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Search for heavy particles in the b-tagged dijet mass distribution with additional b-tagged jets in proton-proton collisions at $\sqrt{s} = 13$ TeV with the ATLAS experiment

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A search optimized for new heavy particles decaying to two b-quarks and produced in association with additional b-quarks is reported. The sensitivity is improved by b-tagging at least one lower-p_{T} jet in addition to the two highest-p_{T} jets. The data used in this search correspond to an integrated luminosity of 103 fb^{-1} collected with a dedicated trijet trigger during the 2017 and 2018 $\sqrt{s} = 13$ TeV proton-proton collision runs with the ATLAS detector at the LHC. The search looks for resonant peaks in the b-tagged dijet invariant mass spectrum over a smoothly falling background. The background is estimated with an innovative data-driven method based on orthonormal functions. The observed b-tagged dijet invariant mass spectrum is compatible with the background-only hypothesis. Upper limits at 95% confidence level on a heavy vector-boson production cross section times branching ratio to a pair of b-quarks are derived.

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I. INTRODUCTION

New particles beyond the Standard Model with preferential couplings to third-generation quarks are predicted by many models [1–6] and have been extensively searched for by experiments at the Tevatron and the LHC. Searches for heavy particles in the dijet invariant mass spectrum of "b-tagged" jets, identified as containing b-hadrons, have probed this scenario [7–12]. Recent results from the LHCb and Belle experiments suggest deviations in lepton-flavor universality (LFU) from Standard Model (SM) expectations [13–17], referred to as LFU anomalies. The phenomenological work in Refs. [18,19] predicts new heavy vector bosons, a Z' boson and W' boson, mainly coupled to third-generation leptons and quarks. This model not only offers an explanation for the LFU anomalies, but also predicts Z' boson production in association with third-generation quarks via gluon splitting in the LHC experiments, due to the vanishingly small b-quark and top-quark parton distribution functions (PDFs) for protons at the TeV scale. The dominant Feynman diagram for this b-quark associated production is shown in Fig. 1.

The additional b-flavor jets, not coming from the heavy-particle decay, can be used to reduce the multijet background contribution since the additional jets in multijet events most likely do not contain b-hadrons. Most previous searches for heavy particles in dijet final states did not require additional b-tagged jets beyond the leading two jets [7–10], i.e., the two jets with the highest transverse momentum (p_{T}). This article presents a search for heavy particles in final states where the two leading jets are b-tagged and either the third or fourth jet is also b-tagged. The b-tagging criterion for the third and fourth jets increases the sensitivity by 20%–50% at a mass scale of 1.3–3 TeV. This is the first search probing the mass region up to 3.6 TeV in this final state. Previous searches for a heavy Higgs boson [11,12] in a similar final state were optimized for masses up to 1.4 TeV. An advanced b-tagging algorithm with better performance at high p_{T} [20] is applied in this search compared to the one used in Ref. [11], enhancing the sensitivity in the high mass region. The model proposed in Refs. [18,19] is compared with data for the first time.

II. ATLAS DETECTOR

The ATLAS detector [21] at the LHC covers nearly the entire solid angle around the collision point.[1] It consists of

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[1] ATLAS uses a right-handed coordinate system with its origin at the nominal interaction point (IP) in the center of the detector and the z-axis along the beam pipe. The x-axis points from the IP to the center of the LHC ring, and the y-axis points upward. Cylindrical coordinates (r, ϕ) are used in the transverse plane, ϕ being the azimuthal angle around the z-axis. The pseudorapidity is defined in terms of the polar angle θ as $\eta = -\ln[\tan(\theta/2)]$. The rapidity is defined as $y = (1/2)\ln[(E + p_z)/(E - p_z)]$, where E is the energy and p_z is the momentum in the z direction. Transverse energy is defined as $E_{\mathrm{T}} = E \sin\theta$.

