Search for heavy resonances decaying to a $Z$ boson and a photon in $pp$ collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector

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1. Introduction

Many models of physics beyond the Standard Model (SM) introduce new bosons through either an extension of the Higgs sector or additional gauge fields. This suggests that a broad experimental survey of physics beyond the SM can be made by searching for new massive bosons. Some models predict that these bosons decay to final states containing the SM electroweak $W$ or $Z$ bosons or photons [1,2]. Attractive decays from an experimental perspective are to $\gamma\gamma$ [3-6], $Z\gamma$ [7,8] or $ZZ$ [9,10] final states, since both the $Z$ bosons and photons in pair production can be measured well with relatively low backgrounds. If new bosons were produced, the complete reconstruction of these final states could be used to precisely measure their properties, such as their mass.

This Letter presents a search for $X \rightarrow Z\gamma$ resonances using an integrated luminosity of 3.2 fb$^{-1}$ of proton–proton ($pp$) collisions at a centre-of-mass energy $\sqrt{s}$ of 13 TeV, collected with the ATLAS detector at the Large Hadron Collider (LHC) in 2015. To enhance the sensitivity of the search, both the leptonic ($Z \rightarrow \ell^+\ell^-$, $\ell = e,\mu$)$^1$ and hadronic ($Z \rightarrow q\bar{q}$) decay modes of the $Z$ boson are used. The combined selection captures about 77% of all $Z$ boson decays. In the following, the search based on the selection of $\ell\ell\gamma$ final states is also referred to as the leptonic analysis, while the search based on the selection of $q\bar{q}\gamma$ final state is also referred to as the hadronic analysis.

The leptonic analysis uses events collected using lepton triggers and is performed in the $X$ boson mass ($m_X$) range 250 GeV-1.5 TeV. The hadronic analysis is performed in the $m_X$ range 700 GeV-2.75 TeV. Due to the large value of $m_X$, the $Z$ bosons from $X \rightarrow Z\gamma$ are highly boosted and the two collimated sprays of energetic hadrons, called jets in the following, that are produced in $Z \rightarrow q\bar{q}$ decays are merged into a single, large-radius, jet $J$. The events used for the hadronic analysis are collected using single-photon triggers. Due to the larger $Z$ boson branching ratio to hadrons, the boosted hadronic analysis dominates the sensitivity at high $m_X$, where the number of events is very small, while the leptonic analysis, with its higher signal-to-background ratio, dominates the sensitivity at low $m_X$.

Previous searches for non-SM bosons decaying into $Z\gamma$ final states were carried out at the Tevatron and the LHC. The D0 Collaboration set limits [11] on $X \rightarrow Z\gamma$ production using $pp$ collisions at $\sqrt{s} = 1.96$ TeV. At the LHC, the ATLAS Collaboration used $pp$ collisions collected in 2011 and 2012 at $\sqrt{s} = 7$ and 8 TeV to extend the mass and sensitivity of $X \rightarrow Z\gamma$ searches [7,8]. The analyses assumed a narrow width for the $X$ boson and used $e^+e^-$ and $\mu^+\mu^-$ decays of the $Z$ boson. No signals were observed and limits on the product of the production cross section $\sigma(pp \rightarrow X)$ times the branching ratio $BR(X \rightarrow Z\gamma)$ were determined for values of $m_X$ in the range $\approx$ 200 to 1600 GeV.

The analyses presented here search for a localized excess in the reconstructed invariant mass distribution of the final state, either a photon and two leptons or a photon and a heavy, large-radius jet. In the leptonic analysis, the main background arises from continuum production of a $Z$ boson in association with a photon, or, to a lesser extent, with a hadronic jet misidentified as a photon. In the hadronic analysis, the background is dominated by non-resonant SM production of $\gamma +$jet events, with smaller contributions from dijet events with a jet misidentified as a photon, and from SM...
$V + \gamma$ events ($V = W, Z$). The invariant mass distribution of the background should be smoothly and steeply decreasing with the mass. It is parameterized by a smooth function with free parameters, which are adjusted to the data. The intrinsic width of the heavy boson is assumed to be small compared to the experimental resolution. The boson is assumed to be a spin-0 particle produced via gluon fusion.

2. The ATLAS detector

The ATLAS detector is a multi-purpose particle detector with approximately forward--backward symmetric cylindrical geometry. Its original design [12] has been complemented with the installation, prior to the 2015 data-taking, of a new innermost silicon pixel layer [13].

