

Measurement of pairs of photons in LHC Run-2 proton–proton collisions with the ATLAS detector

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Abstract

The first differential cross section measurement of the production of pairs of prompt isolated photons in proton–proton collisions at $\sqrt{s} = 13$ TeV is performed. The full LHC Run-2 data recorded by ATLAS corresponding to an integrated luminosity of $\mathcal{L} = 139 \text{ fb}^{-1}$ is used. The differential cross sections are measured as a function of several kinematic variables of the photon pairs in a fiducial phase space characterized by a good detector performance. The event yields are corrected for background, detector resolution effects and detector inefficiencies and are compared to state-of-the-art QCD predictions. Good agreement to the measured results is observed for fixed-order NNLO calculations and for NLO calculations merged with Monte Carlo parton showers within the uncertainties. Furthermore, two auxiliary measurements are performed to determine inputs used for both the photon-pair measurement and other future measurements with the ATLAS detector that use electrons, photons or muons. A data-driven measurement of the pileup dependence of calorimetric isolation variables is performed using $Z \rightarrow ee$ events. The results of the measurement are used to develop an improved η -dependent pileup subtraction and show that the pileup noise is overestimated in MC samples. The second measurement uses $Z \rightarrow \mu\mu\gamma$ events to determine selection efficiencies of photons. The results include values for the inefficiency induced by rejecting electron-like photon candidates, which is part of the ATLAS photon reconstruction. Previously, this inefficiency was assumed to be well modelled in simulated samples, but the results show that a correction needs to be applied. This correction increases the result of the photon-pair cross section measurement by 1.8%.

Kurzfassung

Die erste differenzielle Wirkungsquerschnittsmessung der Produktion von Paaren prompter, isolierter Photonen in Proton–Proton Kollisionen bei Schwerpunktsenergien von $\sqrt{s} = 13$ TeV wird durchgeführt. Dabei wird der komplette LHC Run-2 Datensatz einbezogen, der mit dem ATLAS-Detektor aufgenommen wurde und einer integrierten Luminosität von $\mathcal{L} = 139 \text{ fb}^{-1}$ entspricht. Die differenziellen Wirkungsquerschnitte werden als Funktion unterschiedlicher kinematischer Variablen der Photonpaare in einem Referenz-Phasenraum gemessen, welcher sich durch eine gute Detektorleistungsfähigkeit auszeichnet. Die Ereigniszählraten werden um Untergrund, um Dektorauflösungseffekte und um Detektorineffizienzen korrigiert und mit den besten zur Verfügung stehenden QCD-Vorhersagen verglichen. Gute Übereinstimmung innerhalb der Unsicherheiten der gemessenen Werte mit NNLO-Berechnungen und mit NLO-Berechnungen in Verbindung mit Monte-Carl-Parton-Shower-Algorithmen wird beobachtet. Weiterhin werden zwei Hilfsmessungen durchgeführt die wichtige Eingangsgrößen bestimmen, welche sowohl für die Photonpaarmessung als auch für andere zukünftige Messungen mit dem ATLAS Detektor, die Endzustände mit Elektronen, Photonen oder Myonen untersuchen, verwendet werden. Eine datengetriebene Messung der Pileup-Abhängigkeit kalorimetrischer Isolationsvariablen wird anhand von $Z \rightarrow ee$ Ereignissen durchgeführt. Die Ergebnisse der Messung werden verwendet, um eine Verbesserte η -abhängige Pileup-Subtraktion zu entwickeln und zeigen eine Überschätzung des Pileup-Rauschens in MC Datensätzen. Die zweite Messung verwendet $Z \rightarrow \mu\mu\gamma$ Ereignisse um Selektionseffizienzen von Photonen zu bestimmen. Unter anderem wird die Ineffizienz des Verwerfens elektronenähnlicher Photonenkandidaten, das Teil der ATLAS-Photonenrekonstruktion ist, bestimmt. Bisher wurde davon ausgegangen, dass diese Ineffizienz gut durch die Simulation modelliert ist, aber die Ergebnisse zeigen, dass eine Korrektur erforderlich ist, welche das Ergebnis für den Wirkungsquerschnitt der Photonpaarmessung um 1.8% erhöht.

