Search for new phenomena in high-mass final states with a photon and a jet from $pp$ collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector

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Abstract A search is performed for new phenomena in events having a photon with high transverse momentum and a jet collected in 36.7 fb$^{-1}$ of proton--proton collisions at a centre-of-mass energy of $\sqrt{s} = 13$ TeV recorded with the ATLAS detector at the Large Hadron Collider. The invariant mass distribution of the leading photon and jet is examined to look for the resonant production of new particles or the presence of new high-mass states beyond the Standard Model. No significant deviation from the background-only hypothesis is observed and cross-section limits for generic Gaussian-shaped resonances are extracted. Excited quarks hypothesized in quark compositeness models and high-mass states predicted in quantum black hole models with extra dimensions are also examined in the analysis. The observed data exclude, at 95% confidence level, the mass range below 5.3 TeV for excited quarks and 7.1 TeV (4.4 TeV) for quantum black holes in the Arkani-Hamed–Dimopoulos–Dvali (Randall–Sundrum) model with six (one) extra dimensions.

1 Introduction

This paper reports a search for new phenomena in events with a photon and a jet produced from proton–proton ($pp$) collisions at $\sqrt{s} = 13$ TeV, collected with the ATLAS detector at the Large Hadron Collider (LHC). Prompt photons in association with jets are copiously produced at the LHC, mainly through quark–gluon scattering ($qg \rightarrow q\gamma$). The $\gamma +$ jet(s) final state provides a sensitive probe for a class of phenomena beyond the Standard Model (SM) that could manifest themselves in the high invariant mass ($m_{\gamma j}$) region of the $\gamma +$ jet system. The search is performed by looking for localized excesses of events in the $m_{\gamma j}$ distribution with respect to the SM prediction. Two classes of benchmark signal models are considered.

The first class of benchmark models is based on a generic Gaussian-shaped mass distribution with different values of its mean and standard deviation. This provides a generic interpretation for the presence of signals with different Gaussian widths, ranging from a resonance with a width similar to the reconstructed $m_{\gamma j}$ resolution of $\sim 2\%$ to wide resonances with a width up to 15%. The second class of benchmark models is based on signals beyond the SM that are implemented in Monte Carlo (MC) simulation and appear as broad peaks in the $m_{\gamma j}$ spectrum. This paper considers two scenarios for physics beyond the SM: quarks as composite particles and extra spatial dimensions. In the first case, if quarks are composed of more fundamental constituents bound together by some unknown interaction, new effects should appear depending on the value of the compositeness scale $\Lambda$. In particular, if $\Lambda$ is sufficiently smaller than the centre-of-mass energy, excited quark ($q^*$) states may be produced in high-energy $pp$ collisions at the LHC [1–3]. The $q^*$ production at the LHC could result in a resonant peak at the mass of the $q^*$ ($m_q^*$) in the $m_{\gamma j}$ distribution if the $q^*$ can decay into a photon and a quark ($qg \rightarrow q^* \rightarrow q\gamma$). In the present search, only the SM gauge interactions are considered for $q^*$ production. In the second scenario, the existence of extra spatial dimensions (EDs) is assumed to provide a solution to the hierarchy problem [4–6]. Certain types of ED models predict the fundamental Planck scale $M^*$ in the $4+n$ dimensions ($n$ being the number of extra spatial dimensions) to be at the TeV scale, and thus accessible in $pp$ collisions at $\sqrt{s} = 13$ TeV at the LHC. In such a TeV-scale $M^*$ scenario of the extra dimensions, quantum black holes (QBHs) may be produced at the LHC as a continuum above the threshold mass ($M_{\text{th}}$) and then decay into a small number of final-state particles including photon–quark/gluon pairs before they are able to thermalize [7–10]. In this case a broad resonance-like structure could be observed just above $M_{\text{th}}$ on top of

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The ATLAS detector at the LHC is a multi-purpose, forward-backward symmetric detector\(^1\) with almost full solid angle coverage, and is described in detail elsewhere [20–21]. Most relevant for this analysis are the inner detector (ID) and the calorimeter system composed of electromagnetic (EM) and hadronic calorimeters. The ID consists of a silicon pixel detector, a silicon microstrip tracker and a transition radiation tracker, all immersed in a 2 T axial magnetic field, and provides charged-particle tracking in the range \(|\eta| < 2.5\). The electromagnetic calorimeter is a lead/liquid-argon (LAr) sampling calorimeter with accordion geometry. The calorimeter is divided into a barrel section covering \(|\eta| < 1.475\) and two endcap sections covering 1.375 < \(|\eta| < 3.2\). For \(|\eta| < 2.5\) it is divided into three layers in depth, which are finely segmented in \(\eta\) and \(\phi\). In the region \(|\eta| < 1.8\), an additional thin LAr presampler layer is used to correct for fluctuations in the energy losses in the material upstream of the calorimeters. The hadronic calorimeter is a sampling calorimeter composed of steel/scintillator tiles in the central region (\(|\eta| < 1.7\)), while copper/LAr modules are used in the endcap (1.5 < \(|\eta| < 3.2\) regions. The forward regions (3.1 < \(|\eta| < 4.9\) are instrumented with copper/LAr and tungsten/LAr calorimeter modules optimized for electromagnetic and hadronic measurements, respectively. Surrounding the calorimeters is a muon spectrometer that includes three air-core superconducting toroidal magnets and multiple types of tracking chambers, providing precision tracking for muons within \(|\eta| < 2.7\) and trigger capability within \(|\eta| < 2.4\).