A two-level trigger system [14] selects events to be recorded for offline analysis. The first-level trigger is hardware-based, while the second, high-level trigger is implemented in software and employs algorithms similar to those used offline to identify lepton and photon candidates.

3. Data sample

Data were collected in 2015 during $pp$ collisions at a centre-of-mass energy of 13 TeV. The bunch spacing was 25 ns and the average number of inelastic interactions per bunch crossing was 13.

The search in the $\ell\ell\gamma$ final state is performed in events recorded using the lowest-threshold unprescaled single-lepton or dilepton triggers. The single-muon trigger has a nominal transverse momentum ($p_T$) threshold of 20 GeV and a loose requirement on the track isolation. This quantity, defined as the sum of the transverse momenta of the tracks in the inner detector (ID) found in a cone of size $\Delta R \equiv \sqrt{(\Delta \eta)^2 + (\Delta \phi)^2} = 0.2$ around the muon, excluding the muon track itself, is required to be less than 12% of the muon $p_T$. Only tracks with longitudinal impact parameter $z_0$ within 6 mm of that from the muon track are considered in the calculation. An additional single-muon trigger with a higher $p_T$ threshold (50 GeV) but no isolation requirement is also used. The dimuon trigger has a $p_T$ threshold of 10 GeV for both muon candidates and applies no isolation criteria. The single-electron (di-electron) trigger has a nominal $p_T$ threshold of 24 GeV (12 GeV). Electron candidates are required to satisfy likelihood-based identification criteria looser than those applied offline and described in Section 5. The electron identification likelihood is computed from both the properties of the track reconstructed in the ID and the energy deposited in the electromagnetic (EM) calorimeter.

The search in the $J\gamma$ final state uses events recorded by the lowest-$p_T$ threshold unprescaled single-photon trigger. This trigger requires at least one photon candidate with $p_T > 120$ GeV passing loose identification requirements based on the shape of the shower in the EM calorimeter and on the energy leaking into the hadronic calorimeter.

The trigger efficiency for events satisfying the offline selection criteria described in Section 5 is greater than 99% in the $ee\gamma$ and $J\gamma$ channels and is about 96% in the $\mu\mu\gamma$ channel due to the reduced geometric acceptance of the muon trigger system.

The integrated luminosity after the trigger and data quality requirements is $L_{\text{int}} = 3.2 \text{ fb}^{-1}$.

4. Monte Carlo simulation

Simulated signal and background samples were generated with a Monte Carlo (MC) technique. They are used to optimize the selection criteria and to quantify the signal efficiency of the final selection. Such MC samples are also used to test the analytic parameterization of the $Z\gamma$ invariant mass spectra of signal and background, while the estimate of the background yield after the selection is estimated in situ from the data.

All MC samples are generated assuming a centre-of-mass $pp$ collision energy of 13 TeV. The samples were passed through a detailed simulation of the ATLAS detector response [16] based on GEANT4 [17]. Multiple inelastic proton–proton collisions (referred to as pile-up) are simulated with the soft QCD processes of PYTHIA 8.186 [18] using the A2 set of tuned parameters (A2 tune) [19] and the MSTW2008LO parton distribution function (PDF) set [20], and are overlaid on each MC event. The distribution of the number of pile-up interactions in the simulation is reweighted to match the data. The simulated signals in the detector are passed through the event reconstruction algorithms used for the data. The simulation is tuned to take into account small differences with data. These include corrections to photon, lepton and jet reconstruction and selection efficiencies, and their energy or momentum resolution and scale. The corrections are obtained either from control samples selected in early $\sqrt{s} = 13$ TeV data or from 8 TeV data with additional systematic uncertainties introduced to cover the different conditions between the 2012 and 2015 data-taking.

In the signal simulation, a scalar boson $X$ is produced in $pp$ collisions via gluon fusion, and decays to a photon and a $Z$ boson. Monte Carlo samples are produced for different $m_X$ hypotheses between 200 GeV and 3 TeV. The width of the boson $X$ is set to 4 MeV, which is much smaller than the experimental resolution, regardless of the resonance mass. Due to the assumed narrow width of the $X$ boson and the small contribution of gluon fusion to the non-resonant SM production of $Z + \gamma$ [21], the interference between the $gg \rightarrow X \rightarrow Z\gamma$ signal process and the SM $gg \rightarrow Z\gamma$ background is neglected in the simulation. The signal samples are generated with POWHEG-BOX [22,23] interfaced to PYTHIA 8.186 for the underlying event, parton showering and hadronization. The CT10 [24] PDF set and the AZNLO tune [25] of the underlying event are used.