Contents

1. Introduction	3
2. Foundations	5
2.1. The Standard Model	5
2.2. Quantum Chromo Dynamics	7
2.3. Photon-pair production in hadron collisions	9
2.4. Previous measurements	11
3. The ATLAS Detector at the Large Hadron Collider	13
3.1. The Run-2 of the LHC	14
3.2. The ATLAS Detector	16
3.2.1. Inner Detector	17
3.2.2. Electromagnetic Calorimeter	18
3.2.3. Hadronic Calorimeter	20
3.2.4. Muon Spectrometer	21
3.2.5. Trigger	21
3.2.6. Processing of data and simulated samples	23
4. Photon reconstruction in ATLAS	25
4.1. Low-level inputs	25
4.1.1. Inner-detector tracks	25
4.1.2. Calorimeter clusters	26
4.2. Reconstruction	27
4.2.1. Electron-photon ambiguity resolution	28
4.3. Energy calibration	29
4.4. Photon identification	30
4.5. Isolation	33
5. Pileup dependency of calorimetric isolation variables	37
5.1. Data samples	37
5.2. MC samples	37
5.2.1. Pileup overlay	38
5.2.2. Pileup reweighting	38
5.3. Event Selection	38
5.4. Supercluster based core subtraction	40

5.5. Improved data-driven pileup subtraction	40
5.5.1. Motivation	42
5.5.2. Pileup subtraction as a function of η	43
5.5.3. Signal performance	47
5.5.4. Background rejection	50
5.6. Pileup-dependent correction of isolation variables in simulation	51
5.7. Pileup noise studies	52
6. Photon efficiency measurement using radiative $Z \rightarrow \mu\mu\gamma$ events	57
6.1. Data and MC samples	58
6.2. Event selection	58
6.3. Fit model	59
6.4. Systematic uncertainties	64
6.5. Results	66
6.5.1. Reconstruction efficiency	66
6.5.2. Interplay between conversion fractions and identification efficiencies	67
6.5.3. Identification-isolation correlation $R_{\gamma}^{\text{iso-id}}$	68
6.6. Conclusion	70
7. Diphoton Production Measurement	71
7.1. Data samples	73
7.2. Simulated samples	73
7.2.1. Diphoton signal samples	73
7.2.2. Electron background samples	74
7.2.3. γ +jet background	74
7.3. Event selection	75
7.4. Observables	75
7.5. Background estimation	79
7.5.1. Jet background	79
7.5.2. Signal parameters	83
7.5.3. Prompt-photon isolation and identification efficiencies in γj and $j\gamma$ events	85
7.5.4. Isolation–identification correlation for misidentified jets	85
7.5.5. Correlation parameters in γj and $j\gamma$ events	87
7.5.6. Electron background	88
7.5.7. Pileup background	88
7.5.8. Results	91
7.6. Unfolding	92
7.6.1. Fiducial correction	94
7.6.2. Resolution correction	95
7.6.3. Efficiency correction	97
7.6.4. Overall corrections	98
7.6.5. Particle-level isolation requirement	98
7.7. Uncertainties	101
7.7.1. Overview	102

7.7.2.	Systematic uncertainty estimation and combination method	102
7.7.3.	Background estimation	105
7.7.4.	Photon isolation	106
7.7.5.	Data-period stability	110
7.7.6.	Photon identification and reconstruction	114
7.7.7.	Photon energy scale	115
7.7.8.	Unfolding	118
7.7.9.	Data and MC statistical uncertainties	121
7.8.	Theory predictions	122
7.9.	Results	123
7.9.1.	Integrated fiducial cross section	123
7.9.2.	Differential cross sections	124
8.	Summary and Outlook	129
8.1.	Summary	129
8.2.	Outlook	130
A.	SHERPA-to-PYTHIA particle-level isolation reweighting	147
B.	Optimization of the detector-level isolation requirement	151
C.	Scale factors and anti-scale factors	155
D.	Additional figures of the diphoton measurement	159

Chapter 1.