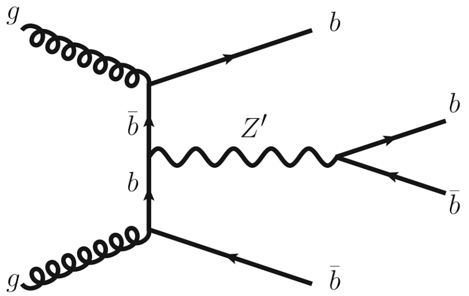

FIG. 1. Representative Feynman diagram for the resonant production of a Z' boson in association with additional b-quarks and its decay into a pair of b-quarks.

an inner tracking detector surrounded by a thin superconducting solenoid, electromagnetic and hadronic calorimeters, and a muon spectrometer. The inner-detector system is immersed in a 2 T axial magnetic field and provides charged-particle tracking in the range $|\eta| < 2.5$. The high-granularity silicon pixel detector covers the vertex region and typically provides four measurements per track, the first hit normally being in the insertable B-layer installed before Run 2 [22,23]. It is followed by the silicon microstrip tracker, which usually provides eight measurements per track. These silicon detectors are complemented by the transition radiation tracker, which enables radially extended track reconstruction up to $|\eta| = 2.0$ and contributes to electron identification. The calorimeter system covers the pseudorapidity range $|\eta| < 4.9$. Within the region $|\eta| < 3.2$, electromagnetic calorimetry is provided by barrel and end cap high-granularity lead/liquid-argon (LAr) calorimeters, with an additional thin LAr presampler covering $|\eta| < 1.8$ to correct for energy loss in material upstream of the calorimeters. Hadronic calorimetry is provided by the steel/scintillator-tile calorimeter, segmented into three barrel structures within $|\eta| < 1.7$, and two copper/LAr hadronic end cap calorimeters. The solid angle coverage is completed with forward copper/LAr and tungsten/LAr calorimeter modules optimized for electromagnetic and hadronic measurements, respectively. The outermost layers of ATLAS consist of a muon spectrometer within $|\eta| < 2.7$, incorporating three large superconducting toroidal magnet systems. Interesting events are selected by the first-level trigger system implemented in custom hardware, followed by selections made by algorithms implemented in software in the high-level trigger computer farm [24,25]. The first-level trigger accepts events from the 40 MHz bunch crossings at a rate below 100 kHz, which the high-level trigger reduces in order to record events to disk at a rate of about 1 kHz. An extensive software suite [26] is used for real and simulated data reconstruction and analysis, for operation and in the trigger and data acquisition systems of the experiment.

III. SIMULATED EVENT SAMPLES

The theory model used in this search considers a Z' boson exclusively coupled to the third generation of the left-handed SM fermions [18,19]. Events with a Z' boson produced in association with up to two additional partons in the final state, with the coupling to the quark sector (g_b) set to unity and the coupling to the lepton sector (g_τ) set to zero, were generated using MadGraph5_aMC@NLO 2.2.4 [27], considering all diagrams at the matrix-element level of the type $pp \to Z'$, $pp \to Z'j$ and $pp \to Z'jj$, and the parton showering was done in PYTHIA 8.212 [28]. Both $Z' \to t\bar{t}$ and $Z' \to b\bar{b}$ are possible with g_b set to unity, but only the latter was included in the generation. The five-flavor scheme leading-order (LO) NNPDF3.0 PDF [29] and a set of tuned parameters called the A14 tune [30] were applied in the generation. CKKW-L k_t-merging [31] was used to match the multileg parton-level events with PYTHIA 8. The intrinsic width of the Z' boson is roughly 4% of the Z' boson mass. This model is referred to as the lepton-universality-violating (LUV) Z' in this article.

Multijet events were generated with PYTHIA 8.186, using the LO NNPDF2.3 PDF [32] and the A14 tune. The background is estimated in a fully data-driven way and the simulated multijet event samples are only used to optimize the event selections.

The simulated multijet events were passed through a full ATLAS detector simulation [33] using GEANT4 [34]. The signal samples were passed through a fast simulation where the response in the calorimeters is provided by a parametrization [35] while GEANT4 is used elsewhere. The decay of b- and c-hadrons was performed using the EvtGen 1.2.0 decay package [36]. Additional proton-proton interactions (pileup) from the same and neighboring bunch crossings were taken into account by generating a number of inelastic pp interactions with PYTHIA 8.186 using the LO NNPDF2.3 PDF set and the A3 tune [37]. These events were then overlaid with the hard-scattering events. All simulated events are weighted so that the distributions of the average number of collisions per bunch crossing match those in data.