Events from SM processes containing a photon and a $Z$ or $W$ boson ($V + \gamma$), a $Z$ boson produced in association with jets, or a prompt photon produced in association with jets ($\gamma + $) are simulated using the SHERPA 2.1.1 [26] generator. The matrix elements for SM $V + \gamma$ ($\gamma + $) production are calculated for real emission of up to three (four) partons at leading order (LO) in the strong coupling constant $\alpha_S$ and are merged with the SHERPA parton shower [27] using the ME-+$\text{PS}@\text{LO}$ prescription [28]. The matrix elements of events containing $Z$ bosons with associated jets are calculated for up to two partons at next-to-leading order (NLO) and four partons at LO and merged with the parton shower using the ME-+$\text{PS}@\text{NLO}$ prescription [29]. The matrix elements are calculated using the Comix [30] and OpenLoops [31] generators. For all the background samples, the CT10 PDF set is used in conjunction with dedicated parton shower tuning developed by the SHERPA authors. The $\gamma + $ and $V + \gamma$ samples are generated in binned ranges of the transverse momentum of the photon to ensure precise predictions over the full spectrum relevant for these analyses. Similarly, $Z + $ events are generated in binned ranges of the dilepton pair $p_T$ from the $Z$ boson decays.
5. Event selection

Events with at least one primary vertex candidate with two or more tracks with $p_T > 400$ MeV are selected. In each event, the primary vertex candidate with the largest sum of the $p_T^2$ of the associated tracks is chosen as the hard interaction primary vertex.

Events are required to contain at least one photon candidate and one $Z$ boson candidate. In the leptonic analysis, the $Z$ boson candidate is formed from a pair of opposite-sign, same-flavour electrons or muons. In the hadronic analysis, $Z$ bosons are required to recoil against a high-momentum photon ($p_T > 250$ GeV); as a consequence of the $Z$ boson’s large Lorentz boost, the two jets from the hadronization of the two quarks are reconstructed as a single, relatively heavy, large-radius jet. Jet-substructure variables and the jet mass are then used to discriminate between a $Z$ boson decay and jets from single quarks or gluons [32]. Events with one or more electron or muon candidates satisfying the selection described below are vetoed in the hadronic analysis. In the following, the selection of photons, leptons, large-radius jets and of the final $X \rightarrow Z\gamma$ candidates is described.

Unconverted photons, photon conversions to electron-positron pairs, and electrons are reconstructed from clusters of energy deposits in the EM calorimeter cells found by a sliding-window algorithm and from tracks reconstructed in the ID and extrapolated to the calorimeter [33,34].

Photon candidates are required to have a pseudorapidity within the regions $|\eta| < 1.37$ or $1.52 < |\eta| < 2.37$, where the first calorimeter layer has high granularity. In the leptonic analysis, the transverse momentum of photon candidates is initially required to pass a loose preselection, $p_T > 15$ GeV, whereas the final photon $p_T$ requirement is applied when a $Z\gamma$ candidate is reconstructed, as described later. In the hadronic analysis, the photon transverse momentum is required to be larger than 250 GeV. To reduce background from hadronic jets, photon candidates are required to satisfy a set of requirements on the shower leakage in the hadronic calorimeter and on the transverse shower profile measured with the first two layers of the electromagnetic calorimeter [33]. The requirements were optimized using simulated samples of photons and hadronic jets produced in 13 TeV pp collisions. The efficiency of the identification criteria is about 98% for converted photon candidates and 94% for unconverted photon candidates with $p_T > 100$ GeV. Background from hadronic jets is further reduced by requiring the transverse energy measured in the calorimeter in a cone of size $\Delta R = 0.4$ around the photon direction ($E_{T,\text{iso}}$ [35], also called calorimeter isolation in the following) to be less than $2.45\text{GeV} + 0.022 \times p_T$.

Electron candidates are required to have $p_T > 10$ GeV and $|\eta| < 2.47$, excluding the transition region between the barrel and endcaps in the EM calorimeter ($1.37 < |\eta| < 1.52$). To suppress background from hadronic jets, electron candidates are required to satisfy likelihood-based identification criteria [36]. Such requirements provide approximately 85% identification efficiency for electrons with a transverse momentum of 20 GeV, increasing to 95% for $p_T > 80$ GeV.