Introduction

The modern understanding of light as an electromagnetic wave consisting of discrete quanta of energy, nowadays referred to as photons, was pioneered in the early 1900s [1, 2] and heralded the era of quantum physics. Today, the Standard Model of particle physics (SM) stands at the end of over a century of experimental insights and theoretical developments and describes physics based on the interaction of indivisible elementary particles. Scattering experiments were a core tool in resolving the internal structure of matter and thus finding these elementary particles: Starting from the discovery of the atomic nucleus [3], to finally arriving at the fundamental quarks [4, 5] and gluons [6–8]. The increasing energy of the incident particles of the collisions in the scattering experiments allowed to probe ever-smaller structures. The last elementary particle predicted by the SM, but evading experimental observation was the Higgs-boson. The Higgs-boson could finally be found in 2012 [9, 10] using proton–proton collisions at unprecedented energies of up to $\sqrt{s} = 8 \text{ TeV}$ produced by the LHC, which is the largest particle accelerator in the world with a circumference of around 27 km. The detection of highly energetic pairs of photons is one of the key experimental signatures used for the discovery of the Higgs-boson and subsequent measurements of its properties.

Quantum Chromo Dynamics (QCD) [11–15] is part of the SM and describes the strong force, which is mediated by gluons binding together quarks and thereby e.g. constituting the protons and neutrons which build up atomic nuclei. The outcome of proton–proton collisions at high energies is almost exclusively caused by the QCD interactions between the quarks and gluons of the different protons.

Already for one of the earliest photon measurements in proton–proton collisions, in a time where QCD was still being established, it was stated in Ref. [16] that: “At present, within the framework of QCD analyses, copious production of direct photons is one of the clearest predictions of this theory: provided this reaction is probed at large enough transverse momentum, the point-like coupling of the photon to the quarks should be at the origin of the dominant source for direct photons.”

This statement is still valid and illustrates two aspects. Photon production in proton–proton collisions is dominantly a QCD process, because photons couple to the electric charge of the quarks. Therefore QCD production of photons represents an important background which needs to be taken into account e.g. for the Higgs measurements mentioned above. Furthermore photons are a very clear signature to test QCD. They can be identified and measured with a very good resolution experimentally by detectors like ATLAS. In contrast to photons the creation of quarks and gluons can not be measured directly, but only by their manifestation as a jet of multiple particles.

The precise measurement of QCD photon-pair production presented in this thesis is a benchmark to

scrutinize QCD prediction on which the understanding of LHC physics is based. Different kinematic properties of the photon-pair system are measured. These kinematics of the photon-pair are related to additional quarks and gluons in the final state by transverse momentum-conservation. Photon pairs in back-to-back configurations are sensitive probes of even very low-energetic QCD emissions perpendicular to the photon-axis, which would be difficult to measure directly with the ATLAS detector.

This thesis is structured as follows. Chapters 2 to 4 summarize the foundations for the original scientific contributions in Chapters 5 to 7. In Chapter 2 an outline of the theoretical foundations and a short overview of previous photon-pair measurements in hadron collisions is given. In Chapter 3 some important aspects about the LHC and the ATLAS detector are summarized. Chapter 4 describes the algorithms used for the reconstruction of photon candidates. In Chapter 5 an auxiliary measurement of calorimetric isolation variables as a function of pileup in $Z \rightarrow ee$ events is presented. In Chapter 6 another measurement is performed which studies photon selection efficiencies in $Z \rightarrow \mu\mu\gamma$ events. Finally, in Chapter 7 the photon-pair measurement is presented, followed by a summary and outlook in Chapter 8.

