$ tagger, as well as the tagging efficiencies for the $\mathrm{T_{bqq}^{PNet}}$ and $\mathrm{T_{bqq}^{DAK8}}$ discriminants, are calibrated in data using the tag-and-probe method [66] with events enriched in $\mathrm{t\bar{t}}$ production. The $\mathrm{T_{Xbb}}$ mistagging uncertainty is applied only to $\mathrm{t\bar{t}}$ MC samples, as top quark induced jets have a nonnegligible, p_{T}-dependent, probability of being misidentified by this tagger as a $\phi \to \mathrm{b\bar{b}}$ candidate. The data-to-simulation correction factors for the $\mathrm{T_{Xbb}}$ mistagging efficiency range from 0.7 to 1.2, depending on the jet p_{T} and data-taking year. The uncertainty in the $\mathrm{T_{bqq}^{DAK8}}$ tagging efficiency is applied only to the $\mathrm{t\bar{t}}$ background in the CR($\mathrm{t\bar{t}}$), which is the only analysis region where this tagger is employed.

Finally, the uncertainty in the QCD multijet background prediction in the SR is derived during the simultaneous fit to data of the SR and CR($\mathrm{t\bar{t}}$). The uncertainty in the best fit TF parameter values enters the Hessian matrix used to calculate the total background uncertainty. The TF parameters are uncorrelated between the SR and CR($\mathrm{t\bar{t}}$) and are treated as nuisance parameters with uniform probability distribution functions in the likelihood.

The fully hadronic and semileptonic searches entering the combination are statistically independent of one another because of a lepton veto applied in the fully hadronic channel, which rejects any event with isolated muons or electrons. For all common $m_{\mathrm{T}'}$ and m_{ϕ} hypotheses, a simultaneous maximum likelihood fit is performed to extract limits on the product of the cross section and branching fraction for the $\mathrm{T}' \to \mathrm{t}\phi$ process, wherein systematic uncertainties that are common between the fully hadronic and semileptonic top quark decay channels are treated as fully correlated. These include uncertainties arising from reconstruction and calibration procedures such as the jet energy scale and resolution and the top quark p_{T} reweighting. Uncertainties in the $\mathrm{T_{Xbb}}$ tagging and

