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Authors
Aaboud, M
Aad, G
Abbott, B
et al.

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A search for resonances decaying into a Higgs boson and a new particle $X$ in the $XH \rightarrow q\bar{q}b\bar{b}$ final state with the ATLAS detector

The ATLAS Collaboration

A search for heavy resonances decaying into a Higgs boson ($H$) and a new particle ($X$) is reported, utilizing 36.1 fb$^{-1}$ of proton–proton collision data at $\sqrt{s} = 13$ TeV collected during 2015 and 2016 with the ATLAS detector at the CERN Large Hadron Collider. The particle $X$ is assumed to decay to a pair of light quarks, and the fully hadronic final state $XH \rightarrow q\bar{q}b\bar{b}$ is analysed. The search considers the regime of high $XH$ resonance masses, where the $X$ and $H$ bosons are both highly Lorentz-boosted and are each reconstructed using a single jet with large radius parameter. A two-dimensional phase space of $XH$ mass versus $X$ mass is scanned for evidence of a signal, over a range of $XH$ resonance mass values between 1 TeV and 4 TeV, and for $X$ particles with masses from 50 GeV to 1000 GeV. All search results are consistent with the expectations for the background due to Standard Model processes, and 95% CL upper limits are set, as a function of $XH$ and $X$ masses, on the production cross-section of the $XH \rightarrow q\bar{q}b\bar{b}$ resonance.
1 Introduction

The Standard Model (SM), including the recently discovered Higgs boson [1, 2], describes collider phenomenology for energy scales up to a few hundred GeV. However, a number of issues with the SM, including sensitivity of the Higgs boson mass to radiative corrections, indicate either extreme fine-tuning or the presence of new physics at an energy scale not far above the Higgs boson mass. Many theoretical extensions to the SM predict the existence of new particles around the TeV scale, and it is natural to expect such particles to exhibit significant coupling to the Higgs boson ($H$). Examples of previous studies at the CERN Large Hadron Collider (LHC) which are motivated by these considerations include ATLAS [3, 4] and CMS [5–8] searches for new resonances decaying into $VH$, where $V$ denotes a $W$ or $Z$ boson, as well as ATLAS [9] and CMS [10, 11] searches for resonances decaying into $HH$.

This Letter presents a new and more general search for heavy resonances which decay into the SM Higgs boson and a new particle ($X$), utilizing a data sample corresponding to 36.1 fb$^{-1}$ of proton–proton ($pp$) collisions at $\sqrt{s} = 13$ TeV collected during 2015 and 2016 with the ATLAS detector. Since the hypothetical particle $X$ has not yet been detected, it has unknown properties. It is assumed that $X$ decays hadronically into a pair of light quarks, $X \rightarrow q\bar{q}'$, and has a natural width which is narrow compared to the detector resolution. It is also assumed that single $X$ production is sufficiently rare that it has not been observed by analyses such as the ATLAS and CMS searches for dijet resonances [12–14].

Examples of theories of physics beyond the SM which predict the existence of $XH$ resonances include pseudo Nambu–Goldstone models [15], extended Higgs sectors [16] and extra-dimension frameworks with warped compactifications [17]. For simplicity, such $XH$ resonances are hereafter denoted by $Y$. It is assumed that the new resonance $Y$ is narrow. This study analyses the decay chain $Y \rightarrow XH \rightarrow q\bar{q}'b\bar{b}$, and considers the regime of high $Y$ masses, in the range between 1 TeV and 4 TeV, with $m(Y) \gg m(X)$, which implies that the $X$ and $H$ bosons are both highly Lorentz-boosted. The $X$ and $H$ boson candidates are each reconstructed in a single jet with large radius parameter; these jets are called “large-$R$ jets” throughout this Letter and are denoted by $J$. Jet substructure techniques and $b$-tagging are used to suppress the dominant background from multijet events, to enhance the sensitivity to the dominant $H \rightarrow b\bar{b}$ decay mode, and to distinguish between the two bosons.

Given their assumed decay modes, both $X$ and $Y$ must be bosons. However, the search does not impose explicit requirements on their electric charge, spin or polarization states, and utilizes a simple event selection that does not seek to exploit angular correlations or other variables that would be sensitive to particular spin states. The analysis utilizes the reconstructed $Y$ mass as the final discriminant, searching for an excess due to a resonance in the $Y \rightarrow XH \rightarrow JJ$ mass distribution, separately in a large number of overlapping ranges of $X$ mass.

A modified form of the benchmark heavy vector triplet (HVT) model [18, 19] is used to provide a measure of the implications of the results of the search within one particular theoretical framework. The HVT model provides a simplified phenomenological Lagrangian that predicts heavy spin-1 resonances which are produced via $q\bar{q}$ annihilation, and which can have significant branching ratios for decays into boson pairs, with longitudinally polarized bosons. The search results are used to set limits on the production cross-section $\sigma(pp \rightarrow Y \rightarrow XH \rightarrow q\bar{q}'b\bar{b})$ within the HVT theoretical framework, to provide an interpretation in the case where both $X$ and $Y$ have spin 1. The search overlaps with the $VH$ and $HH$ searches, when the $X$ mass window extends around the $V$ and $H$ mass values, respectively, in which cases the results are found to be compatible with those analyses. However, the current search considers a much wider range of $X$ masses, from 50 GeV to 1000 GeV.
2 ATLAS detector

The ATLAS detector [20] is a general-purpose particle physics detector used to investigate a broad range of physics processes. ATLAS includes an inner detector (ID) surrounded by a superconducting solenoid, electromagnetic (EM) and hadronic calorimeters, and a muon spectrometer (MS). The ID consists of a silicon pixel detector, including the insertable B-layer [21] installed after Run 1 of the LHC, a silicon microstrip detector and a straw-tube tracker. The ID is immersed inside a 2 T axial magnetic field from the solenoid and provides precision tracking of charged particles with pseudorapidity $|\eta| < 2.5$. The straw-tube tracker also provides transition radiation measurements for electron identification. The calorimeter system consists of finely segmented sampling calorimeters using lead/liquid-argon for the detection of EM showers up to $|\eta| = 3.2$, and copper or tungsten/liquid-argon for hadronic showers for $1.5 < |\eta| < 4.9$. In the central region ($|\eta| < 1.7$), a steel/scintillator hadronic calorimeter is used. Outside the calorimeters, the MS incorporates multiple layers of trigger and tracking chambers within a magnetic field produced by a system of superconducting toroids, enabling an independent precise measurement of muon track momenta for $|\eta| < 2.7$. The ATLAS detector has a two-level trigger system. The first-level (L1) trigger is implemented in hardware and uses the calorimeter and muon systems to reduce the accepted event rate to 100 kHz. The L1 trigger is followed by a software-based high-level trigger to reduce the accepted event rate to approximately 1 kHz for offline analysis [22].