Muons with $|\eta| < 2.5$ are reconstructed by combining tracks in the ID with tracks in the muon spectrometer (MS) [37]. The acceptance is extended to the region $2.5 < |\eta| < 2.7$ by also selecting muons whose trajectory is reconstructed only in the MS. Muon candidates are required to have transverse momentum above 10 GeV. Background muons, originating mainly from pion and kaon decays, are rejected by applying a set of quality requirements on the number of hits in the muon spectrometer and (for $|\eta| < 2.5$) on the compatibility between the ID and MS momentum measurements. The muon identification efficiency is around 97% for transverse momenta above 10 GeV.

If two electron candidates share the same track, or have clusters in the calorimeter separated by $|\Delta \eta| < 0.075$ and $|\Delta \phi| < 0.125$, only the candidate with the higher energy measured by the calorimeter is kept. In addition, if the track associated with an electron candidate is within a distance $\Delta R = 0.02$ from the track associated with a muon candidate, the electron candidate is rejected.

Track and calorimeter isolation requirements are further applied to the selected leptons. For electrons, combined criteria are applied to the calorimeter isolation, $E_{T,\text{iso}}$, in a cone of radius $\Delta R = 0.2$, and to the track isolation, $\sum_{\text{other}} p_T$, in a cone of radius $\Delta R = 0.2$ for electron transverse momenta $p_T < 50$ GeV and of radius $\Delta R = (10 \text{ GeV})/p_T$ for $p_T > 50$ GeV. In the calculation of the track isolation, the contribution from the electron track itself is not included. The criteria are chosen to provide an efficiency of about 95% independent of the electron transverse momentum and pseudorapidity, as determined in a control sample of $Z \rightarrow ee$ decays selected with a tag-and-probe technique [36]. For muons, combined criteria are imposed on $E_{T,\text{iso}}$ in a cone of radius $\Delta R = 0.2$ and on $\sum_{\text{other}} p_T$ inside a cone of radius $\Delta R = 0.3$ for muon transverse momenta $p_T < 33$ GeV and of radius $\Delta R = (10 \text{ GeV})/p_T$ for $p_T > 33$ GeV. The efficiency of these criteria increases with the muon transverse momentum, reaching 95% at 25 GeV and 99% at 60 GeV, as measured in $Z \rightarrow \mu\mu$ events selected with a tag-and-probe method [37].

In the hadronic analysis, topological clusters of energy in the calorimeter that were locally calibrated and assumed to be massless [38] are used as inputs to reconstruct large-radius jets, based on the anti-$k_t$ algorithm [39] with radius parameter $R = 1.0$ [40]. Within the large-radius jets, smaller “subjets” are reconstructed using the $k_t$ algorithm [41,42] with a radius parameter $R = R_{\text{sub}} = 0.2$. The large-radius jet is trimmed [43] by removing subjets that carry fractional $p_T$ less than $\text{cut} = 5\%$ of the $p_T$ of the original jet. The pseudorapidity, energy and mass of these trimmed large-radius jets are calibrated using a simulation-based calibration scheme [44]. The large-radius jets are required to have $p_T > 200$ GeV and $|\eta| < 2.0$. Large-radius jets within $\Delta R = 1.0$ from selected photons are discarded. A $p_T$-dependent requirement on the substructure observable $D_2^{(\beta=1)}$ [45], defined as the ratio $E_2^{(\beta=1)}/E_1^{(\beta=1)}$ of $N$-point energy correlation functions $E_j^{(\beta=1)}$ of the jet constituents [46], is used to select hadronically decaying bosons while rejecting jets from single quarks or gluons. The ratio makes use of the sensitivity of the $E_2$ functions to the “pronginess” character of the jet. In particular, it relies on the sensitivity of $E_2$ to radiation around a single hard core, and of $E_3$ to radiation with two cores. The powers of the $E_2$ and $E_3$ functions in the ratio are chosen to optimize the discrimination between one- and two-prong jets following an analysis of the $(E_2, E_3)$ phase-space of these two types of jets.

The jet mass $m_j$, computed from its topological cluster constituents that remain after the trimming procedure, is required to be in the range 80 GeV $< m_j < 110$ GeV. The jet is required to be associated with less than 30 tracks with $p_T > 500$ MeV originating from the hard-interaction primary vertex (before trimming). The efficiency of the $D_2^{(\beta=1)}$, $m_j$ and number-of-track requirements is around 22% for the signal jet and 2.2% for jets from single quarks or gluons.