A dedicated two-level trigger system is used for the online event selection [22]. Events are selected using a first-level trigger implemented in custom electronics, which reduces the event rate to a design value of 100kHz using a subset of the detector information. This is followed by a software-based trigger that reduces the accepted event rate to 1kHz on average by refining the first-level trigger selection.

3 Data and Monte Carlo simulations

The data sample used in this analysis was collected from \(pp\) collisions in the 2015–2016 LHC run at a centre-of-mass energy of 13 TeV, and corresponds to an integrated luminosity

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\(^1\) ATLAS uses a right-handed coordinate system with its origin at the nominal interaction point (IP) in the centre of the detector and the \(z\)-axis along the beam pipe. The \(x\)-axis points from the IP to the centre of the LHC ring, and the \(y\)-axis points upwards. Cylindrical coordinates \((r, \phi)\) are used in the transverse plane, \(\phi\) being the azimuthal angle around the \(z\)-axis. The pseudorapidity is defined in terms of the polar angle \(\theta\) as \(\eta = -\ln \tan(\theta/2)\). Angular distance is measured in units of \(\Delta R = \sqrt{(\Delta\eta)^2 + (\Delta\phi)^2}\).
of $36.7 \pm 1.2$ fb$^{-1}$. The uncertainty was derived, following a methodology similar to that detailed in Ref. [23], from a preliminary calibration of the luminosity scale using $x-y$ beam-separation scans performed in August 2015 and May 2016. The data are required to satisfy a number of quality criteria ensuring that the relevant detectors were operational while the data were recorded.

Monte Carlo samples of simulated events are used to study the background modelling for the dominant $\gamma + \text{jet}$ processes, to optimize the selection criteria and to evaluate the acceptance and selection efficiencies for the signals considered in the search. Events from SM processes containing a photon with associated jets were simulated using the SHERPA 2.1.1 [24] event generator, requiring a photon transverse energy $E_T^{\gamma}$ above 70 GeV at the generator level. The matrix elements were calculated with up to four final state partons at leading order (LO) in quantum chromodynamics (QCD) and merged with the parton shower [25] using the ME+PS@LO prescription [26]. The CT10 [27] parton distribution function (PDF) set was used in conjunction with dedicated parton shower tuning developed by the SHERPA authors. A second sample of SM $\gamma + \text{jet}$ events was generated using the LO PYTHIA 8.186 [28] event generator with the LO NNPDF 2.3 PDFs [29] and the A14 tuning of the underlying-event parameters [30]. The PYTHIA simulation includes leading-order $\gamma + \text{jet}$ events from both the direct processes (the hard subprocesses $qg \rightarrow q\gamma$ and $g\bar{q} \rightarrow g\gamma$) and bremsstrahlung photons in QCD dijet events. To estimate the systematic uncertainty associated with the background modelling, a large sample of events was generated with the next-to-leading-order (NLO) JETPHOX v1.3.1.2 [31] program. Events were generated at parton level for both the direct and fragmentation photon contributions using the NLO photon fragmentation functions [32] and the NLO NNPDF 2.3 PDFs, and setting the renormalization, factorization and fragmentation scales to the photon $E_T^{\gamma}$. Jets of partons are reconstructed using the anti-$k_t$ algorithm [33,34] with a radius parameter of $R = 0.4$. The generated photon is required to be isolated by ensuring that the total transverse energy of partons inside a cone of size $\Delta R = 0.4$ around the photon is smaller than $7.07 \text{ GeV} + 0.03 \times E_T^{\gamma}$, equivalent$^2$ to the photon selection for the data described in Sect. 4.