3 Signal and background simulation

Samples of simulated signal and background events are used to optimize the event selection and to estimate the background contributions from various SM processes.

The $Y \to XH$ signal was simulated by modifying the HVT [18, 19] configuration for $W' \to WH$ decays, replacing the $W'$ boson with a narrow resonance $Y$, and the $W$ boson by $X$. The new $X$ boson was assumed to have spin 1, a natural width of 2 GeV, and a branching ratio (B) of 100% for decays $X \to u\bar{d}$. The properties of the Higgs boson were assumed to be as described in the SM, with its mass set to 125.5 GeV and decays into $b\bar{b}$ and $c\bar{c}$ enabled in the simulation. Given the SM branching ratios and the relevant experimental performance factors, Higgs boson decays to $b\bar{b}$ dominate the signal efficiency. The signal samples were generated with Madgraph5_aMC@NLO 2.2.2 [23] interfaced to Pythia 8.186 [24] for parton shower and hadronization, with the NNPDF2.3 next-to-leading-order (NLO) parton distribution function (PDF) set [25] and the ATLAS A14 set of tuned parameters (tune) [26] for the underlying event. Approximately 100 signal samples were generated, each with individual values of $Y$ and $X$ masses, chosen in a two-dimensional grid of values ranging from 1 TeV to 4 TeV for $m(Y)$ and from 50 GeV to 1000 GeV for $m(X)$. The requirements $m(Y) > 1$ TeV and $m(Y) \gg m(X)$ were applied, to focus on the kinematic regime where the $X$ and $H$ bosons are highly Lorentz-boosted.

The dominant SM background is due to multijet processes and, as described in Section 7, is evaluated using data-driven techniques. Some cross-checks were performed using simulated multijet events generated with Pythia 8.186, with the NNPDF2.3 NLO PDF and the ATLAS A14 tune.
Minor background contributions, which are estimated using simulated samples, are due to $t\bar{t}$ production and to vector boson production in association with jets (V+jets). The $t\bar{t}$ samples were generated with POWHEG Box v2 [27] with the CT10 PDF set [28], interfaced with PYTHIA 6.428 [29] and the Perugia 2012 tune for the parton shower [30] using the CTEQ6L1 PDF set [31]. The cross-section of the $t\bar{t}$ process was normalized to the result of a QCD calculation at next-to-next-leading order and next-to-next-leading logarithmic accuracy (NNLO+NNLL), as implemented in Top++ 2.0 [32]. The V+jets background samples were generated with SHHERPA 2.1.1 [33] interfaced with the CT10 PDF set, including only hadronic V decays. Matrix elements of up to four extra partons were calculated at leading order in QCD. The V+jets events are normalized to the NNLO cross-sections [34].

For all simulated samples except those produced using SHHERPA, EVTGEN v1.2.0 [35] was used to model the properties of bottom and charm hadron decays. The effect of multiple $pp$ interactions in the same and neighbouring bunch crossings (pile-up) was included by overlaying minimum-bias events simulated with PYTHIA 8.186 on each generated event [36]. The detector response was simulated with a GEANT4 [37] based framework [38] and the events were processed with the same reconstruction software as that used for data.

4 Event reconstruction

The reconstruction and identification of hadronically decaying bosons is performed using jets. Large-$R$ jets are reconstructed with the anti-$k_t$ algorithm [39, 40] with radius parameter $R = 1.0$ from three-dimensional topological clusters of energy deposits in the calorimeter [41]. The large-$R$ jets are required to have transverse momentum $p_T > 250$ GeV and $|\eta| < 2.0$.

Track-jets are formed from charged-particle tracks with $p_T > 0.4$ GeV and $|\eta| < 2.5$ that satisfy a set of hit and impact parameter criteria to reduce the contamination from pile-up interactions, and are clustered using the anti-$k_t$ algorithm with $R = 0.2$ [42]. Only track-jets with $p_T > 25$ GeV that are constructed from at least two tracks are considered in this analysis.

To mitigate pile-up effects and soft radiation, the large-$R$ jets are trimmed [43], and then are subsequently reclustered into subjets using the $k_t$ algorithm [44]. To compensate for the limited angular resolution of the calorimeter, the mass of large-$R$ jets is computed using a combination of calorimeter and tracking information [45]. The combined jet mass is defined as

$$m_J \equiv w_{\text{calo}} m_{\text{calo}}^J + w_{\text{track}} \left( m_{\text{track}}^J \frac{P_T^{\text{calo}}}{P_T^{\text{track}}} \right),$$

where $m_{\text{calo}}^J$ is the calorimeter-only estimate of the jet mass. The variable $m_{\text{track}}^J$ is the jet mass estimated via tracks with $p_T > 0.4$ GeV associated with the large-$R$ jet using “ghost association” [39], and is scaled in the combined mass formula by the ratio of calorimeter to track $p_T$ estimates in order to account for the missing neutral-particle component in the track-jet. The ghost association technique relies on repeating the jet clustering process with the addition of measured tracks that have the same direction but infinitesimally small $p_T$, so that the jet properties remain unaffected. A track is associated with a jet if it is contained in the jet after this re-clustering procedure. The weighting factors $w_{\text{calo}}$ and $w_{\text{track}}$ depend on $p_T$ so that $w_{\text{calo}} + w_{\text{track}} = 1$, and are used to optimize the combined mass resolution. To partially account for the energy carried by muons from semileptonic $b$-hadron decays, the four-momentum of the closest muon candidate satisfying “Tight” muon identification criteria [46] with $p_T > 4$ GeV and $|\eta| < 2.5$ that
is within $\Delta R = 0.2$ of a track-jet that is $b$-tagged is added to the calorimeter jet four-momentum \cite{47}. In this study, only large-$R$ jets with $m_J > 50$ GeV are considered for further analysis.