IV. DATA SAMPLE AND EVENT SELECTION

The data used for this analysis were collected with the ATLAS detector from proton-proton (pp) collisions at the LHC with a center-of-mass energy of $\sqrt{s} = 13$ TeV in 2017 and 2018, requiring that all detector systems were functional and recording high-quality data [38]. The dataset corresponds to an integrated luminosity of 103 fb^{-1} [39], using the LUCID-2 detector [40] for the primary luminosity measurements. Data were collected using a newly developed trijet trigger with asymmetric thresholds, first deployed in 2017. This trigger required two jets to have transverse energy E_{T} greater than 250 GeV and a third jet to have E_{T} greater than 120 GeV. All three jets were required to have $|\eta| < 3.2$, with intermediate preselections at lower p_T requiring $|\eta| < 2.4$. This trigger allows this search to reach an invariant mass (m_{jj}) of the two highest-p_T jets about 100 GeV lower than a single-jet trigger would allow. The trigger efficiency exceeds 99.95% after applying the kinematic selections on jets described below.

Collision vertices are reconstructed from at least two tracks with $p_T > 0.5$ GeV. The one with the highest $\sum p_T^2$ of the associated tracks is considered to be the primary vertex. Jets are reconstructed using the anti-k_t algorithm [41–43] with a radius parameter of $R = 0.4$ from noise-suppressed topological energy depositions [44]. A calibration sequence is applied to jet energies and directions as described in Ref. [45]. Jets with $p_T > 25$ GeV are removed if they are compatible with noise bursts, beam-induced background or cosmic rays with the "loose" criteria defined in Ref. [46].

A deep-learning neural network, DL1r, is applied to identify jets containing b-hadrons [20]. This algorithm utilizes the distinctive characteristics of b-hadron decays such as the large impact parameters of tracks and the displaced vertices reconstructed in the inner detector. Therefore it is only applied to jets with $|\eta| < 2.5$. In addition, it includes the output from a recurrent neural network (RNNIP) [47], which exploits the correlations between tracks originating from the same b-hadron. Operating points (OP) are defined by a single cut-value on the discriminant output distribution and are chosen to yield a certain b-tagging efficiency in a simulated inclusive $t\bar{t}$ event sample. The 77% efficiency b-tagging OP is selected as it gives the best overall signal sensitivity across the m_{jj} range under consideration. In simulated multijet events, the efficiency drops from 77% on average for b-jets with $p_T < 250$ GeV to 10% for a p_T of 2 TeV. The corresponding mistag rate for charm-flavor (light-flavor) jets changes from 20% (< 1%) to 2% (< 1%).

The analysis considers events with at least four jets. The leading two jets must have $p_T > 250$ GeV and the third leading jet must have $p_T > 120$ GeV. The leading three jets must be within $|\eta| < 2.4$ to match the preselections applied in the trigger chain. The fourth leading jet must have $p_T > 25$ GeV and be within $|\eta| < 4.5$. To suppress low-p_T jets from underlying events, a multivariate classification algorithm based on tracking information, the jet vertex tagger (JVT), is applied and jets within $|\eta| < 2.5$ with $p_T < 60$ GeV must satisfy the "medium" OP [48]. Jet pairs from the decay of heavy particles are more central than those from multijet events, thus the rapidity separation of two leading jets, defined as $y^* = (y_1 - y_2)/2$, is a powerful discriminant. The optimal choice is found to be $|y^*| < 0.8$. The m_{jj} is required to be greater than 730 GeV above which the spectrum starts to decrease continually. An event is preselected if it passes all the above requirements.

The signal region (SR) selection requires both the leading two jets and either the third or fourth jet to satisfy the 77% b-tagging OP. The full selection is summarized in Table I. The acceptance of the benchmark signal is 1.9%, 2.4%, and 1.1% for an LUV Z' mass of 1.3, 1.6, and 2.5 TeV respectively, rising then falling due to increasing kinematic acceptance and decreasing b-tagging efficiency with jet p_T. The corresponding m_{jj} spectra after applying the full selection are shown in Fig. 2. The m_{jj} distributions are wide due to the significant low Z' mass tails introduced by off-shell production, which occurs due to the steeply falling PDF of the two colliding partons at large values of Bjorken x. This feature is commonly referred to as a "parton-luminosity tail," and its size increases with the resonance mass. This effect is more significant for LUV Z' as the b-quark PDF has a larger proportion at low Bjorken x values than those of light quarks, c-quarks and gluons.