After the selection of photons, leptons and large-radius jet candidates, the $Z\gamma$ candidate is chosen. If an event has multiple photon or jet candidates, only the photon or jet candidate with highest transverse momentum is kept. In the leptonic analysis, only $Z \rightarrow \ell\ell$ candidates with invariant mass $m_{\ell\ell}$ within $\pm 15$ GeV of the $Z$ boson mass [47] are retained: in case of multiple dilepton candidates, only the one with invariant mass closest to the $Z$ bo-
son mass is kept. Moreover, the triggering leptons are required to match one, or both in the case of events collected with dilepton triggers, of the $Z$ boson candidate's leptons.

The invariant mass $m_{Z'}$ of the selected $Z'$ candidate is computed from the four-momenta of the photon candidate and either the selected leptons or the jet ($m_{Z'} = m_{\ell\ell}$ or $m_{J}$). In the leptonic analysis, the four-momentum of the photon is recalculated using the identified primary vertex as the photon's origin, while the four-momenta of the leptons are first corrected for collinear FSR (muons only) and then recomputed by means of a $Z$-mass-constrained kinematic fit [48]. The $Z'$ invariant mass is required to be larger than 200 (640) GeV for the leptonic (hadronic) analysis, to be sufficiently far from the kinematic turn-on due to the $Z$ boson mass and the photon transverse momentum requirement.

Finally, the leptonic analysis only retains candidates in which the photon transverse momentum is larger than 30% of $m_{Z'}$, significantly suppressing background at large invariant mass while maintaining high efficiency over a large range of signal masses.

6. Signal and background models

The final discrimination between signal and background events in the selected sample is achieved by means of an unbinned maximum-likelihood fit of a signal+background model to the invariant mass distribution of the selected data events. Both the signal and background models are described in this section.

6.1. Signal model

Fig. 1 illustrates the distributions of $m_{\ell\ell}$ and $m_{J}$ for simulated signal events for a resonance mass of 800 GeV. The intrinsic width of the simulated resonance (4 MeV) is negligible compared to the experimental resolution. The $m_{Z'}$ resolution ranges between 2 GeV at $m_{X} = 200$ GeV and 15 GeV at $m_{X} = 1500$ GeV (1% relative resolution). The $m_{J}$ resolution ranges between 22 GeV at $m_{X} = 750$ GeV (3%) and 50 GeV at $m_{X} = 3$ TeV (1.7%).

The $m_{\ell\ell}$ distribution is modelled with a double-sided Crystal Ball function (a Gaussian function with power-law tails on both sides). The $m_{J}$ distribution is modelled with the sum of a Crystal Ball function [49] (a Gaussian function with a power-law tail on one side) and a second small, wider Gaussian component. The fraction of signal $J\gamma$ events described by the Crystal Ball function is above 90% for resonance masses up to 1.8 TeV and decreases with $m_{X}$, reaching 85% at $m_{X} = 3$ TeV. Polynomial parameterizations of the signal shape parameters as a function of the resonance mass $m_{X}$ are obtained from a simultaneous fit to the invariant mass distributions of all the simulated signal samples, for each $Z$ boson decay channel.

The signal detection efficiency (including the acceptance of the kinematic criteria) as a function of $m_{X}$ is computed in the leptonic analysis by interpolating the efficiencies predicted by all the simulated signal samples up to $m_{X} = 1.5$ TeV with a function of the form $a + b e^{m_{X}}$. In the hadronic analysis, the efficiency at any value of $m_{X}$ is obtained through a linear interpolation between the efficiencies obtained from the two simulated signal samples with masses closest to $m_{X}$. The signal detection efficiency of the leptonic analysis ranges between 28% at $m_{X} = 250$ GeV and 43% at $m_{X} = 1.5$ TeV, while that of the hadronic analysis increases from 11% at $m_{X} = 700$ GeV to 15% at $m_{X} = 3$ TeV, as shown in Fig. 2.