Chapter 2.

Foundations

In this section the theoretical foundations of this thesis and previous photon-pair measurements are discussed. Only an overview is given fixing the terminology important for the measurement presented in this thesis. The Standard Model of particle physics is outlined in Section 2.1 and a few aspects of Quantum Chromo Dynamics are further discussed in Section 2.2. Theoretical predictions for the production of photon pairs in hadron collisions are discussed in Section 2.3. In Section 2.4 an overview of previous measurements is given.

2.1. The Standard Model

The Standard Model of particle physics (SM) is a relativistic quantum field theory describing all known elementary particles and their interactions. The SM is extremely successful in predicting experimental results with a high precision. The SM is based on the local gauge symmetries:

$$U(1)_Y \times SU(2)_L \times SU(3)_C. \quad (2.1)$$

The generators of the symmetry groups are connected to the particles mediating the three fundamental forces of nature described by the SM: The electromagnetic force, the weak force and the strong force. Gravitation is not part of the SM as it is much weaker than the other forces and thus not accessible at all planned or current particle-physics experiments.

The electroweak symmetry $U(1)_Y \times SU(2)_L$ is the basis for the electroweak theory [17–19] and is spontaneously broken by the Higgs mechanism [20–22] giving rise to the massless photon γ responsible for the electromagnetic interaction, the massive $W^\pm$ - and Z -boson responsible for the weak interaction and the Higgs particle h . Most of the everyday perception like light, mechanical forces or chemistry can be explained with electromagnetic interactions on a fundamental level. The weak interaction is important for nuclear physics, e.g. in the decay of natural radio-isotopes or in the fusion processes in stars.

The $SU(3)_C$ symmetry underpins Quantum Chromo Dynamics (QCD) [11–15], the theory of the strong interaction mediated by the massless gluons g . Although the Higgs mechanism is creating the mass of elementary particles the dynamics of QCD are responsible for most of the visible mass in the universe by building up protons and neutrons [23].

The conserved quantities, which are related to the symmetries of the SM through Noethers theorem