Samples of excited quark events were produced using PYTHIA 8.186 with the LO NNPDF 2.3 PDFs and the A14 set of tuned parameters for the underlying event. The Standard Model gauge interactions and the magnetic-transition type couplings [1–3] to gauge bosons were considered in the production processes of the excited states of the first-generation quarks ($u^*, d^*$) with degenerate masses. The compositeness scale $\Lambda$ was taken to be equal to the mass $m_{q^*}$ of the excited quark, and the coefficients $f_s$, $f_f$ and $f'$ of magnetic-transition type couplings to the respective SU(3), SU(2) and U(1) gauge bosons were chosen to be unity. The $q^*$ samples were generated with $m_{q^*}$ values between 0.5 and 6.0 TeV in steps of 0.5 TeV.

The QBH samples were generated using the QBH 2.02 [35] event generator with the CTEQ6L1 [36] PDF set and PYTHIA 8.186 for the parton shower and underlying event tuned with the A14 parameter set. The $M_{th}$ values were chosen to vary between 3.0 (1.0) and 9.0 (7.0) TeV in steps of 0.5 TeV for the QBH signals in the ADD (RS1) model. All the $qg$, $\bar{q}g$, $gg$ and $q\bar{q}$ processes were included in the QBH signal production while only final states with a photon and a quark/gluon were considered for the decay. All six quark flavours were included together with their anti-quark counterparts in both the production and decay processes.

Apart from the sample generated with JETPHOX which is a parton-level calculator, all the simulated samples include the effects of multiple $pp$ interactions in the same and neighbours bunch crossings (pile-up) and were processed through the ATLAS detector simulation [37] based on GEANT4 [38]. Pile-up effects were emulated by overlaying simulated minimum-bias events from PYTHIA 8.186, generated with the A2 tune [39] for the underlying event and the MSTW2008LO PDF set [40]. The number of overlaid minimum-bias events was adjusted to match the one observed in data. All the MC samples except for the JETPHOX sample were reconstructed with the same software as that used for collision data.

4 Event selection

Photons are reconstructed from clusters of energy deposits in the EM calorimeter as described in Ref. [41]. A photon candidate is classified depending on whether the EM cluster is associated with a conversion track candidate reconstructed in the ID. If no ID track is matched, the candidate is considered as an unconverted photon. If the EM cluster is matched to either a conversion vertex formed from two tracks constrained to originate from a massless particle or a single track with its first hit after the innermost layer of the pixel detector, the candidate is considered to be a converted photon. Both the converted and unconverted photon candidates are used in the analysis. The energy of each photon candidate is corrected using MC simulation and data as described in Ref. [42]. The EM energy clusters are calibrated separately for converted and unconverted photons, based on their properties including the longitudinal shower development. The energy scale and resolution of the photon candidates after the MC-based calibration are further adjusted based on a correction derived using $Z \rightarrow e^+e^-$ events from
data and MC simulation. Photon candidates are required to have $E_T > 25$ GeV and $|\eta| < 2.37$ and satisfy the “tight” identification criteria defined in Ref. [41]. Photons are identified based on the profile of the energy deposits in the first two layers of the EM calorimeter and the energy leakage into the hadronic calorimeter. To further reduce the contamination from $\pi^0 \rightarrow \gamma\gamma$ or other neutral hadrons decaying into photons, the photon candidates are required to be isolated from other energy deposits in an event. The calorimeter isolation variable $E_{T,iso}$ is defined as the sum of the $E_T$ of all positive-energy topological clusters [43] reconstructed within a cone of $\Delta R = 0.4$ around the photon direction excluding the energy deposits in an area of size $\Delta \eta \times \Delta \phi = 0.125 \times 0.175$ centred on the photon cluster. The photon energy expected outside the excluded area is subtracted from the isolation energy while the contributions from pile-up and the underlying event are subtracted event by event [44]. The photon candidates are required to have $E_{T,iso} > 0.022 \times E_T^\gamma$ less than 2.45 GeV. This $E_T^\gamma$-dependent selection requirement is used to guarantee an efficiency greater than 90% for signal photons in the $E_T^\gamma$ range relevant for this analysis. The efficiency for the signal photon selection varies from (90 ± 1)% to (83 ± 1)% for signal events with masses from 1 to 6 TeV. The dependency on the signal mass is mainly from the efficiency of the tight identification requirement while the isolation selection efficiency is approximately (99 ± 1)% over the full mass range.