6.2. Background model

In both the leptonic and hadronic final states, the total background exhibits a smoothly falling spectrum as a function of the invariant mass $m_{Z'}$ of the final-state products. The $m_{Z'}$ distribution of the background is parameterized with a function similar to the one used in previous searches in the $g +$ jet and diphoton final states [5,50]:

$$f_{bkg}(m_{Z'}) = \mathcal{N}(1 - x^{k})p_{1} + x^{k}p_{2}.$$  

(1)

Here $\mathcal{N}$ is a normalization factor, $x = m_{Z'}/\sqrt{3}$, the exponent $k$ is 1/3 for the leptonic analysis and 1 for the hadronic analysis, and $p_{1}$ and $p_{2}$ are dimensionless shape parameters that are fitted to the data. The constant $\xi$ is set to zero in the leptonic analysis and to the value (ten) that minimizes the correlation between the maximum-likelihood estimates of $p_{1}$ and $p_{2}$ in a fit to the background simulation for the hadronic analysis.

These parameterizations were chosen since they satisfy the following two requirements: (i) the bias in the fitted signal due to the
choice of this functional form is estimated to be sufficiently small compared to the statistical uncertainties from the background, and (ii) the addition of further degrees of freedom to Eq. (1) does not lead to a significant improvement in the goodness of the fit to the data distribution.

The bias is checked by performing signal+background fits to large background control samples, scaled to the luminosity of the data. A functional form is retained if the absolute value of the fitted signal yield \( N_{\text{sig}} \) (spurious signal in the following) is less than 20% (25%) of its statistical uncertainty in the leptonic (hadronic) analysis [51].

For the leptonic analysis, the control sample for the spurious signal study is obtained by summing the invariant mass distributions of \( Z + \gamma \) and \( Z + \text{jets} \) simulated events, normalized according to their relative fractions measured in data (90% and 10% respectively). These fractions are determined by means of a simultaneous fit of the \( E_T^{\text{miss}} \) distributions of the photon candidates passing or failing the identification requirements. To increase the number of \( Z + \gamma \) MC events, a very large (up to one thousand times more events than in data) simulated sample is obtained by passing the events generated by SHERPA through a fast simulation of the calorimeter response [52]. The agreement of the \( m_{Z\gamma} \) distribution in the parametric simulation with that of the full-simulation \( Z + \gamma \) sample described in Section 4 was evaluated with a \( \chi^2 \) test. The \( \chi^2 \) was found to be 23 for 28 degrees of freedom, corresponding to a \( p \)-value of 75%, indicating that the shapes agree well within statistical uncertainties. The \( m_{Z\gamma} \) distribution of \( Z + \text{jets} \) events is obtained by reweighting that of the large \( Z + \gamma \) sample by a second-order polynomial function. The parameters of this function are determined from a fit to the ratio of the \( m_{Z\gamma} \) distributions of a \( Z + \text{jets} \)-enriched data control sample to that of the paramerized simulation of \( Z + \gamma \).

For the hadronic analysis, the spurious signal is studied in a data control sample enriched in jets not originating from \( Z \) boson decays. This sample passes the selection described in Section 5, with the exception that the jet mass \( m_1 \) is either between 50 GeV and 65 GeV, or between 110 GeV and 140 GeV. Based on simulation and data-driven studies, the \( m_{Y\gamma} \) distribution of \( \gamma + \text{jets} \) events has a similar shape to that of the total background in the signal region, where the latter also includes contributions at the 10% level from \( V + \gamma \) and dijet events. Thus, this control region (dominated by \( \gamma + \text{jets} \) events) can be used to study the background in the hadronic \( Z \gamma \) signal region.

Tests to check whether the degrees of freedom of the chosen function are sufficient to accurately describe the background distribution in data are performed by comparing the goodness of the fits to the data using either the nominal background function or a function with one or two additional degrees of freedom. A test statistic \( \Lambda_{12} \) to discriminate between two background models \( f_1 \) and \( f_2 \) is built. This uses either the \( \chi^2 \) and number of degrees of freedom computed from a binned comparison between the data and the fit (leptonic analysis) or directly the maximum value of the likelihood (hadronic analysis), for the fits performed to data using either \( f_1 \) or \( f_2 \). The simpler model \( f_1 \) is then rejected in favour of \( f_2 \) if the probability of finding values of \( \Lambda_{12} \) more extreme than the one measured in data is lower than 5%. No significant improvement in goodness of fit over the model of Eq. (1) is found when adding one or two extra degrees of freedom to it.

7. Systematic uncertainties

The systematic uncertainty in the measured \( \sigma(pp \to X) \times BR(X \to Z\gamma) \) has contributions from uncertainties in the integrated luminosity \( L_{\text{int}} \) of the analyzed data, in the estimated signal yield \( N_{\text{sig}} \), and in the signal efficiency \( \varepsilon \).