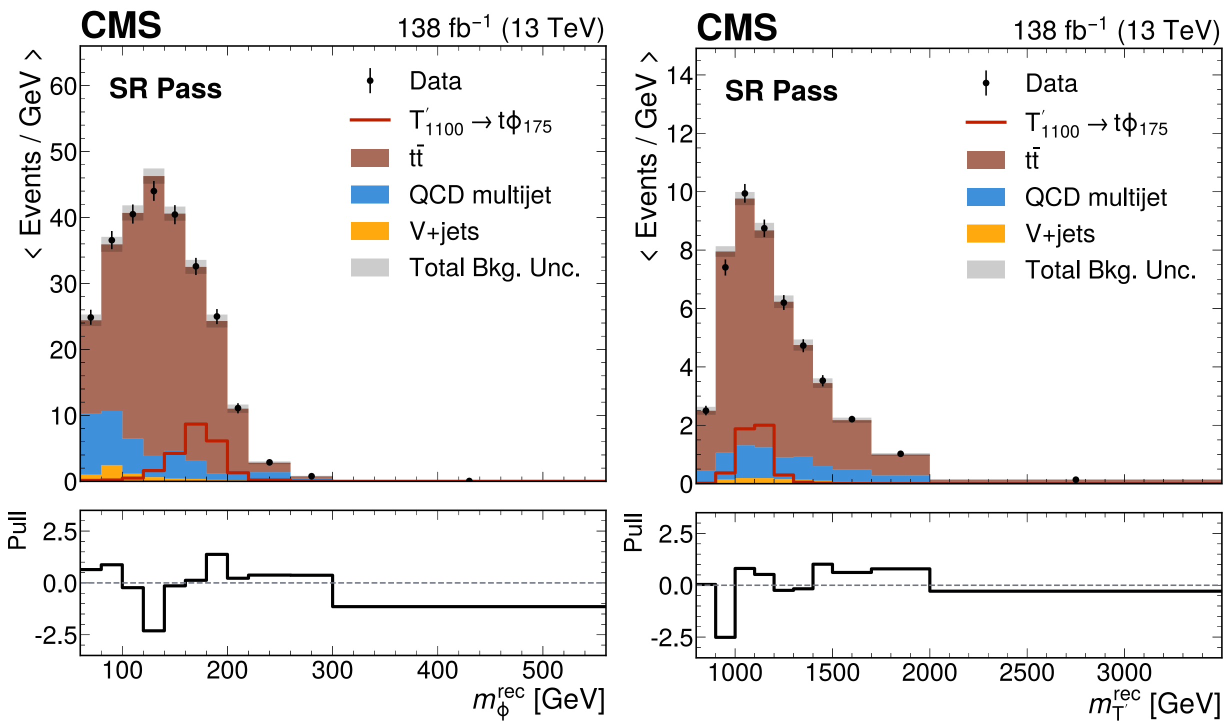

Fig. 1. Postfit distributions of data and predicted background in the SR under the background-only hypothesis, projected onto the m_{ϕ}^{rec} (left) and $m_{T'}^{rec}$ (right) axes in the T_{Xbb} Pass tagging region, SR_P. A $m_{\phi} = 175$ GeV, $m_{T'} = 1100$ GeV signal sample normalized to a cross section of 220 fb is overlaid for visualization. The y axes of the top panels have been rescaled to display the number of events per bin, divided by the width of each bin.

mistagging efficiency correction factors are correlated between the two analyses, since both use this tagger at the same WP for boosted ϕ boson identification. Theoretical uncertainties in both the renormalization and factorization scales as well as in the PDFs used in the generators are also taken to be correlated. Finally, uncertainties inherent to the accelerator and detector in both analyses are correlated, including those in the integrated luminosity and the L1 prefiring correction factors. Systematic uncertainties inherent to the QCD multijet background estimates are uncorrelated between the two channels, as these background estimates are performed in statistically independent regions. A detailed description of the uncertainty sources exclusive to the semileptonic channel, which include those arising from lepton identification and semileptonic top quark reconstruction, can be found in Ref. [17].

8. Results

A 2D binned maximum likelihood fit to data of the $(m_{T'}^{rec}, m_{\phi}^{rec})$ distributions is performed simultaneously for events in the SR and CR($t\bar{t}$), using MC simulation to model $t\bar{t}$ and V + jets, and control samples in data to predict the QCD multijet background. The inclusion of the CR($t\bar{t}$) background model in the likelihood constrains the systematic uncertainties affecting $t\bar{t}$ MC simulation, helping to model this dominant background in the SR more accurately. The product of a data-driven estimate in the T_{Xbb} Fail region and an unconstrained constant TF is used to predict the QCD multijet background yield in the T_{Xbb} Pass region of the SR, and the same estimation is performed in the CR($t\bar{t}$) using a separate constant TF.

The results of the 2D fit to data in the hadronic channel are represented in Fig. 1 as projections onto the reconstructed mass axes, and it is observed that the data are in agreement with the SM background prediction within uncertainties. A deficit in data relative to the predicted background is observed for the reconstructed T′ quark masses near 900 GeV and ϕ boson masses near 125 GeV. The deficit has a local (global) significance of 2.7 (1.5) standard deviations. The figure on the left shows the projection of the postfit distributions onto the m_{ϕ}^{rec} axis and the one on the right the projection onto the $m_{T'}^{rec}$ axis. The lower panels show the pull distributions, defined for each bin as the difference between the observed data and the postfit background prediction divided by the square root of the difference between the squared Poisson uncertainty in the data and the squared postfit uncertainty in the total background estimate in that particular bin.

The results from the fully hadronic channel are combined with those from the semileptonic channel in a global maximum likelihood fit using the CMS statistical analysis tool COMBINE [67], which is based on the ROOFIT [68] and ROOSTATS [69] frameworks. Shared sources of systematic uncertainty are correlated between the two channels in the fit and are listed in Section 7, while those exclusive to each channel are considered uncorrelated. The signal strength for each $m_{T'}$ hypothesis is extracted from a simultaneous fit of both channels' SRs, while utilizing their respective CRs to constrain the backgrounds.

The data are in agreement with the SM background prediction within uncertainties in both searches. The 95% confidence level (CL) expected and observed upper limits on the product of the cross section and branching fraction for T′ quark production are calculated using the CL_s criterion [70,71] with the profile likelihood ratio as the test statistic [72] using an asymptotic approximation [73]. The observed 95% CL upper limit is shown as a function of $(m_{T'}, m_{\phi})$ in Fig. 2. No assumption is made for $\mathcal{B}(T' \to t\phi)$, and $\mathcal{B}(\phi \to b\bar{b})$ is assumed to be 100%. For $m_{T'} < 1.5$ TeV, the combination achieves an improvement on the upper limits on the product of cross section and branching fraction for each channel by up to a factor of two for certain m_{ϕ}. When interpreting the results in the case where the neutral scalar is the SM Higgs boson, the combination improves the mass exclusion limits by 100 GeV over the fully hadronic limits alone. For $m_{T'} > 2$ TeV the combination converges to the results obtained by the semileptonic channel, which is more sensitive primarily due to lower backgrounds.