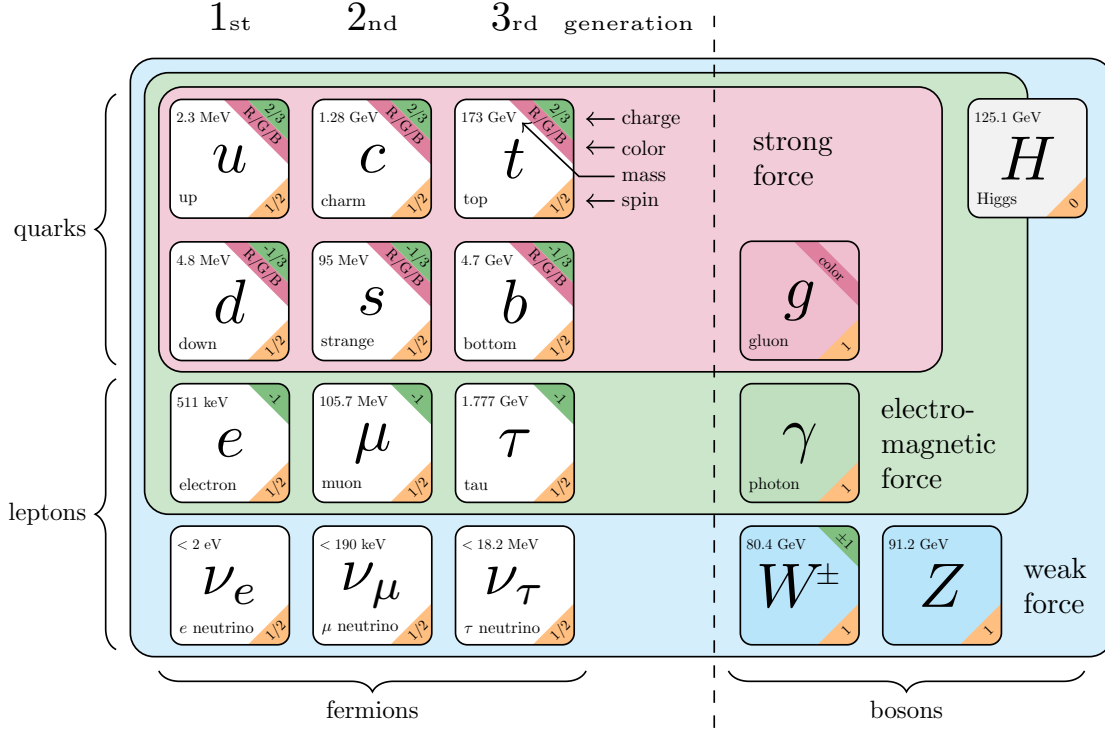


Figure 2.1.: Each small box represents one particle of the SM and its respective properties. The particles are grouped by their spin into fermions (left) and bosons (right). The fermions are subdivided into quarks (top) and leptons (bottom). The large coloured boxes contain all fermions which participate in a certain interaction. Adapted from [26].

[24, 25], are the electroweak charge Y , electroweak isospin I_W^3 and the colour charge C of QCD. After the electroweak symmetry breaking the $U(1)_Y \times SU(2)_L$ is reduced to $U(1)_Q$ with the electric charge $Q = \frac{1}{2}Y + I_W^3$ as the corresponding conserved quantity.

The particles contained in the SM with their respective charges and mass are summarized in Fig. 2.1. The integer-spin bosons γ , $W^\pm$, Z and g mediate the interactions between the spin-1/2 fermions, which are the building blocks of matter. The fermions are subdivided into quarks and leptons.

The quarks participate in all three forces of the SM including the strong force, because they carry a colour charge, which distinguishes them from the leptons. Quarks form colour neutral bound states called hadrons. Two-quark states are referred to as mesons and are unstable decaying to combinations of lighter hadrons, leptons and photons. Three-quark states, referred to as baryons, form the bulk of the stable matter as they include protons and neutrons, which consist of up quarks (u) and down quarks (d). The up and down quark are the lightest of the six quarks and form the so-called first generation, which is followed by the similar but heavier quarks charm (c) and strange (s) constituting the second generation; and the even heavier top (t) and bottom (b) forming the third generation.

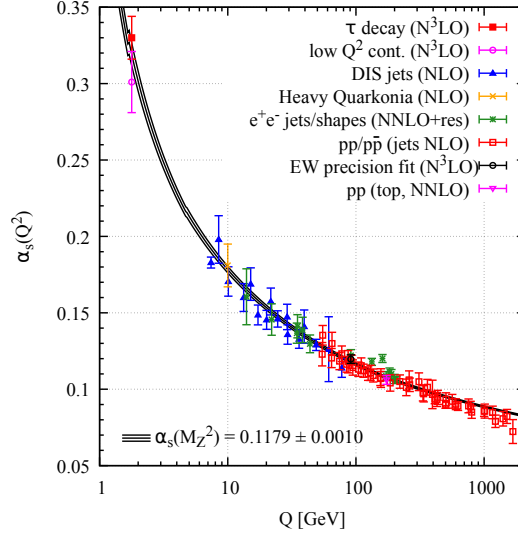


Figure 2.2.: Summary of measurements of the strong coupling α_s at different energy scales Q [30].

The leptons occur also in three generations consisting of the electrically charged electron e , muon μ and tau lepton τ and the respective electrically neutral neutrinos ν_e , ν_μ , ν_τ . Only the lightest charged lepton, the electron e , is stable. The neutrinos are the only particles which interact only via the weak force.

The quarks and leptons form left-handed doublets $(u, d)_L$, $(\ell, \nu_\ell)_L$ and right-handed singlets. The left-handed doublets undergo charged-current weak interactions with the $W^\pm$, while the right-handed singlets couple only to the neutral current of the Z -boson. The mass eigenstates of the particles are mixtures of these weak eigenstates of different generations and related to them by the CKM matrix [27, 28] for quarks and the PMNS matrix [29] for leptons. This mixture is enabling transitions between the different generations.