An integrated-luminosity uncertainty of \( \pm 5\% \) is derived, following a methodology similar to that detailed in Ref. [53], from a preliminary calibration using \( x-y \) beam-separation scans performed in August 2015.

The uncertainties in the signal yield arise from the choice of functional forms used to describe the signal and the background in the final fit to \( m_{Z\gamma} \), as well as from the parameters of the signal model, which are determined from the simulation. Uncertainties due to the parameterization of the signal distribution chosen in Section 6.1 are negligible compared to the other uncertainties. Effects of spurious signals from the choice of background function on the signal are included as described in Section 6.2. The uncertainties in the signal model parameters arise from the uncertainties in the energy scales and resolutions of the final-state particles (photons, electrons, muons, and large-radius jets).

Contributions to the uncertainty in the signal detection efficiency \( \varepsilon \) originate from the trigger and the reconstruction, identification and isolation requirements of the selected final-state particles. There is also a contribution from the kinematic requirements used to select the final-state particles due to uncertainties in the energy scale and resolution. The effects of the lepton and photon trigger, reconstruction, identification and isolation efficiency uncertainties are estimated by varying the simulation-to-data efficiency correction factors by their \( \pm 1\sigma \) uncertainties and recalculating the signal efficiency. The impact of the lepton and photon energy scale and resolution uncertainties is estimated by computing the relative change in efficiency and in the peak position and the width of the invariant mass distribution of the signal after varying these quantities by their uncertainties in the simulation.

The uncertainties in the jet \( p_T \), mass and \( D_0^{a=1} \) scales and resolutions are evaluated by comparing the ratio of calorimeter-based track-based measurements in dijet data and simulation [32, 54]. Their effect is estimated by recomputing the efficiency of the hadronic \( Z \) boson selection and the signal \( m_{Z\gamma} \) distribution after varying the \( p_T \), mass and \( D_0^{a=1} \) scales and resolutions by their uncertainties. The requirement on the number of primary-vertex tracks associated with the jet induces a 6% systematic uncertainty in the corresponding efficiency, as estimated from the comparison of simulation and control samples of data.

In the leptonic analysis, the systematic uncertainties have a small effect on the final results, which are dominated by the statistical uncertainties originating from the small size of the selected sample. The main contributions arise from the uncertainty in the photon and electron resolution, from the spurious signal and from the luminosity uncertainty. They worsen the search sensitivity by only 4.0%–0.5%, 3.0%–2.0% and 0.5% respectively, over the \( m_X \) range from 250 GeV to 1.5 TeV.

In the hadronic analysis, the systematic uncertainties are dominated by estimates of the jet mass resolution and the jet energy resolution. The search sensitivity worsens by 4.3% (5.3%), 4.3% (1.1%) and 2.1% (1.0%) at \( m_{Z\gamma} \) masses of 0.7 TeV, 1.5 TeV and 2.7 TeV, from the effects of the jet mass resolution (jet energy resolution) uncertainty. The degradation of the search sensitivity due to the uncertainty in the efficiency of the requirement on the number of tracks associated with the large-radius jet is less than 1% at all tested masses.

8. Statistical procedure

A profile-likelihood-ratio method [55] is used to search for a localized excess over a smoothly falling background in the \( m_{Z\gamma} \) distribution of the data, as well as to quantify its significance and estimate its production cross section. The extended likelihood function \( L(\alpha, \theta) \) is given by the product of a Poisson term, the
values of the probability density function $f_{\text{tot}}(m_{Z'}^i, \alpha, \theta)$ of the invariant mass distribution for each candidate event $i$ and constraint terms $G(\theta)$:

$$
\mathcal{L} \left( (\alpha, \theta) \left| m_{Z'}^i \right. \right)_{i=1,n} = \frac{e^{-N(\alpha, \theta)} N^\alpha(\alpha, \theta)}{n!} \prod_{i=1}^{n} f_{\text{tot}}(m_{Z'}^i, \alpha, \theta) \times G(\theta).
$$