Limits at 95% CL on the product of the T′ quark production cross section and branching fraction are shown in Fig. 3 as a function of $m_{T'}$

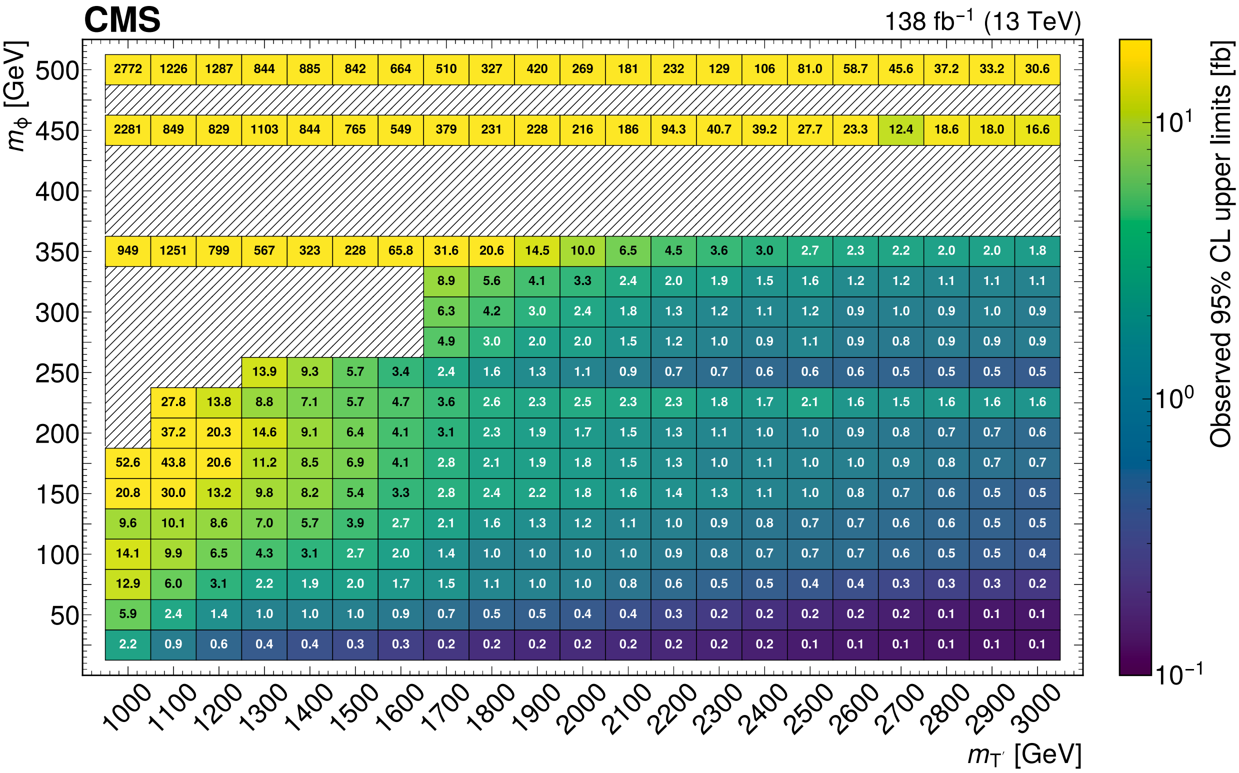

Fig. 2. The upper limit at 95% CL on the product of cross section for the $T' \to t\phi$ process and branching fraction $\mathcal{B}(t \to bq\bar{q}')$ as a function of $(m_{T'}, m_\phi)$, assuming $\mathcal{B}(\phi \to b\bar{b}) = 100\%$. Masses of the ϕ boson below 75 GeV are exclusive to the semileptonic channel, while $m_\phi > 250$ GeV are exclusive to the fully hadronic channel. Besides $m_\phi = 225$ GeV, also exclusive to the fully hadronic channel, upper limits for $75 < m_\phi < 250$ GeV are obtained from the combination of the two channels. Gaps in m_ϕ above 250 GeV are due to the limitations in the signal interpolation scheme in the hadronic channel, while gaps in $m_\phi < 250$ GeV correspond to signals not considered by the semileptonic channel due to poor signal efficiency. All such gaps in coverage are represented by the hatched regions.