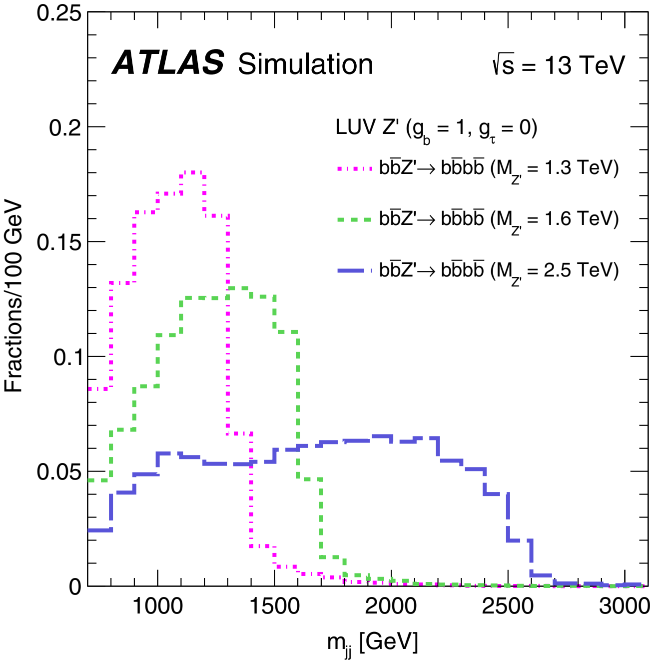

FIG. 2. m_{jj} distributions of three benchmark LUV Z' mass points, 1.3 TeV, 1.6 TeV, and 2.5 TeV after applying the full signal region selections, normalized to unity.

V. BACKGROUND ESTIMATION

The main background in this search originates from multijet events. A novel data-driven method is used to estimate the background contribution by performing a fit to the m_{jj} spectrum. The shape of this spectrum is impacted by the asymmetric thresholds of the trijet trigger used to collect the data. The empirical functional forms used in previous heavy-particle searches [9] are not able to model this effect adequately. The background is estimated with the "functional decomposition" (FD) method [49,50], which uses a truncated series. First it performs a power-law transformation on m_{jj}, as given by

$$z \equiv \left(\frac{m_{\mathrm{jj}} - m_{\mathrm{jj}}^0}{\lambda}\right)^{\alpha},$$

where m_{jj}^0 is the start of the spectrum (730 GeV), λ is a positive scale factor and α is a positive exponent. The spectrum can then be modeled by

$$\Omega(z) = \sum_{n=1}^{N} c_n E_n(z),$$

where $E_n(z)$ is the nth member of an orthonormal basis constructed from exponential functions, c_n is the corresponding nth coefficient and N is the total number of terms used. Equation (1) shows the first three orthonormal functions.

$$\begin{aligned} E_1(z) &= \sqrt{2}e^{-z}, \\ E_2(z) &= 6e^{-2z} - 4e^{-z}, \\ E_3(z) &= 10\sqrt{6}e^{-3z} - 12\sqrt{6}e^{-2z} + 3\sqrt{6}e^{-z}. \end{aligned} \quad (1)$$

Each pair of (λ, α) defines a hyperspace of functions. For a given pair of (λ, α), the m_{jj} spectrum can be modeled precisely as $N \to \infty$. Since a falling m_{jj} spectrum can be described adequately using lower moments, while a localized structure in m_{jj} needs higher moments to model it well, truncating the series at a certain N allows the background to be modeled mostly independently of the presence of signal [49]. There exists an optimal set of (λ, α, N) that gives the most succinct representation of the data. It is identified by using two steps: dataset decomposition and parameter optimization. In the dataset decomposition step, the m_{jj} spectrum is converted to an unbinned dataset and the FD method creates a complete representation of this dataset in an initial hyperspace defined by (λ_0, α_0), considering 4096 moments as an approximation of $N \to \infty$. Values of c_n and the covariance matrix are calculated. The parameter optmization step performs a grid scan on the λ-α plane followed by a gradient-descent minimization starting from the best point obtained in the grid scan. The grid scan covers a large space, with α ranging from 0.6 to 1.3 and λ ranging from 50 to 750. Each axis has 140 evenly distributed steps and there are 19600 points scanned in total. The starting point is (0.6, 50). The covariance matrix and c_n in another hyperspace can be obtained by a matrix transformation between the initial hyperspace and the new one [49], thus the dataset decomposition is only carried out once at the starting point. Only the first 128 moments are considered in the parameter optimization step as it is already well above the number of moments needed for the spectrum under consideration. Every combination of (λ, α) and N is considered and the quantity to minimize is [49]:

$$\mathcal{L} = D_{\mathrm{KL}}(\tilde{\mathbf{f}}||\tilde{\mathbf{c}}) + D_{\mathrm{KL}}(\tilde{\mathbf{c}}||\tilde{\mathbf{p}}), \quad (2)$$

which contains two Kullback–Leibler divergences (D_{KL}) [51] and measures how a probability distribution differs from a reference probability distribution. The first term is the divergence of the estimate ($\tilde{\mathbf{c}}$) with respect to data ($\tilde{\mathbf{f}}$). A better description of the data results in a smaller divergence. The second term is the divergence of some prior background assumption ($\tilde{\mathbf{p}}$) with respect to the estimate ($\tilde{\mathbf{c}}$). It is a penalty term as $\tilde{\mathbf{p}}$ is constructed such that the divergence increases as the value of N increases [49]. As a consequence, the minimization prefers a smaller number of terms and the series is truncated. The truncated series, given by the optimized (λ, α), N and the corresponding coefficients (c_n), determines the background estimate. Even though the penalty term in Eq. (2) prevents overfitting the data, the upper limit on N is fixed using background-only pseudodata samples introduced below. A lower limit on N is also identified using the same pseudodata samples to ensure the background estimate is adequate. In the application to data, the parameter optimization step only considers values of N within this fixed range while other parameters are not constrained by background-only pseudodata samples. The background estimate is converted to a histogram as the input to the statistical analysis, where the binning is determined by the m_{jj} resolution measured in Ref. [9].

Background-only pseudodata samples are generated by scaling the events passing the preselections listed in Table I with the expected event-level b-tagging selection efficiency of multijet events in data. The event-level b-tagging selection efficiency is defined as the probability, as a function of the m_{jj}, of a preselected event to enter the signal region. The measured efficiency points are fitted by a third-order polynomial to smooth any features introduced by local fluctuations or by the presence of signal events. It is verified that a third-order polynomial is insensitive to possible signal contamination by artificially introducing different signal width and mass combinations. The event-level b-tagging selection efficiency for the target signal region is calculated using data to be 0.14% at 730 GeV and

TABLE I. Signal region event selection criteria. The superscripts refer to the ranking given by jet p_{T}.

Preselection	
Jet p_{T}	$p_{\mathrm{T}}^{1,2} > 250$ GeV
	$p_{\mathrm{T}}^{3} > 120$ GeV
	$p_{\mathrm{T}}^{4} > 25$ GeV
Jet $\lvert\eta\rvert$	$\lvert\eta^{1,2,3}\rvert < 2.4$
	$\lvert\eta^{4}\rvert < 4.5$
JVT	“medium” OP
$\lvert y^*\rvert$	< 0.8
b-tagging Selection	
DL1r	Leading two jets: 77% OP
	Third or fourth jet: 77% OP
m_{jj}	>730 GeV

decreases to 0.01% at 3 TeV. Pseudodata samples are generated by varying the fitted efficiency curve according to the uncertainties associated with the fit.

A background-enhanced control region with negligible signal contamination, where both the third and fourth jets are required to fail the b-tagging requirements, is constructed to validate this procedure for generating pseudodata samples. In this control region, the corresponding event-level b-tagging selection efficiency is the probability that an event fails to satisfy the b-tagging criteria for the third and fourth jets but has both the leading two jets b-tagged. The pseudodata samples generated by this procedure provide a good description of the target spectrum in this control region.

The background-only pseudodata samples approximating the signal region are used to check whether a given FD configuration models the background adequately by performing two sets of tests. A χ^2 test is applied to check whether the estimate agrees well with the background. More than 90% of the pseudoexperiments are required to have a χ^2 p-value greater than 0.01. In addition to the χ^2 test, the BumpHunter algorithm [52,53] described in Sec. VII is used to check whether the background estimate introduces strong biases in the statistical analysis. More than 90% of the pseudoexperiments must give a BumpHunter p-value greater than 0.01 when the background-only pseudodata samples are considered.