Identifying a large-$R$ jet as a hadronically decaying Higgs boson candidate is aided by using track-jets matched via ghost association to the large-$R$ jet \cite{48}. The identification of $b$-hadrons relies on a multivariate $b$-tagging algorithm \cite{49} applied to a set of tracks in a region of interest around each track-jet axis. The $b$-tagging requirements result in an efficiency of 77% for track-jets containing $b$-hadrons, and the misidentification rate is $\sim 2\%$ ($\sim 24\%$) for light-flavour (charm) jets. These were determined in a sample of simulated $t\bar{t}$ events. For simulated samples the $b$-tagging efficiencies are corrected, based on the jet $p_T$, to match those measured in data \cite{50}.

Identifying a large-$R$ jet as a hadronically decaying $X \to q\bar{q}'$ boson candidate is aided by using jet substructure techniques. The variable $D_2$ is defined\footnote{The angular exponent $\beta$, defined in Ref. \cite{51}, is set to unity.} as a ratio of two- and three-point energy correlation functions \cite{51, 52}, which are based on the energies and pairwise angular distances of particles within a jet. This variable is optimized \cite{53} to distinguish between jets originating from a single parton and those from the two-body decay of a heavy particle. A detailed description of the optimization, performed using simulated $V$ decays, can be found in Refs. \cite{54, 55}. Studies of boosted $W$ boson decays \cite{54} demonstrate that the $D_2$ variable is well modeled, with good agreement observed between data and simulation.

“Loose” electrons and muons are reconstructed and identified as described in Refs. \cite{46, 56}. These leptons have $p_T > 7$ GeV, $|\eta| < 2.5$ (2.47) for muons (electrons), $|d_0|/\sigma_{d_0} < 3$ (5) and $|z_0 \sin \theta| < 0.5$ mm, where $d_0$ is transverse impact parameter with respect to the beam line, $\sigma_{d_0}$ is the corresponding uncertainty, and $z_0$ is the distance between the longitudinal position of the track along the beam line at the point where $d_0$ is measured and the longitudinal position of the primary vertex. An isolation criterion is also applied. Specifically, within a cone of size $\Delta R = 0.2$ (0.3) around an electron (muon), the scalar sum of transverse momenta of tracks divided by the lepton $p_T$ is required to be less than a cut-off value, chosen to provide a constant efficiency of around 99% as a function of $p_T$ and $|\eta|$.

5 Event selection

Events are selected from the 2015 (2016) running period using a trigger that requires a single large-$R$ jet with $p_T > 360$ (420) GeV. Selected events are required to have at least one primary vertex (PV) that has at least two associated tracks, each with transverse momentum $p_T > 0.4$ GeV. For events with more than one PV candidate, the one with the largest track $\sum p_T$ is chosen as the hard-scatter PV. To select a hadronic final state, events with one or more “Loose” charged leptons (electrons or muons) are vetoed.

Events are kept only if they contain at least two large-$R$ jets. For events with more than two large-$R$ jets, only the two “leading” jets, namely those with highest $p_T$, are considered as possible $X$ and $H$ candidates. To ensure high and uniform trigger efficiency, the leading large-$R$ jet must satisfy $p_T > 450$ GeV.

Additional requirements are imposed to distinguish hadronically decaying boson candidates from background jets. To be identified as a Higgs jet candidate, the combined mass of the jet is required to satisfy $75$ GeV < $m_J$ < $145$ GeV, a criterion that is $\sim 90\%$ efficient for Higgs boson jets. The number of $b$-tagged jets inside the Higgs jet is used to categorize the events in two orthogonal signal regions: the “1-tag” signal region (SR1) and “2-tag” signal region (SR2) definitions require Higgs candidates to contain exactly one and two $b$-tagged jets, respectively. The SR1 region recovers some efficiency loss in the high
$Y$ mass region where the angular separation between the two $b$-quarks from the Higgs decay is small and the fragmentation products are merged [47]. As depicted in Fig. 1 and described in Section 7, a number of different samples of events are selected to be used as part of the background estimation strategy. These samples include events with the Higgs jet candidate with a mass in the so-called “high sideband” (HSB) region with $145 \text{ GeV} < m_J < 200 \text{ GeV}$, as well as events in a “low sideband” (LSB) region with $50 \text{ GeV} < m_J < 75 \text{ GeV}$. In addition, “0-tag” samples, with Higgs candidates that pass these various mass requirements but have no associated $b$-tagged jets, are also selected. The 0-tag sideband samples are denoted by LSB0 and HSB0. The 0-tag sample satisfying the SR mass cut is denoted by CR0 to emphasize its use as a control region in the background determination (see Section 7), rather than as an additional signal region.

![Figure 1: Illustration of the definitions of the various mutually exclusive data regions. The data are divided into Low Sidebands (LSB), Signal Regions (SR), and High Sidebands (HSB) according to the mass of the candidate Higgs jet. Each region is subdivided further according to the number of $b$-tagged jets associated with the candidate Higgs jet. The 0-tag sample satisfying the SR mass cut is denoted by CR0 to emphasize its use as a control region in the background determination, rather than as an additional signal region.](image)

If both large-$R$ jets fulfill the Higgs mass requirement, the jet with the highest number of associated $b$-tagged jets is chosen as the Higgs candidate. In case both have the same number of $b$-tagged jets, the ambiguity is resolved by assigning the leading $p_T$ large-$R$ jet as the Higgs candidate. Studies of signal samples with $m(X) = 110 \text{ GeV}$ demonstrate that, in the lower $m(Y)$ region, the probability to correctly identify the $H$ and $X$ jets is 98.8%. This value decreases to 89.5% for $m(Y) = 4 \text{ TeV}$, due to the falling efficiency in the very high mass region to tag two separate $b$-tagged jets within the $H$ jet.

The large-$R$ jet which is not chosen as the Higgs candidate is assigned to the $X$ hypothesis. The jet substructure variable $D_2$, described previously, is used to check whether the $X$ candidate jet is compatible with the two-prong structure expected due to its assumed $X \rightarrow q\bar{q}'$ decay. The requirement on the value of $D_2$ corresponds to that defined in Refs. [54, 55] to provide a constant efficiency of 50% for selecting hadronic $V$ decays, when applied along with an associated requirement that $m_J$ lies within a window around the $V$ mass. Given that the $X$ mass is a priori unknown, the event selection does not make any requirement on the mass of the $X$ candidate jet beyond the $m_J > 50 \text{ GeV}$ restriction applied to all large-$R$ jets, however the data are interpreted in windows of $m_X$.