In this expression $\alpha$ represents the parameter of interest, $\alpha = \sigma(pp \rightarrow X) \times BR(X \rightarrow Z')$, $\theta$ are nuisance parameters, $n$ is the observed number of events, and the expected event yield $N$ is the sum of the number of signal events $N_{\text{sig}} = \text{Int} \times (\sigma \times BR) \times \epsilon$, the number of background events $N_{\text{bkg}}$, and the spurious signal yield $N_{\text{spur}}$ described in Section 6.2. The function $f_{\text{tot}}(m_{Z'}^i, \alpha, \theta)$ is built from the signal and background probability density functions of $m_{Z'}$, $f_{\text{sig}}$ and $f_{\text{bkg}}$:

$$
f_{\text{tot}}(m_{Z'}^i, \alpha, \theta) = \frac{1}{N} \left[ (N_{\text{sig}}(m_X, \alpha, \theta_{\text{sig}}) + N_{\text{spur}}(m_X) \times \theta_{\text{spur}}) \times f_{\text{sig}}(m_{Z'}^i, \theta_{\text{sig}}) + N_{\text{bkg}} \times f_{\text{bkg}}(m_{Z'}^i, \theta_{\text{bkg}}) \right].
$$

The uncertainties in the signal parameterization, efficiency and bias in the signal yield due to the choice of the background model are included in the fit via nuisance parameters which are constrained with Gaussian or log-normal penalty terms for signal modelling and a Gaussian penalty term for the spurious signal uncertainty.

The significance of the signal is estimated by computing the $p$-value of the compatibility of the data with the background-only hypothesis ($p_0$). A modified frequentist ($CL_s$) method is used to set upper limits on the signal cross-section times branching ratio at 95% confidence level (CL), by identifying the value of $\sigma \times BR$ for which $CL_s$ is equal to 0.05.

Closed-form asymptotic formulae are used to derive the results. Due to the small size of the selected dataset and of the expected background for large values of $m_X$, the results for some values of $m_X$, spread over the full tested range, are checked using ensemble tests. The results obtained using the asymptotic formulae are in good agreement (differences on the cross-section limits < 10%) with those from the ensemble tests for most of the $m_X$ range, except at high $m_X$ where the differences on the cross-section limits can be as large as 30%.

9. Results

In the data, there are 382 $Z(\rightarrow \ell\ell)\gamma$ candidates with $m_{Z'} > 200$ GeV and 534 $Z(\rightarrow j\gamma)$ candidates with $m_{Z'} > 640$ GeV. The candidates with largest invariant mass in the leptonic and hadronic analyses have $m_{\ell\ell\gamma} = 1.47$ TeV and $m_{jj\gamma} = 2.58$ TeV respectively.

The invariant mass distributions of the selected $Z\gamma$ candidates in data in the leptonic and hadronic final states are shown in Fig. 3. The solid lines represent the expected results of a background-only fit.

There is no significant excess with respect to the background-only hypothesis, and the largest deviations are observed around $m_X = 350$ GeV in the leptonic analysis (2.0σ local significance) and around $m_X = 1.9$ TeV in the hadronic analysis (1.8σ local significance).

For a narrow scalar boson $X$ of mass $m_X$, 95% CL upper limits on $\sigma(pp \rightarrow X) \times BR(X \rightarrow Z\gamma)$ are set for $m_X$ between 250 GeV and 1.5 TeV in the leptonic analysis and between 700 GeV and 2.75 TeV in the hadronic analysis. In the $m_X$ range between 700 GeV and 1.5 TeV the results of the two analyses are then combined. The observed limits range between 295 fb for $m_X = 340$ GeV and 8.2 fb for $m_X = 2.15$ TeV, while the expected limits range between 230 fb for $m_X = 250$ GeV and 10 fb for $m_X = 2.75$ TeV. The observed and expected limits as a function of $m_X$ are shown in Fig. 4.

10. Conclusion

A search for new resonances with masses between 250 GeV and 2.75 TeV decaying to a photon and a $Z$ boson has been performed using 3.2 fb$^{-1}$ of proton–proton collision data at a centre-of-mass energy of $\sqrt{s} = 13$ TeV collected by the ATLAS detector at the Large Hadron Collider. The $Z$ bosons were reconstructed through their decays either to charged, light, lepton pairs ($e^-e^+$, $\mu^-\mu^+$) or to boosted quark–antiquark pairs giving rise to a single, large-radius, heavy jet of hadrons.

No significant excess in the invariant-mass distribution of the final-state particles due to a scalar boson with a narrow width (4 MeV) was found over the smoothly falling background.

Limits at 95% CL using a profile-likelihood ratio method were set on the production cross section times decay branching ratio to $Z\gamma$ of such a boson. The observed limits range between 295 fb for $m_X = 340$ GeV and 8.2 fb for $m_X = 2.15$ TeV, while the expected limits range between 230 fb for $m_X = 250$ GeV and 10 fb for $m_X = 2.75$ TeV.
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