The lower and upper limits on N are determined by the above tests, starting without any constraints on N and gradually shrinking the allowed range. First the lower limit is optimized by increasing it until the above criteria are met. Once the lower limit is determined, the upper limit is decreased until the above criteria are no longer satisfied. The tests show that requiring N to be 2 or 3 is sufficient to obtain a good estimate of the background. Therefore, the minimization only considers these two options in the signal injection tests described below and in the final application to data.

Another set of tests is performed with signal events injected into the background-only pseudodata samples to evaluate the sensitivity to signal. The sensitivity to a given signal model is considered to be optimal if more than 90% of pseudoexperiments return a BumpHunter p-value less than 0.01 with a significant number of signal events injected. The number of events injected satisfies $N_{\mathcal{S}}/\sqrt{N_{\mathcal{B}}} = 5$, in which $N_{\mathcal{S}}$ and $N_{\mathcal{B}}$ are the numbers of signal and background events, respectively, within a m_{jj} window corresponding to twice the signal width on each side of the signal mass point. A large set of Gaussian-like signal hypotheses across the entire m_{jj} region, with various widths, are tested; and they show that this search has optimal sensitivity above 1.3 TeV. The low m_{jj} region is sculpted more significantly by the trigger and kinematic selections. The truncated series determined by FD is too flexible and absorbs more of the signal in this region, resulting in lower sensitivities. Therefore, the signal search is conducted only in the region $m_{\mathrm{jj}} > 1.3$ TeV despite the whole region, $m_{\mathrm{jj}} > 730$ GeV, being considered in the FD. The lower m_{jj} region is used as a sideband.

VI. SYSTEMATIC UNCERTAINTIES

The main systematic uncertainties in the simulated signal samples consist of those associated with the modeling of the jet energy scale (JES), the jet energy resolution (JER) and the b-tagging efficiency. JES and JER variations are applied to the signals to obtain varied signal templates. They are estimated using jets in $\sqrt{s} = 13$ TeV data and simulation in various methods [45]. The impact of these uncertainties on the expected number of signal events across the whole m_{jj} range is 24%–30% (35%–40%) from JES (JER) variations. The systematic uncertainty of the b-tagging efficiency is measured using data enriched in $t\bar{t}$ events for jet $p_{\mathrm{T}} < 400$ GeV and extrapolated to higher p_{T} regions using a method similar to the one described in Ref. [54]. This uncertainty ranges from 12% to 20% depending on the reconstructed signal mass. A luminosity uncertainty of 2.4% [39] is applied to the normalization of the signal samples.

The background modeling uncertainties come from both the statistical uncertainty in the fit parameters, referred to as the fit parameter uncertainty, and the biases introduced by the fit model itself. The fit parameter uncertainty is evaluated by propagating the covariance matrix returned by the fit to each m_{jj} bin, giving an uncertainty ranging from 2% to 5% relative to the background estimate. The biases from the fit model are evaluated with pseudoexperiments using signal-injected pseudodata samples, quantifying how much the background estimate is biased by injected signal events in the spectrum that are not able to create significant excesses. The number of signal events injected corresponds to the mean of the expected limits obtained for each signal hypothesis when background-only pseudodata samples are considered. The background estimate is increased by 5% to 40% at the injected signal mass point compared to the nominal case. This is referred to as the fit bias uncertainty.

The fit model may not describe the background perfectly, so that signal-like features can arise in data relative to the fit even if there are no signal events in data, introducing spurious signals. A spurious-signal uncertainty is included to address this. It is evaluated using pseudoexperiments, for each of which a fixed background template, obtained from an FD fit to the background-only pseudodata sample, and the signal templates have their normalizations fitted to the background-only m_{jj} spectrum in the manner described in Sec. VII, and the obtained number of signal events is taken as the spurious signal. It is measured for each signal mass point and a smooth envelope is constructed following the method described in Ref. [50]. The size of this uncertainty relative to the background estimate increases from 0.5% at 1.3 TeV to 14% at 3.0 TeV.

VII. RESULTS AND INTERPRETATION

The BumpHunter algorithm is adopted to quantify the statistical significance of any localized excess in the binned m_{jj} distribution. It calculates the significance of any excess found in continuous intervals in all possible locations. The search window has a width ranging from two bins up to half of the full m_{jj} distribution. In each window it evaluates the significance of the discrepancy between the data and the background yield. The most significant interval is the set of bins with the smallest probability of arising from background fluctuations. A p-value is reported by BumpHunter, corresponding to the probability of random fluctuations in the background-only hypothesis creating an excess at least as significant as the one observed anywhere in the spectrum. This is obtained by performing a series of pseudoexperiments constructed from the background estimate so that the look-elsewhere effect [55] is taken into account.