The mass of the $Y \rightarrow XH$ candidate is required to be larger than 1 TeV. The efficiencies for the 1-tag and 2-tag signal region selections are presented as a function of $m(Y)$ and $m(X)$ in Fig. 2 for the various signal samples. No signal samples with $m(Y) > 4 \text{ TeV}$ were simulated, due to the low expected sensitivity for
such high masses with the current data sample. However, data events with higher reconstructed \( Y \) mass values are included in the overflow bin in the mass distributions.

\[
m(X) \ 	ext{[GeV]} \quad m(Y) \ 	ext{[TeV]} \quad m(X) \ 	ext{[GeV]} \quad m(Y) \ 	ext{[TeV]}
\]

\[
\begin{array}{cccccccc}
1.0 & 1.5 & 2.0 & 2.5 & 3.0 & 3.5 & 4.0 \\
0 & 200 & 400 & 600 & 800 & 1000 & \\
\end{array}
\]

\text{(a) ATLAS Simulation (b) ATLAS Simulation}

Figure 2: Efficiencies, as a function of \( m(Y) \) and \( m(X) \) for all the generated signal samples, for the selection defining (a) the 1-tag signal region (SR1) and (b) the 2-tag signal region (SR2).

6 Signal modelling

The signal search in the two-dimensional space of \( m(Y) \) versus \( m(X) \) employs a sliding-window technique to the \( m_J \) spectrum of the \( X \) candidate jet, dividing the data into a series of overlapping \( m_J \) ranges. As described in Section 9, for each \( m_J \) window of the \( X \) candidate jet, the corresponding \( m_{JJ} \) distribution is examined for evidence of an excess due to a signal, where \( m_{JJ} \) denotes the invariant mass of the system formed by the \( H \) and \( X \) candidate large-\( R \) jets.

The reconstructed \( X \) mass resolution varies from 12 GeV to 40 GeV. The widths of the overlapping \( m_J \) windows for the \( X \) candidate jet are chosen to be around twice the \( X \) mass resolution, but also take into account the limited number of data events. The central values of neighbouring \( m_J \) windows are shifted by roughly half of the \( X \) mass resolution, ensuring that they overlap and do not leave gaps in the search coverage. Studies in which simulated signals were injected at various mass values were used to demonstrate the reasonableness of the window choices.

The reconstructed \( Y \to XH \) mass resolution varies from about 65 GeV to 100 GeV. For each \( m_J \) window of the \( X \) candidate jet, the binning for the corresponding \( m_{JJ} \) distribution is chosen to be at least as large as the \( Y \) mass resolution, dependent on the size of the data sample.

Given the large number of possible \( m(Y) \) and \( m(X) \) values in the ranges considered, a parameterization of the signal is used to interpolate between the mass values for which signal samples were generated. Probability distribution functions for the \( m_{JJ} \) and \( m_J \) shapes are built using the RooKeysPdf class of the RooFit package [57]. Multidimensional morphing methods, implemented in the RooMomentMorphND
class [58], are subsequently applied to parameterize grid points using the surrounding four nearby points. The normalization of the parameterized signals is estimated using linear interpolation.

7 Background Estimation

After the event selection, over 96% of the SM background originates from multijet processes. A data-driven method is used to determine the shape of the dominant multijet background, with its normalization in the signal regions being determined with the fit procedure described in Section 9. The small additional background contributions from $t\bar{t}$ and $V$+jets production are estimated via simulation. The background determination is performed separately in each of the $m_J$ windows considered for the $X$ candidate jet mass.

As depicted in Fig. 1, the event sample, before any specific requirements are made on the mass of the $X$ candidate jet, is separated into mutually exclusive categories according to the mass and number of $b$-tagged jets of the Higgs boson candidate. The SR1 and SR2 regions are used to perform the signal search, while the other seven regions are used as control regions to develop and validate the background model. The multijet background component in each of the seven control regions is determined by subtracting from the data the $t\bar{t}$ and $V$+jets contributions predicted by simulation.

The modelling of the dominant multijet background in the SR1 and SR2 signal regions starts from the CR0 sample, for which the candidate Higgs jet satisfies the SR requirement on the jet mass but has no associated $b$-tagged jets. The CR0 sample should contain negligible signal contamination. The basic strategy is to use events in the CR0 sample with at least one (two) track-jet(s) associated with the Higgs jet to model the shape of the multijet background in the SR1 (SR2) signal region. However, sources of possible differences between the multijet components of CR0 versus SR1 and SR2 include changes in the underlying event populations due to the absence or presence of $b$-quarks as well as kinematic differences arising from the application of $b$-tagging, since the $b$-tagging efficiency depends on the $p_T$ and $\eta$ of the track-jet. The corrections required to take these differences into account are extracted from the HSB events.

In each of the HSB regions with different number of $b$-tags (HSB0, HSB1, HSB2), a pair of two-dimensional histograms is filled, one of $p_T$ versus $\eta$ for the leading track-jet, and the other for the subleading track-jet. Subsequently, leading and subleading track jet reweighting maps are created by dividing the HSB1 and HSB2 histograms by the corresponding HSB0 histogram. A Gaussian kernel, similar to that applied in Ref. [59], is used to smooth out statistical fluctuations by taking a weighted sum of neighbouring bins. The weight is inversely proportional to the width of the Gaussian kernel and depends on the statistical uncertainty of each bin. The result is a reduction of statistical fluctuations, while adding negligible bias to the distributions.

To describe the SR multijet background shapes, the CR0 events are reweighted using the maps in bins of track-jet $p_T$ and $\eta$ extracted from the sideband. The reweighting is performed only for the 2-tag samples, as the modelling of the shape of the multijet background in the 1-tag sideband regions without reweighting is observed to be adequate. Due to the correlations between the kinematic variables of the two leading track-jets used for the reweighting, multiple reweighting iterations are performed, until the track-jet properties, $p_T$ and $\eta$, are matched within statistical uncertainties.

The background modelling is validated by using the same method to predict the background in the LSB regions in the low mass sidebands, and then comparing with the data and obtaining good agreement.
Agreement is also confirmed in the signal region by integrating over all values of the mass of the $X$ candidate jet, thereby diluting any possible signal contamination to a negligible level.