Jets are reconstructed from topological clusters calibrated at the electromagnetic scale using the anti-$k_t$ algorithm with a radius parameter $R = 0.4$. The jets are calibrated to the hadronic energy scale by applying corrections derived from MC simulation and in situ measurements of relative jet response obtained from $Z + \text{jets}$, $\gamma + \text{jets}$ and multijet events at $\sqrt{s} = 13$ TeV [45–47]. Jets from pile-up interactions are suppressed by applying the jet vertex tagger [48], using information about tracks associated with the hard-scatter and pile-up vertices, to jets with $p_T^\text{jet} < 60$ GeV and $|\eta| < 2.4$. In order to remove jets due to calorimeter noise or non-collision backgrounds, events containing at least one jet failing to satisfy the loose quality criteria defined in Ref. [49] are discarded. Jets passing all the requirements and with $p_T^\text{jet} > 20$ GeV and $|\eta| < 4.5$ are considered in the rest of the analysis. Since a photon is also reconstructed as a jet, jet candidates in a cone of $\Delta R = 0.4$ around a photon are not considered.

This analysis selects events based on a single-photon trigger requiring at least one photon candidate with $E_T^\gamma > 140$ GeV which satisfies loose identification conditions [41] based on the shower shape in the second sampling layer of the EM calorimeter and the energy leakage into the hadronic calorimeter. Selected events are required to contain at least one primary vertex with two or more tracks with $p_T > 400$ MeV. Photon candidates are required to satisfy the “tight” identification and isolation conditions discussed above. The kinematic requirements for the highest-$E_T$ photon in the events are tightened to $E_T^\gamma > 150$ GeV and $|\eta| < 1.37$. The $E_T^\gamma$ requirement is used to select events with nearly full trigger efficiency [50] while the $|\eta|$ requirement is imposed to enhance the signal-to-background ratio. Moreover, an event is rejected if there is any jet with $p_T^\text{jet} > 30$ GeV within $\Delta R < 0.8$ around the photon. The presence of additional tight and isolated photons with $E_T^\gamma > 150$ GeV in events is negligible for both signal and background events, and therefore allowed. The $\gamma + \text{jet}$ system is formed from the highest-$E_T$ photon and the highest-$p_T$ jet in the event. Finally, the highest-$p_T$ jet in the event is required to have $p_T^\text{jet} < 60$ GeV and the pseudorapidity difference between the photon and the jet ($\Delta \eta_{\gamma j} \equiv |\eta^\gamma - \eta^\text{jet}|$) must be less than 1.6 to enhance signals over the $\gamma +$ jet background, which typically has a large $\Delta \eta_{\gamma j}$ value. After applying all the selection requirements, $6.34 \times 10^5$ events with an invariant mass $(m_{\gamma j})$ of the selected $\gamma +$ jet system greater than 500 GeV remain in the data sample.

5 Statistical analysis

The data are examined for the presence of a significant deviation from the SM prediction using a test statistic based on a profile likelihood ratio [51]. Limits on the visible cross-section times branching ratio for specific benchmark models are computed using the CLS prescription [52]. The details of the signal and background modelling used for the likelihood function construction are discussed in Sects. 5.1 and 5.2 while a summary of the statistical procedures used to establish the presence of a signal or set limits on the production cross-sections for new phenomena is given in Sect. 5.3.

5.1 Signal modelling

The signal model is built starting from the probability density function (pdf), $f_{\text{sig}}(m_{\gamma j})$, of the $m_{\gamma j}$ distribution at the reconstruction level. For a Gaussian-shaped resonance with mass $m_G$, the $m_{\gamma j}$ pdf is modelled by a normalized Gaussian distribution with the mean located at $m_{\gamma j} = m_G$. The standard deviation of the Gaussian distribution is chosen to be 2, 7 or 15% of $m_G$, where 2% approximately corresponds to the effect of the detector resolution on the reconstruction of the photon–jet invariant mass. For the $q^+q^-$ and QBH signals, the $m_{\gamma j}$ pdfs are created from the normalized reconstructed $m_{\gamma j}$ distributions after applying the selection requirements described in Sect. 4 using the simulated MC events, and a kernel density estimation technique [53] is applied to smooth the distributions. The signal pdfs for intermediate mass points at
which signal events were not generated are obtained from the simulated signal samples by using a moment-morphing method [54]. The signal template for the \(q^*\) and QBH signals is then constructed as \(f_{\text{sig}}(m_{\gamma j}) \times (\sigma \cdot B \cdot A \cdot \varepsilon) \times \mathcal{L}_{\text{int}}\), where the \(f_{\text{sig}}\) is scaled by the product of the cross-section times branching ratio to a photon and a quark or gluon \(\sigma \cdot B\), acceptance \((A)\), selection efficiency \((\varepsilon)\) and the integrated luminosity \(\mathcal{L}_{\text{int}}\) for the data sample. The product of the acceptance times efficiency \((A \cdot \varepsilon)\) is found to be about 50% for all the \(q^*\) and QBH models, varying only by a few percent with \(m_{q^*}\) or \(M_{\text{th}}\). This dependence is accounted for in the model by interpolating between the generated mass points using a third-order spline. For the \(q^*\) and QBH signals, limits are set on \(\sigma \cdot B\) after correcting for the acceptance and efficiency \(A \cdot \varepsilon\) of the selection criteria.