Three moments are used ($N = 3$) after applying the optimization procedure described in Sec. V. The corresponding fit describes the data very well across the entire m_{jj} region, obtaining $\chi^2/\mathrm{nDoF} = 0.72$ and a χ^2 p-value of 0.89 [56]. BumpHunter reports a p-value of 0.55 after scanning the m_{jj} range starting at 1.3 TeV with the most significant interval found to be [1.92, 2.11] TeV, as shown in Fig. 3.

A binned likelihood is constructed with the signal templates obtained from simulation and the background template given by FD. The likelihood function, $\mathcal{L}(\mu, \vec{\theta})$, is a product of Poisson probability terms over all the m_{jj} bins, where the parameter of interest, μ, is defined as the cross section, $\sigma(pp \to b\bar{b}Z')$, times the branching ratio, $B(Z' \to b\bar{b})$, of the LUV Z' boson, and a set of nuisance parameters (NPs), $\vec{\theta}$, is used to encode systematic uncertainties in the signal and background expectations. The background normalization and shape are estimated by FD prior to the likelihood fit, and corresponding uncertainties are included as NPs in the likelihood function. The NPs allow variations of the expectations for signal and background according to the systematic uncertainties, subject to Gaussian constraints in the likelihood fit. The maximum-likelihood fit to the observed m_{jj} spectrum is performed independently for each LUV Z' boson mass hypothesis with the starting point of the m_{jj} spectrum set to 1 TeV so that the majority of signal events are included.

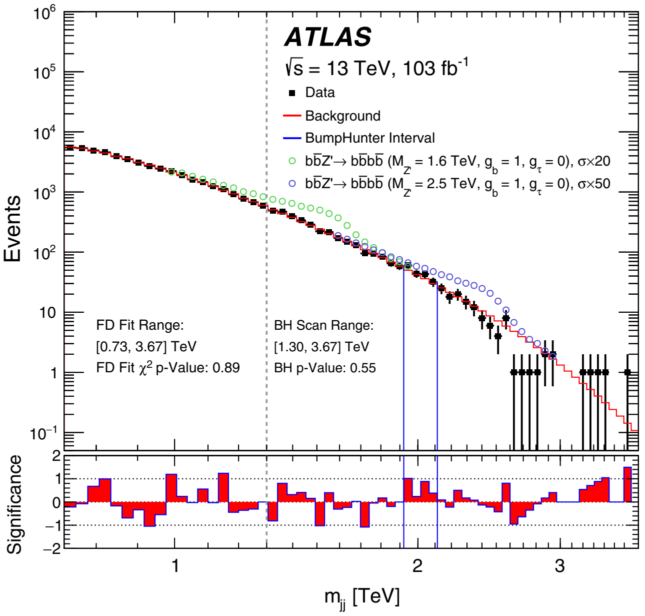

FIG. 3. Background estimate from the FD method with $N = 3$ and data in the SR. The solid squares show the m_{jj} spectrum in data and the solid curve is the background estimated by the FD method. The BumpHunter algorithm scans the m_{jj} region above 1.3 TeV as indicated by the vertical dashed line. The vertical solid lines refer to the boundaries of the most significant interval flagged by BumpHunter; this is found to be [1.92, 2.11] TeV for which the p-value is stated in the figure. Open squares (circles) are the signal distributions of the 1.6 (2.5) TeV LUV Z' boson on top of the data with the cross sections inflated by a factor of 20 (50). The lower panel shows the significance calculated using the background estimate and data. The significance is defined as $(d_i - b_i)/\delta$, where d_i refers to the data count while b_i refers to the background estimate, and δ is an uncertainty taking both the uncertainty on the data count and background estimate into account [57].