8 Systematic uncertainties

The main systematic uncertainty in the background estimate arises from the potential mis-modelling of the background processes. As described in Section 7, the multijet background shapes in the two signal regions are estimated directly from data using sideband regions. To determine the systematic uncertainty in this method, the multijet background shapes in the HSB1 and HSB2 regions are compared, in each $m_J$ window of the $X$ candidate jet, to those of the reweighted HSB0 multijet distributions. The differences, in bins of $m_{JJ}$, fitted with a line are used as the multijet modelling systematic uncertainties. The largest observed shape difference is found to be approximately 12%, while the smallest is 3%. A normalization uncertainty of 30% is assigned to the small $t\bar{t}$ background, based on the ATLAS $t\bar{t}$ differential cross-section measurement [60]. The same uncertainty is conservatively applied to the small $V+$jets background component.

The uncertainty in the combined 2015+2016 integrated luminosity is 2.1%. It is derived, following a methodology similar to that detailed in Ref. [61], from a calibration of the luminosity scale using $x$–$y$ beam–separation scans performed in August 2015 and May 2016. This uncertainty is applied to the yields of both the signal and the small $t\bar{t}$ and $V+$jets backgrounds, which are not determined from data.

Additional systematic uncertainties in the signal acceptance arise from the choice of PDF set and the uncertainty in the amount of initial- and final-state radiation. For all the two-dimensional mass grid points, a constant 5% uncertainty is applied and covers both effects.

Uncertainties related to the signal parameterization method are estimated by comparing the mass distributions of generated signal points to those predicted from morphing nearby points in the two-dimensional space of $m(Y)$ versus $m(X)$. The largest observed normalization deviation is $\sim$8%, while differences in the signal shape also reach levels up to $\sim$8%. Both effects are included as uniform uncorrelated systematic uncertainties.

Systematic uncertainties which account for experimental effects on the signal shape include the large-$R$ jet mass scale and mass resolution, as well as $D_2$ and the $b$-tagging. The impact of each of these effects is evaluated by shifting each variable according to these systematic uncertainties and then re-performing the signal parameterization. Based on the measurements documented in Refs. [55, 62], a 2% uncertainty is assigned for the large-$R$ jets $p_T$ scale, while uncertainties of 20% and 15%, respectively, are assigned for the large-$R$ jet mass resolution and $D_2$ resolution. Uncertainties in the correction factors for the $b$-tagging are applied to the simulated event samples by looking at dedicated flavour-enriched samples in data. An additional term is included to extrapolate the measured uncertainties to the high-$p_T$ region of interest.

This term is calculated from simulated events by considering variations of the quantities affecting the $b$-tagging performance such as the impact parameter resolution, percentage of poorly measured tracks, description of the detector material, and track multiplicity per jet. The dominant effect on the uncertainty when extrapolating to high $p_T$ is related to the change in tagging efficiency when smearing the track impact parameters based on the resolution measured in data and simulation. The uncertainty in the $b$-tagging efficiency is measured as a function of $b$-jet $p_T$ and $\eta$ for track-jets with $p_T < 250$ GeV while for higher $p_T$ values it is extrapolated using simulation [50]. These uncertainties vary between 2% and 8% in the lower $p_T$ range, and rise to approximately 9% for track-jets with $p_T > 400$ GeV.
9 Statistical treatment and results

The signal search in the two-dimensional space of \( m(Y) \) versus \( m(X) \) is performed by applying a sliding-window technique to the \( m_{\ell} \) spectrum of the \( X \) candidate jet, which divides the data into a series of overlapping \( m_{\ell} \) ranges. For each \( m_{\ell} \) window, a binned maximum-likelihood fit is then performed to the resultant \( m_{\ell \ell} \) distributions in both SR1 and SR2 signal regions simultaneously. A test statistic based on the profile likelihood ratio [63] is used to test hypothesized values of the global signal strength (\( \mu \)), corresponding to the HVT model. The systematic uncertainties, described previously, are modelled with Gaussian or log-normal constraint terms (nuisance parameters) in the definition of the likelihood function.

Each \( m_{\ell} \) window of the \( X \) candidate jet is fitted independently, but as the mass ranges overlap, the fit results are correlated. In each fit, the normalizations of the multijet backgrounds in the SR1 and SR2 signal regions are treated as free parameters. All of the systematic uncertainties are treated as correlated between the two signal regions.

The data distributions and fit results are shown for three example \( m_{\ell} \) windows of the \( X \) candidate jet in Fig. 3–5. In each case, the left (right) upper plot shows the \( m_{\ell \ell} \) distribution in the SR1 (SR2) signal region, and the results of the simultaneous fit are superimposed on the plots. Examples of possible signal models are also shown, with arbitrary overall normalization, illustrating the corresponding contributions that would be expected in the SR1 and SR2 regions. The data distributions are well described by the fitted SM background, and there is no significant evidence of a signal. The same conclusion is valid for all \( m_{\ell} \) windows of the \( X \) candidate jet.

The fits to the data are used to set upper limits on the production cross-section, \( \sigma(pp \rightarrow Y \rightarrow XH \rightarrow q\bar{q}'b\bar{b}) \). Exclusion limits are computed using the CL\(_s\) method [64], with a value of \( \mu \) regarded as excluded at the 95% confidence level (CL) when CL\(_s\) is less than 5%. The corresponding limit plots are included in panel (c) of Fig. 3–5.

A summary of the expected and observed 95% CL limits on the production cross-section, \( \sigma(pp \rightarrow Y \rightarrow XH \rightarrow q\bar{q}'b\bar{b}) \), is given in the two-dimensional plane of \( m(Y) \) versus \( m(X) \) in Fig. 6. For \( X \) mass windows around the \( V \) and Higgs boson mass values, the results are found to be compatible with the dedicated ATLAS \( VH \) and \( HH \) searches reported in Refs. [4] and [9], respectively. To visualize both the magnitude and the sign of discrepancies between the expected and observed limits, Fig. 7 presents the differences between the expected and observed limits, expressed in multiples of \( \sigma \), the equivalent Gaussian significance. The maximum observed deviation has a local significance of about 2.5\( \sigma \), corresponding to a global deviation of 1.2\( \sigma \).
Figure 3: The $m_{jj}$ mass distributions in the $m_j$ window of the X candidate jet from 133 GeV to 171 GeV after the likelihood fit for events in (a) the 1-tag signal region (SR1) and (b) the 2-tag signal region (SR2). The highest mass bin includes any overflows. The background expectation is given by the filled histograms and the ratio of the observed data to the background (Data/Bkg) is shown in the lower panel. The uncertainties shown are those after the fit described in the text. One particular example of a possible signal model, namely with $m(X) = 152$ GeV and $m(Y) = 1.8$ TeV, is overlaid with an arbitrary overall normalization, illustrating the corresponding contributions that would be expected in the SR1 and SR2 regions. Panel (c) shows the resultant 95% CL upper limit on the production cross-section, $\sigma(pp \to Y \to XH \to q\bar{q}' b\bar{b})$. 