Experimental uncertainties in the signal yield arise from uncertainties in the luminosity \((\pm 3.2\%)\), photon identification efficiency \((\pm 2\%)\), trigger efficiency \((\pm 1\%\) as measured in Ref. [50]) and pile-up dependence \((\pm 1\%)\). The impact of the uncertainties in the photon isolation efficiency, photon and jet energy scales and resolutions is negligible. A 1% uncertainty in the signal yield is included to account for the statistical error in the acceptance and selection efficiency estimates due to the limited size of the MC signal samples. The impact of the PDF uncertainties on the signal acceptance is found to be negligible compared to the other uncertainties. The photon and jet energy resolution uncertainties \((\pm 2\%\) of the mass) are accounted for as a variation of the width for the Gaussian-shaped signals. The impact of the resolution uncertainty on intrinsically large width signals is found to be negligible and thus not included in the signal models for the \(q^*\) and QBH. The typical difference between the peaks of the reconstructed and generator-level \(m_{\gamma j}\) distributions for the excited-quark signals is well below 1%.

A summary of systematic uncertainties in the signal yield and shape included in the statistical analysis is given in Table 1.

In order to facilitate the re-interpretation of the present results in alternative physics models, the fiducial acceptance and efficiency for events with the invariant mass of the \(\gamma + \) jet system around \(m_{q^*}\) or \(M_{\text{th}}\) (referred to as “on-shell” events hereafter) are also provided. The chosen \(m_{\gamma j}\) ranges are \(0.6m_{q^*} < m_{\gamma j} < 1.2m_{q^*}\) for the \(q^*\) signal and \(0.8M_{\text{th}} < m_{\gamma j} < 3.0M_{\text{th}}\) for the QBH signal. The fiducial region at particle level, as summarized in Table 2, is chosen to be close to the one used in the event selection at reconstruction level.

The fiducial acceptance \(A_f\), defined as the fraction of generated on-shell signal events falling into the fiducial region, increases from 56 to 63% with increasing signal mass \(M_{\text{th}}\) from 1.0 to 6.5 (9.0) TeV for the QBH in the RS1 (ADD) model. The \(A_f\) value for the \(q^*\) model varies very similarly to that for the RS1 QBH signal. The rise in the fiducial acceptance as a function of \(M_{\text{th}}\) \((m_{q^*})\) is driven mainly by the increase of the efficiency for the photon \(\eta\) requirement since the photons tend to be more central as \(M_{\text{th}}\) \((m_{q^*})\) becomes larger.

The fiducial selection efficiency \(\varepsilon_f\) is defined as the ratio of the number of on-shell events in the particle-level fiducial region passing the selection at the reconstruction level, including photon identification, isolation and jet quality criteria, to the number of generated on-shell events in the particle-level fiducial region. The migration of generated on-shell events outside the particle-level fiducial region into the selected sample at the reconstruction level is found to be negligible. The fiducial selection efficiency decreases from 88 (86) to 82 (80)% within the same \(M_{\text{th}}\) ranges as above for the RS1 (ADD) QBH model and is not highly dependent on the kinematics of the assumed signal production processes. The \(\varepsilon_f\) for the \(q^*\) model behaves very similarly to that for the RS1 QBH model. The reduction in the fiducial selection efficiency is caused mainly by the inefficiency of the shower shape requirements used in the photon identification for high-\(E_T\) photons. The fiducial acceptance and selection efficiencies for the three benchmark signal models are shown in Fig. 1 as functions of \(m_{q^*}\) or \(M_{\text{th}}\).

### Table 1 Summary of systematic uncertainties in the signal event yield and shape included in the fit model. The signal mass resolution uncertainty affects the generic Gaussian signal shape, while the other uncertainties affect the signal yield.

<table>
<thead>
<tr>
<th>Uncertainty</th>
<th>(q^*) and QBH</th>
<th>Generic Gaussian</th>
</tr>
</thead>
<tbody>
<tr>
<td>Signal mass resolution</td>
<td>N/A</td>
<td>\pm 2% \cdot m_G</td>
</tr>
<tr>
<td>Photon identification</td>
<td>\pm 2%</td>
<td>N/A</td>
</tr>
<tr>
<td>Trigger efficiency</td>
<td>\pm 1%</td>
<td>N/A</td>
</tr>
<tr>
<td>Pile-up dependence</td>
<td>\pm 1%</td>
<td>N/A</td>
</tr>
<tr>
<td>MC event statistics</td>
<td>\pm 1%</td>
<td>N/A</td>
</tr>
<tr>
<td>Luminosity</td>
<td>\pm 3.2%</td>
<td>N/A</td>
</tr>
</tbody>
</table>

### Table 2 Requirements on the photon and jet at particle level to define the fiducial region and on the detector-level quantities for the selection efficiency.