Since the observed data are consistent with the smoothly falling background expectation, upper limits on the production cross section of the LUV Z' model are obtained at 95% confidence level (CL) using the $\mathrm{CL_s}$ [58–60] method. Various signal mass hypothesis tests and $\mathrm{CL_s}$ values are calculated using a frequentist framework, HistFitter [61], which is an interface to the RooFit package [62], with a profile likelihood ratio, $q_\mu = -2\ln(\mathcal{L}(\mu, \hat{\hat{\vec{\theta}}}_\mu)/\mathcal{L}(\hat{\mu}, \hat{\vec{\theta}}_{\hat{\mu}}))$, as the test statistic. The values of $\hat{\mu}$ and $\hat{\vec{\theta}}_{\hat{\mu}}$ maximize the likelihood function, while $\hat{\hat{\vec{\theta}}}_\mu$ maximizes the likelihood function for a given value of μ. For each signal mass hypothesis, a $\mathrm{CL_s}$ value is evaluated using the asymptotic formula [58]. The predicted LUV Z' boson production cross sections times the branching ratio to $b\bar{b}$ are overlaid in Fig. 4. At 3 TeV, where the number of events is small, the results from pseudoexperiments are consistent with the ones using the asymptotic formula. The difference in the mean is at the few-percent level and that in the uncertainty band is about 10%. A coverage test using an ensemble of pseudodata samples is performed to validate the overall implementation of systematic uncertainties. When signal events are injected with a strength corresponding to the mean cross section excluded at 95% CL obtained by considering the background-only pseudodata samples,

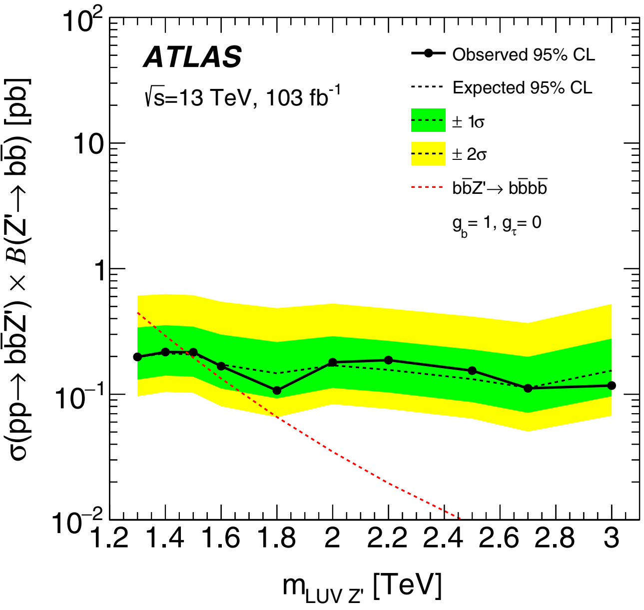

FIG. 4. The observed (solid) and expected (dashed) 95% CL upper limits on the production of $Z' \to b\bar{b}$ in association with b-quarks. The bands surrounding the expected limit show the 68% and 95% confidence intervals. The predicted cross sections of the LUV Z' model times the branching ratio to $b\bar{b}$, with g_b set to unity and g_τ set to zero, calculated at LO with MadGraph5_aMC@NLO, are also overlaid.

the probability of excluding the given signal is less than 5% for a range of signal masses spanning 1.3–3 TeV. An additional cross-check is performed to validate the robustness of the complete analysis procedure against possible signal contamination. This cross-check, which considers two LUV Z' masses (1.3 TeV and 3 TeV), is carried out by subtracting signal events corresponding to the expected limit from data, and creating a new set of pseudodata samples using the signal-subtracted data. The allowed range of N for FD and the uncertainties associated with FD, such as the fit parameter uncertainty, spurious signal uncertainty and the fit bias uncertainty, are rederived and then applied in the statistical analysis of the original data. The resulting limits on N are the same as the ones obtained in Sec. V and the expected and observed limits are shifted by less than 2% compared to the nominal result.

VIII. CONCLUSION

A search for new heavy particles in the final state with the two leading jets b-tagged and at least one additional b-tagged jet among the third and fourth jets is performed in a previously uncovered m_{jj} region using 103 fb^{-1} of pp collision data recorded at $\sqrt{s} = 13$ TeV with the ATLAS detector at the LHC during 2017 and 2018. The m_{jj} spectrum of the two leading b-tagged jets is analyzed with an innovative background estimation method, functional decomposition, utilizing a truncated series. The observed data are compatible with the hypothesis of a smoothly falling background within the m_{jj} region from 1.3 to 3.6 TeV. Upper limits on the production of lepton-universality-violating Z' bosons times the branching ratio to $b\bar{b}$ are derived, and exclude such Z' bosons with masses between 1.3 and 1.45 TeV at 95% CL.

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