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Figure 4: The $m_{jj}$ mass distributions in the $m_j$ window of the X candidate jet from 288 GeV to 340 GeV after the likelihood fit for events in (a) the 1-tag signal region (SR1) and (b) the 2-tag signal region (SR2). The highest mass bin includes any overflows. The background expectation is given by the filled histograms and the ratio of the observed data to the background (Data/Bkg) is shown in the lower panel. The uncertainties shown are those after the fit described in the text. One particular example of a possible signal model, namely with $m(X) = 314$ GeV and $m(Y) = 2.3$ TeV, is overlaid with an arbitrary overall normalization, illustrating the corresponding contributions that would be expected in the SR1 and SR2 regions. Panel (c) shows the resultant 95% CL upper limit on the production cross-section, $\sigma(pp \rightarrow Y \rightarrow XH \rightarrow q\bar{q}b\bar{b})$. 
Figure 5: The $m_{JJ}$ mass distributions in the $m_J$ window of the $X$ candidate jet from 500 GeV to 584 GeV after the likelihood fit for events in (a) the 1-tag signal region (SR1) and (b) the 2-tag signal region (SR2). The highest mass bin includes any overflows. The background expectation is given by the filled histograms and the ratio of the observed data to the background (Data/Bkg) is shown in the lower panel. The uncertainties shown are those after the fit described in the text. One particular example of a possible signal model, namely with $m(X) = 542$ GeV and $m(Y) = 2.9$ TeV, is overlaid with an arbitrary overall normalization, illustrating the corresponding contributions that would be expected in the SR1 and SR2 regions. Panel (c) shows the resultant 95% CL upper limit on the production cross-section, $\sigma(pp \rightarrow Y \rightarrow XH \rightarrow q\bar{q}'b\bar{b})$. 
Figure 6: The (a) expected and (b) observed 95% CL limits on the production cross-section $\sigma(pp \to Y \to XH \to q\bar{q}'b\bar{b})$ (z-axis) in the two-dimensional space of $m(Y)$ versus $m(X)$.

Figure 7: Differences between the observed and the expected 95% CL limits on the resonance production cross-section $\sigma(pp \to Y \to XH \to q\bar{q}'b\bar{b})$, expressed in terms of multiples of $\sigma$, the equivalent Gaussian significance.

10 Conclusion

A search for new heavy resonances $Y$ decaying into a Higgs boson and a new particle $X$ was carried out using 36.1 fb$^{-1}$ of $pp$ collision data collected at $\sqrt{s} = 13$ TeV by ATLAS during the 2015 and 2016 runs of the CERN Large Hadron Collider. The $Y \to XH \to q\bar{q}'b\bar{b}$ channel was studied using a generic approach in the topological regime where both bosons are highly Lorentz-boosted, and each is reconstructed as a single jet with a large radius parameter. Jet substructure and $b$-tagging techniques are exploited to tag the $X$ and Higgs bosons and to reduce the dominant multijet background. Values of $Y$ ($X$) mass in the range of 1 TeV to 4 TeV (50 GeV to 1000 GeV) were considered.

A search for evidence of an excess in the $XH$ mass spectrum was made in a large number of overlapping sliding windows in the mass of the $X$ particle. The data are found to be in agreement with the Standard Model background expectations and only small deviations are observed, with local (global) significance of no more than 2.5$\sigma$ (1.2$\sigma$). Within the framework of a modified Heavy Vector Triplet model, upper
limits on the resonance production cross-section $\sigma(pp \rightarrow Y \rightarrow XH \rightarrow q\bar{q}'b\bar{b})$ were set at 95% CL in the two-dimensional space of the $Y$ mass versus the $X$ mass.