<table>
<thead>
<tr>
<th>Requirement</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Photon-level selection for fiducial region</td>
<td></td>
</tr>
<tr>
<td>Photon: (E_T^\gamma &gt; 150) GeV, (</td>
<td>\eta^\gamma</td>
</tr>
<tr>
<td>Jet: (p_T^{\text{jet}} &gt; 60) GeV, (</td>
<td>\eta^{\text{jet}}</td>
</tr>
<tr>
<td>Photon–Jet (\eta) separation: (</td>
<td>\Delta \eta_{\gamma j}</td>
</tr>
<tr>
<td>No jet with (p_T^{\text{jet}} &gt; 30) GeV within (</td>
<td>\Delta R &lt; 0.8) around the photon</td>
</tr>
<tr>
<td>Detector-level selection for selection efficiency</td>
<td></td>
</tr>
<tr>
<td>Tight photon identification</td>
<td></td>
</tr>
<tr>
<td>Photon isolation</td>
<td></td>
</tr>
<tr>
<td>Jet identification including quality and pile-up rejection requirements</td>
<td></td>
</tr>
</tbody>
</table>
5.2 Background modelling

The $m_{\gamma j}$ distribution of the background is modelled using a functional form. A family of functions, similar to the ones used in the previous searches for $\gamma + \text{jet}$ [13,14,16] and $\gamma \gamma$ resonances [55] as well as dijet resonances [17] is considered:

$$f_{\text{bg}}(x) = N (1 - x)^p \sum_{i=0}^k a_i (\log x)^i,$$

where $x$ is defined as $m_{\gamma j}/\sqrt{s}$, $p$ and $a_i$ are free parameters, and $N$ is a normalization factor. The number of free parameters describing the normalized mass distribution is thus $k + 2$ with a fixed $N$, where $k$ is the stopping point of the summation in Eq. (1). The normalization $N$ as well as the shape parameters $p$ and $a_i$ are simultaneously determined by the final fit of the signal plus background model to data. The goodness of a given functional form in describing the background is quantified based on the potential bias introduced in the fitted number of signal events. To quantify this bias the functional form under test is used to perform a signal + background prediction. The large sample of background events built from the JETPHOX prediction. The large JETPHOX event sample is used for this purpose as the shape of the background prediction can be extracted with sufficiently small statistical uncertainty.

The parton-level JETPHOX calculations do not account for effects from hadronization, the underlying event and the detector resolution. Therefore, the nominal JETPHOX prediction is corrected by calculating the ratio of reconstructed jet $p_T$ to parton $p_T$ in the SHERPA $\gamma + \text{jet}$ sample and applying the parameterized ratio to the JETPHOX parton $p_T$. In addition, an $m_{\gamma j}$-dependent correction is applied to the JETPHOX prediction to account for the contribution from multijet events where one of the jets is misidentified as a photon (fake photon events). This correction is estimated from data as the inverse definition is detailed in Table 2. The description of the selection criteria can be found in the text

![Fig. 1](a) Fiducial acceptance and (b) selection efficiencies for the three signal models considered in the analysis as a function of the excited-quark mass $m_{\gamma^*}$ or the QBH threshold mass $M_{\text{th}}$. The fiducial region
purity (4% at $1.0 < m_{\gamma j} < 1.1$ TeV). The measured purity is approximately constant at 93% over the $m_{\gamma j}$ range above 500 GeV, indicating that the fake-photon contribution does not depend significantly on $m_{\gamma j}$. Figure 3 shows the $m_{\gamma j}$ distribution in data compared to the corrected JETPHOX $\gamma$ + jet prediction normalized to data in the $m_{\gamma j} > 500$ GeV region.

Theoretical uncertainties in the JETPHOX prediction are computed by considering the variations induced by $\pm 1\sigma$ of the NNPDF 2.3 PDF uncertainties, by switching between the nominal NNPDF 2.3 and CT10 or MSTW2008 PDFs, by the variation of the value of the strong coupling constant by $\pm 0.002$ around the nominal value of 0.118 and by the variation of the renormalization, factorization and fragmentation scales between half and twice the photon transverse momentum. The differences between data and the corrected JETPHOX prediction shown in Fig. 3 are well within the uncertainties associated with the perturbative QCD prediction.