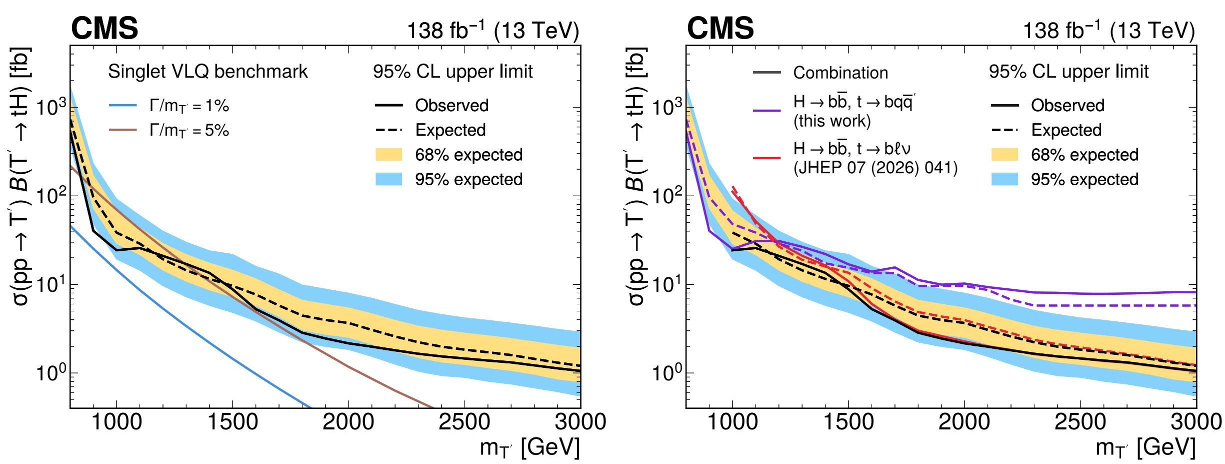

Fig. 3. Upper limits at 95% CL on the product of the cross section and branching fraction for $pp \to T' \to tH$ as functions of the T′ quark mass for fixed $m_\phi = m_H = 125$ GeV. The limits differ from those in Fig. 2 due to the assumption of the SM branching fraction for the $H \to b\bar{b}$ decay. In the left panel, the solid blue (brown) curves indicate the theoretical cross sections for the singlet T′ quark model assuming its width is 1% (5%) of its mass [36,37]. The contributions to the combination from the semileptonic (red) and fully hadronic (purple) channels are detailed in the right panel, where it is shown that upper limits for T′ quark masses below 1 TeV are obtained from the fully hadronic channel only, while limits for all other mass points are obtained from the combination of the semileptonic and fully hadronic channels. The same holds for the shaded 68% and 95% expected upper limits in the right panel. In both panels, the median expected and the observed limits are depicted using dashed and solid lines, respectively.

for $m_\phi = 125$ GeV, corresponding to the SM Higgs boson. The limits for the two channels are shown alongside the results of the statistical combination. The results are interpreted here in the context of the singlet T′ quark, for resonances whose widths Γ are 1 and 5% of their mass. Masses of the T′ quark between 0.85–1.3 TeV are excluded at 95% CL for the scenario where the T′ quark width is 5% of its mass, while no such exclusion can be made for the 1% relative width scenario. Limits on the T′ quark coupling strength κ as a function of the T′ quark mass can be found in Ref. [74] for several different VLQ analyses in CMS alongside the results presented in this Letter. Here, κ represents the strength of the coupling between the T′ quark, a standard model quark, and an EW gauge boson at the production vertex.

9. Summary

A search for single production of a vector-like top quark partner T' decaying to a top quark (t) and a neutral scalar boson ϕ in the fully hadronic final state is presented, using proton-proton collision data recorded by the CMS experiment at $\sqrt{s} = 13$ TeV in 2016–2018 and corresponding to a total integrated luminosity of 138 fb^{-1}. The hadronic decay products of the top quark and ϕ boson are expected to be highly Lorentz boosted from the decay of the massive T' resonance, resulting in two large-radius jets in the final state. The results of this hadronic search are combined with those from a previous search in the semileptonic channels in a simultaneous maximum likelihood fit. No significant excess of data with respect to the background prediction is observed. Upper limits at 95% confidence level (CL) are set on the product of the production cross section and branching fraction for the decay $\mathrm{T}' \to \mathrm{t}\phi$, representing the first results for the decay $\mathrm{T}' \to \mathrm{t}(\mathrm{b}\overline{\mathrm{q}}{}')\phi(\mathrm{b}\overline{\mathrm{b}})$ at the LHC. For the case where the neutral scalar is the standard model Higgs boson (H), upper limits are set on the product of the production cross section and the $\mathrm{T}' \to \mathrm{tH}$ branching fraction ranging from 23 fb for T' quarks of mass $m_{\mathrm{T}'} = 1$ TeV to 1 fb at $m_{\mathrm{T}'} = 3$ TeV. They exclude T' quark masses of 0.85–1.3 TeV assuming the T' quark is a weak-isospin singlet with a resonance width of 5% of its mass, improving on all previous searches by the CMS Collaboration [9] by up to a factor of three and representing the most stringent limits to date for masses above 2 TeV. For other ϕ boson masses, upper limits as low as 0.1 fb are set at 95% CL on the product of the T' production cross section and branching fraction to $\mathrm{t}\phi$.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data availability

Release and preservation of data used by the CMS Collaboration as the basis for publications is guided by the CMS data preservation, re-use and open access policy.

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