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The ATLAS Collaboration

32 CERN, Geneva, Switzerland
33 Enrico Fermi Institute, University of Chicago, Chicago IL, United States of America
34 (a) Departamento de Física, Pontificia Universidad Católica de Chile, Santiago; (b) Departamento de Física, Universidad Técnica Federico Santa María, Valparaíso, Chile
35 (a) Institute of High Energy Physics, Chinese Academy of Sciences, Beijing; (b) Department of Physics, Nanjing University, Jiangsu; (c) Physics Department, Tsinghua University, Beijing 100084; (d) University of Chinese Academy of Science (UCAS), Beijing, China
36 (a) Department of Modern Physics and State Key Laboratory of Particle Detection and Electronics, University of Science and Technology of China, Anhui; (b) School of Physics, Shandong University, Shandong; (c) Department of Physics and Astronomy, Key Laboratory for Particle Physics, Astrophysics and Cosmology, Ministry of Education; Shanghai Key Laboratory for Particle Physics and Cosmology, Shanghai Jiao Tong University, Tsung-Dao Lee Institute, China
37 Université Clermont Auvergne, CNRS/IN2P3, LPC, Clermont-Ferrand, France
38 Nevis Laboratory, Columbia University, Irvington NY, United States of America
39 Niels Bohr Institute, University of Copenhagen, Kobenhavn, Denmark
40 (a) INFN Gruppo Collegato di Cosenza, Laboratori Nazionali di Frascati; (b) Dipartimento di Fisica, Università della Calabria, Rende, Italy
41 (a) AGH University of Science and Technology, Faculty of Physics and Applied Computer Science, Krakow; (b) Marian Smoluchowski Institute of Physics, Jagiellonian University, Krakow, Poland
42 Institute of Nuclear Physics Polish Academy of Sciences, Krakow, Poland
43 Physics Department, Southern Methodist University, Dallas TX, United States of America
44 Physics Department, University of Texas at Dallas, Richardson TX, United States of America
45 DESY, Hamburg and Zeuthen, Germany
46 Lehrstuhl für Experimentelle Physik IV, Technische Universität Dortmund, Dortmund, Germany
47 Institut für Kern- und Teilchenphysik, Technische Universität Dresden, Dresden, Germany
48 Department of Physics, Duke University, Durham NC, United States of America
49 SUPA - School of Physics and Astronomy, University of Edinburgh, Edinburgh, United Kingdom
50 INFN e Laboratori Nazionali di Frascati, Frascati, Italy
51 Fakultät für Mathematik und Physik, Albert-Ludwigs-Universität, Freiburg, Germany
52 Departement de Physique Nucleaire et Corpusculaire, Université de Genève, Geneva, Switzerland
53 (a) INFN Sezione di Genova; (b) Dipartimento di Fisica, Università di Genova, Genova, Italy
54 (a) E. Andronikashvili Institute of Physics, Iv. Javakhishvili Tbilisi State University, Tbilisi; (b) High Energy Physics Institute, Tbilisi State University, Tbilisi, Georgia
55 Il Physikalisches Institut, Justus-Liebig-Universität Giessen, Giessen, Germany
56 SUPA - School of Physics and Astronomy, University of Glasgow, Glasgow, United Kingdom
57 Il Physikalisches Institut, Georg-August-Universität, Göttingen, Germany
58 Laboratoire de Physique Subatomique et de Cosmologie, Université Grenoble-Alpes, CNRS/IN2P3, Grenoble, France
59 Laboratory for Particle Physics and Cosmology, Harvard University, Cambridge MA, United States of America
60 (a) Kirchhoff-Institut für Physik, Ruprecht-Karls-Universität Heidelberg, Heidelberg; (b) Physikalisches Institut, Ruprecht-Karls-Universität Heidelberg, Heidelberg, Germany
61 Faculty of Applied Information Science, Hiroshima Institute of Technology, Hiroshima, Japan
62 (a) Department of Physics, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong; (b) Department of Physics, The University of Hong Kong, Hong Kong; (c) Department of Physics and Institute for Advanced Study, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong, China
Department of Physics, National Tsing Hua University, Taiwan, Taiwan
Department of Physics, Indiana University, Bloomington IN, United States of America
Institut für Astro- und Teilchenphysik, Leopold-Franzens-Universität, Innsbruck, Austria
University of Iowa, Iowa City IA, United States of America
Department of Physics and Astronomy, Iowa State University, Ames IA, United States of America
Joint Institute for Nuclear Research, JINR Dubna, Dubna, Russia
KEK, High Energy Accelerator Research Organization, Tsukuba, Japan
Graduate School of Science, Kobe University, Kobe, Japan
Faculty of Science, Kyoto University, Kyoto, Japan
Kyoto University of Education, Kyoto, Japan
Research Center for Advanced Particle Physics and Department of Physics, Kyushu University, Fukuoka, Japan
Instituto de Física La Plata, Universidad Nacional de La Plata and CONICET, La Plata, Argentina
Physics Department, Lancaster University, Lancaster, United Kingdom

(a) INFN Sezione di Lecce; (b) Dipartimento di Matematica e Fisica, Università del Salento, Lecce, Italy

Oliver Lodge Laboratory, University of Liverpool, Liverpool, United Kingdom
Department of Experimental Particle Physics, Jožef Stefan Institute and Department of Physics, University of Ljubljana, Ljubljana, Slovenia
School of Physics and Astronomy, Queen Mary University of London, London, United Kingdom
Department of Physics, Royal Holloway University of London, Surrey, United Kingdom
Department of Physics and Astronomy, University College London, London, United Kingdom
Louisiana Tech University, Ruston LA, United States of America
Laboratoire de Physique Nucléaire et de Hautes Energies, UPMC and Université Paris-Diderot and CNRS/IN2P3, Paris, France

Fysiska institutionen, Lunds universitet, Lund, Sweden
Departamento de Física Teórica C-15, Universidad Autonoma de Madrid, Madrid, Spain
Institut für Physik, Universität Mainz, Mainz, Germany
School of Physics and Astronomy, University of Manchester, Manchester, United Kingdom
CPPM, Aix-Marseille Université and CNRS/IN2P3, Marseille, France
Department of Physics, University of Massachusetts, Amherst MA, United States of America
Department of Physics, McGill University, Montreal QC, Canada
School of Physics, University of Melbourne, Victoria, Australia
Department of Physics, The University of Michigan, Ann Arbor MI, United States of America
Department of Physics and Astronomy, Michigan State University, East Lansing MI, United States of America

(a) INFN Sezione di Milano; (b) Dipartimento di Fisica, Università di Milano, Milano, Italy
B.I. Stepanov Institute of Physics, National Academy of Sciences of Belarus, Minsk, Republic of Belarus
Research Institute for Nuclear Problems of Byelorussian State University, Minsk, Republic of Belarus
Group of Particle Physics, University of Montreal, Montreal QC, Canada
P.N. Lebedev Physical Institute of the Russian Academy of Sciences, Moscow, Russia
Institute for Theoretical and Experimental Physics (ITEP), Moscow, Russia
National Research Nuclear University MEPhI, Moscow, Russia
D.V. Skobeltsyn Institute of Nuclear Physics, M.V. Lomonosov Moscow State University, Moscow, Russia

Fakultät für Physik, Ludwig-Maximilians-Universität München, München, Germany
Max-Planck-Institut für Physik (Werner-Heisenberg-Institut), München, Germany
Nagasaki Institute of Applied Science, Nagasaki, Japan
Graduate School of Science and Kobayashi-Maskawa Institute, Nagoya University, Nagoya, Japan
(a) INFN Sezione di Napoli; (b) Dipartimento di Fisica, Università di Napoli, Napoli, Italy
Department of Physics and Astronomy, University of New Mexico, Albuquerque NM, United States of America
Institute for Mathematics, Astrophysics and Particle Physics, Radboud University Nijmegen/Nikhef, Nijmegen, Netherlands
(b) Dipartimento di Fisica, Università di Napoli, Napoli, Italy
Department of Physics, Northern Illinois University, DeKalb IL, United States of America
Budker Institute of Nuclear Physics, SB RAS, Novosibirsk, Russia
Department of Physics, New York University, New York NY, United States of America
Ohio State University, Columbus OH, United States of America
Faculty of Science, Okayama University, Okayama, Japan
(b) Dipartimento di Fisica, Università di Pavia, Pavia, Italy
Department of Physics, University of Pennsylvania, Philadelphia PA, United States of America
National Research Centre "Kurchatov Institute" B.P.Konstantinov Petersburg Nuclear Physics Institute, St. Petersburg, Russia
(a) INFN Sezione di Roma; (b) Dipartimento di Fisica, Sapienza Università di Roma, Roma, Italy
(a) INFN Sezione di Roma Tor Vergata; (b) Dipartimento di Fisica, Università di Roma Tor Vergata, Roma, Italy
(a) INFN Sezione di Roma Tre; (b) Dipartimento di Matematica e Fisica, Università Roma Tre, Roma, Italy
137 (a) Faculté des Sciences Ain Chock, Réseau Universitaire de Physique des Hautes Energies - Université Hassan II, Casablanca; (b) Centre National de l’Énergie des Sciences Techniques Nucléaires, Rabat; (c) Faculté des Sciences Semlalia, Université Cadi Ayyad, LPHEA-Marrakech; (d) Faculté des Sciences, Université Mohamed Premier and LPTPM, Oujda; (e) Faculté des sciences, Université Mohammed V, Rabat, Morocco