The number of signal events extracted by the signal + background fit to the pure background model described above is called the spurious signal [57] and it is used to select the optimal functional form and the $m_{\gamma j}$ range of the fit. In order to account for the assumption that the corrected JETPHOX prediction itself is a good representation of the data, the fit is repeated on modified samples obtained by changing the nominal shape to account for several effects: firstly, the nominal distribution is corrected to follow the envelope of the changes induced by $\pm 1\sigma$ variations of the NNPDF 2.3 PDF uncertainty, the variations between the nominal NNPDF 2.3 and CT10 or MSTW2008 PDFs, the variation of the value of the strong coupling constant by $\pm 0.002$ around the nominal value of 0.118 and the variation of the renormalization, factorization and fragmentation scales between half and twice the photon transverse momentum; secondly the corrections for the hadronization, underlying event and detector effects are removed; and finally the corrections for the photon purity are changed within their estimated uncertainty. The largest absolute fitted signal from all variations of the nominal background sample discussed above is taken to be the spurious signal.

The spurious signal is evaluated at a number of hypothetical masses over a large search range. It is required to be less than 40% of the background’s statistical uncertainty, as
quantified by the statistical uncertainty of the fitted spurious signal, anywhere in the investigated search range. In this way the impact of the systematic uncertainties due to background modelling on the analysis sensitivity is expected to be subdominant with respect to the statistical uncertainty. Functional forms that cannot meet this requirement are rejected. For different signal models, the functional form and fit range are determined separately. All considered functions with \( k \) up to two (four parameters) are found to fulfills the spurious-signal requirement when fitting in the range \( 1.1 < m_{\gamma j} < 6.0 \) TeV for the \( q^* \) signal and \( 1.5 (2.5) < m_{\gamma j} < 6.0 (8.0) \) TeV for the RS1 (ADD) QBH signal. To further consolidate the choice of nominal background functional form, an \( F \) test [58] is performed to determine if the change in the \( \chi^2 \) value obtained by fitting the JETPHOX sample with an additional parameter is significant. The test indicates that the \( k = 0 (1) \) functional form with two (three) parameters can describe the present data sufficiently well over the entire fit range for the QBH \( (q^*) \) signal search, and there is no improvement by adding more parameters to the background fit function.

<table>
<thead>
<tr>
<th>Search boundaries (TeV)</th>
<th>(q^*)</th>
<th>RS1 QBH</th>
<th>ADD QBH</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \sigma_{\text{spur}} ) (fb)</td>
<td>3.9</td>
<td>4.0</td>
<td>8.7 \times 10^{-2}</td>
</tr>
<tr>
<td>( \sigma_{\text{spur}/\sigma_{\text{spur}}}(%) )</td>
<td>37</td>
<td>39</td>
<td>20</td>
</tr>
<tr>
<td>( \sigma_{\text{spur}/\sigma_{\text{model}}}(%) )</td>
<td>0.16</td>
<td>1.0</td>
<td>0.0017</td>
</tr>
</tbody>
</table>

5.3 Statistical tests

A profile-likelihood-ratio test statistic is used to quantify the compatibility between the data and the SM background prediction, and to set limits on the presence of possible signal contributions in the \( m_{\gamma j} \) distribution. The likelihood function \( \mathcal{L} \) is built from a Poisson probability for the numbers of observed events, \( n \), and expected events, \( N \), in the selected sample:

\[
\mathcal{L} \propto \text{Pois}(n|N(\theta)) \times \left( \prod_{i=1}^{n} f(m_{\gamma j}^i, \theta) \right) \times G(\theta),
\]

where \( N(\theta) \) is the expected number of candidates, \( f(m_{\gamma j}^i, \theta) \) is the value of the probability density function of the invariant mass distribution evaluated for each candidate event \( i \) and \( \theta \) are nuisance parameters. The \( G(\theta) \) term collects the set of constraints on the nuisance parameters associated with the systematic uncertainties in the signal yield, in the spurious signal and in the resolution (only for Gaussian signals) and it is represented by normal distributions centred at zero and with unit variance.

The pdf of the \( m_{\gamma j} \) distribution is given as the normalized sum of the signal and background pdfs:

\[
f(m_{\gamma j}^i, \theta) = \frac{1}{N} \left[ N_{\text{sig}}(\theta_{\text{yield}}) f_{\text{sig}}(m_{\gamma j}^i) + N_{\text{bg}} f_{\text{bg}}(m_{\gamma j}^i, \theta_{\text{bg}}) \right],
\]