138 DSM/IRFU (Institut de Recherches sur les Lois Fondamentales de l’Univers), CEA Saclay (Commissariat à l’Energie Atomique et aux Energies Alternatives), Gif-sur-Yvette, France

139 Santa Cruz Institute for Particle Physics, University of California Santa Cruz, Santa Cruz CA, United States of America

140 Department of Physics, University of Washington, Seattle WA, United States of America

141 Department of Physics and Astronomy, University of Sheffield, Sheffield, United Kingdom

142 Department of Physics, Shinshu University, Nagano, Japan

143 Department Physik, Universität Siegen, Siegen, Germany

144 Department of Physics, Simon Fraser University, Burnaby BC, Canada

145 SLAC National Accelerator Laboratory, Stanford CA, United States of America

146 (a) Faculty of Mathematics, Physics & Informatics, Comenius University, Bratislava; (b) Department of Subnuclear Physics, Institute of Experimental Physics of the Slovak Academy of Sciences, Kosice, Slovak Republic

147 (a) Department of Physics, University of Cape Town, Cape Town; (b) Department of Physics, University of Johannesburg, Johannesburg; (c) School of Physics, University of the Witwatersrand, Johannesburg, South Africa

148 (a) Department of Physics, Stockholm University; (b) The Oskar Klein Centre, Stockholm, Sweden

149 Physics Department, Royal Institute of Technology, Stockholm, Sweden

150 Departments of Physics & Astronomy and Chemistry, Stony Brook University, Stony Brook NY, United States of America

151 Department of Physics and Astronomy, University of Sussex, Brighton, United Kingdom

152 School of Physics, University of Sydney, Sydney, Australia

153 Institute of Physics, Academia Sinica, Taipei, Taiwan

154 Department of Physics, Technion: Israel Institute of Technology, Haifa, Israel

155 Raymond and Beverly Sackler School of Physics and Astronomy, Tel Aviv University, Tel Aviv, Israel

156 Department of Physics, Aristotle University of Thessaloniki, Thessaloniki, Greece

157 International Center for Elementary Particle Physics and Department of Physics, The University of Tokyo, Tokyo, Japan

158 Graduate School of Science and Technology, Tokyo Metropolitan University, Tokyo, Japan

159 Department of Physics, Tokyo Institute of Technology, Tokyo, Japan

160 Tomsk State University, Tomsk, Russia

161 Department of Physics, University of Toronto, Toronto ON, Canada

162 (a) INFN-TIFPA; (b) University of Trento, Trento, Italy

163 (a) TRIUMF, Vancouver BC; (b) Department of Physics and Astronomy, York University, Toronto ON, Canada

164 Faculty of Pure and Applied Sciences, and Center for Integrated Research in Fundamental Science and Engineering, University of Tsukuba, Tsukuba, Japan

165 Department of Physics and Astronomy, Tufts University, Medford MA, United States of America

166 Department of Physics and Astronomy, University of California Irvine, Irvine CA, United States of America

167 (a) INFN Gruppo Collegato di Udine, Sezione di Trieste, Udine; (b) ICTP, Trieste; (c) Dipartimento di
Also at Fakultät für Mathematik und Physik, Albert-Ludwigs-Universität, Freiburg, Germany

Also at Institute for Mathematics, Astrophysics and Particle Physics, Radboud University Nijmegen/Nikhef, Nijmegen, Netherlands

Also at Department of Physics, The University of Texas at Austin, Austin TX, United States of America

Also at Institute of Theoretical Physics, Ilia State University, Tbilisi, Georgia

Also at CERN, Geneva, Switzerland

Also at Georgian Technical University (GTU), Tbilisi, Georgia

Also at Ochadai Academic Production, Ochanomizu University, Tokyo, Japan

Also at Manhattan College, New York NY, United States of America

Also at The City College of New York, New York NY, United States of America

Also at Departamento de Física Teórica y del Cosmos, Universidad de Granada, Granada, Portugal

Also at Department of Physics, California State University, Sacramento CA, United States of America

Also at Moscow Institute of Physics and Technology State University, Dolgoprudny, Russia

Also at Departement de Physique Nucleaire et Corpusculaire, Université de Genève, Geneva, Switzerland

Also at Institut de Física d’Altes Energies (IFAE), The Barcelona Institute of Science and Technology, Barcelona, Spain

Also at School of Physics, Sun Yat-sen University, Guangzhou, China

Also at Institute for Nuclear Research and Nuclear Energy (INRNE) of the Bulgarian Academy of Sciences, Sofia, Bulgaria

Also at Faculty of Physics, M.V.Lomonosov Moscow State University, Moscow, Russia

Also at National Research Nuclear University MEPhI, Moscow, Russia

Also at Department of Physics, Stanford University, Stanford CA, United States of America

Also at Institute for Particle and Nuclear Physics, Wigner Research Centre for Physics, Budapest, Hungary

Also at Giresun University, Faculty of Engineering, Turkey

Also at CPPM, Aix-Marseille Université and CNRS/IN2P3, Marseille, France

Also at Department of Physics, Nanjing University, Jiangsu, China

Also at Institute of Physics, Academia Sinica, Taipei, Taiwan

Also at University of Malaya, Department of Physics, Kuala Lumpur, Malaysia

* Deceased