where \( f_{\text{sig}} \) and \( f_{\text{bg}} \) are the normalized signal and background \( m_{\gamma j} \) distributions described in the previous sections. The \( \theta_{\text{yield}} \) are nuisance parameters associated with the signal yield uncertainties (constrained) while \( \theta_{\text{bg}} \) are the nuisance parameters of the background shape (unconstrained). The expected number of events \( N \) is given by the sum of the expected numbers of signal events \( (N_{\text{sig}}) \) and background events \( (N_{\text{bg}}) \). The \( N_{\text{sig}} \) term can be expressed as...
Fig. 4 Distributions of the invariant mass of the $\gamma + \text{jet}$ system of the observed events (dots) in 36.7 $fb^{-1}$ of data at $\sqrt{s} = 13$ TeV and fits to the data (solid lines) under the background-only hypothesis for searches in the a excited quarks, b QBH (RS1) with $n = 1$ and c QBH (ADD) with $n = 6$ models. The $\pm 1\sigma$ uncertainty in the background prediction originating from the uncertainties in the fit function parameter values is shown as a shaded band around the fit. The predicted signal distributions (dashed lines) for the $q^*$ model with $m_{q^*} = 5.5$ TeV and the QBH model with $M_B = 4.5$ (7.0) TeV based on RS1 (ADD) are shown on top of the background predictions. The bottom panels show the bin-by-bin significances of the data–fit differences, considering only statistical uncertainties.

Fig. 5 Observed (solid lines) and expected (dotted lines) 95% CL upper limits on the visible cross-sections $\sigma \cdot B \cdot A \cdot \varepsilon$ in 36.7 $fb^{-1}$ of data at $\sqrt{s} = 13$ TeV as a function of the mass $m_{\gamma}$ of the Gaussian resonances with three different Gaussian widths between 2 and 15%. The calculation is performed using ensemble tests at mass points separated by 100 GeV over the search range $m_{\gamma}$.

$$N_{\text{sig}}(\theta_{\text{yield}}) = N_{\text{sig}}^{\text{model}} + N_{\text{sig}}^{\text{spur}}$$

$$= (\sigma_{\text{model}} \cdot B \cdot A \cdot \varepsilon \cdot F(\delta_{\gamma}, \theta_{\gamma}) + \sigma_{\text{spur}} \cdot \theta_{\text{spur}}) \cdot \mathcal{L}_{\text{int}} \times F(\delta_{\mathcal{L}}, \theta_{\mathcal{L}}),$$

where $\sigma_{\text{spur}}$ and $\theta_{\text{spur}}$ are the spurious-signal cross-section and its nuisance parameter while $\mathcal{L}_{\text{int}}$ and $F(\delta_{\mathcal{L}}, \theta_{\mathcal{L}})$ are the integrated luminosity and its uncertainty. Apart from the spurious signal, systematic uncertainties with an estimated size $\delta_{\mathcal{X}}$ are incorporated into the likelihood by multiplying the relevant parameter of the statistical model by a factor $F(\delta_{\gamma}, \theta_{\gamma}) = e^{\delta_{\mathcal{X}}\theta_{\gamma}}$. The parameter of interest in the fit to Gaussian-shaped resonances is the visible cross-section $\sigma_{\text{model}} \cdot B \cdot A \cdot \varepsilon$ while that in the fit to $q^*$ and QBH signals is $\sigma_{\text{model}} \cdot B$. For the latter case, the additional nuisance parameters for the signal efficiency uncertainties $F(\delta_{\gamma}, \theta_{\gamma})$ are included.

The significance of a possible deviation from the SM prediction is estimated by computing the $p_0$ value, defined as the probability to observe, under the background model hypothesis, an excess at least as large as the one observed in data. Upper limits are set at 95% confidence level (CL) with a modified frequentist CL$_S$ method on the visible cross-section $(\sigma_{\text{model}} \cdot B \cdot A \cdot \varepsilon)$ for the Gaussian-shaped resonances or on the signal cross-section times branching ratio $(\sigma_{\text{model}} \cdot B)$ for the $q^*$ and QBH signals by identifying the value for which the CL$_S$ value is equal to 0.05.

6 Results

The photon–jet invariant mass distributions obtained from the selected data are shown in Fig. 4, together with the
Fig. 6 Observed 95% CL upper limits (solid line with dots) on the production cross-section times branching ratio to a photon and a quark or gluon for the excited-quark and QBH signals. The limits are placed as a function of $m_\gamma$ for the excited quarks and $M_{QBH}$ for the QBH signals. The calculation is performed using ensemble tests at mass points separated by 200 (500) GeV for the RS1 (ADD) model over the search range. For the $q^*$ model the step size is 250 GeV up to 5 TeV and then 200 GeV up to 6 TeV. The limits expected if a signal is absent (dashed lines) are shown together with the $\pm 1\sigma$ and $\pm 2\sigma$ intervals represented by the green and yellow bands, respectively. The theoretical predictions of $\sigma \cdot B$ for the respective benchmark signals are shown by the red solid lines.
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