For each particle there is an anti-particle with opposite quantum numbers (charges).

2.2. Quantum Chromo Dynamics

One of the core pieces of the perturbative description of QCD is the running of the strong coupling constant $\alpha_s(Q)$ as a function of the energy scale Q of the interaction [13, 14]. The evolution of $\alpha_s(Q)$ is described by the renormalisation group equations of QCD. This means with a measured $\alpha_s(Q_{\text{meas}})$ at a fixed Q_{meas} the values at an arbitrary Q value can be predicted and measurements at different Q values can be used to check these predictions of QCD. In Fig. 2.2 measurements of α_s at different Q values are compared.

At low values of Q the strong coupling diverges indicating the breakdown of perturbative QCD calculations. The diverging coupling constant at low Q leads to the so-called confinement property of QCD, which prevents free colour charged particles. In contrast at high values of Q the coupling α_s becomes small, which is referred to as asymptotic freedom and enables precise predictions with fixed-order perturbative calculations at the renormalisation energy scale $\mu_R = Q$:

$$\sigma(\mu_R) = \sigma_{\text{LO}} + \left(\frac{\alpha_s(\mu_R)}{2\pi} \right) \Delta\sigma_{\text{NLO}} + \left(\frac{\alpha_s(\mu_R)}{2\pi} \right)^2 \Delta\sigma_{\text{NNLO}} + \dots \quad (2.2)$$

In high energy hadron collisions like at the LHC both aspects are relevant: The non-perturbative low Q physics of the confined partons¹ constituting the initial state protons and the large Q physics of the hard interaction between two partons which can be described perturbatively. Both aspects can be factorised [31] in the calculations of the cross sections:

$$\sigma_{pp \rightarrow X} = \sum_{i,j} \int_0^1 dx_1 \int_0^1 dx_2 f_i(x_1, \mu_F) f_j(x_2, \mu_F) \sigma_{ij \rightarrow X}(\mu_F), \quad (2.3)$$

by using the parton density functions (PDF) $f_i(x, \mu_F)$ which can be interpreted at leading order as the probability density for a parton i to carry the momentum fraction x of the proton. The PDFs depend on the factorisation energy scale μ_F of the interaction and especially for high μ_F are not only relevant for up-and down quarks, but also for gluons and all other kinds of quarks and anti-quarks occurring as quantum-fluctuations in the proton. The PDFs are not calculated from first principles, but are constrained using measurements. The evolution of the parton density function between different energy scales is described by the DGLAP equations [32–34]. This means PDF sets can be determined by fitting measurements at different energy scales and the results can be extrapolated.

Both the dependency on the factorisation scale μ_F and on the renormalisation scale μ_R are unphysical and a feature of the truncated perturbative calculation. The sensitivity of a cross-section calculation to the scale choice is commonly used as an uncertainty. In practice this is evaluated e.g. by 7-point variations, changing μ_F and μ_R in the calculation by factors c_F and c_R in the set:

$$(c_F, c_R) \in \{(0.5, 0.5), (0.5, 1), (1, 0.5), (1, 1), (1, 2), (2, 1), (2, 2)\}, \quad (2.4)$$

and assigning the maximal changes of the result (the envelope) as the uncertainty. The scale variations are usually reduced by taking higher orders in the perturbative calculation into account. The scale uncertainty is nonetheless not reliably covering missing higher order contributions in the perturbative calculations, as illustrated e.g. by the process of photon-pair production measured in this thesis.

Fixed-order calculations of the hard process can involve high energetic quarks and gluons in the final state. This parton level prediction does not match the measurable final state which consists e.g. for a proton-proton collision at the LHC of hundreds of colourless particles like hadrons or photons. There are different approaches to describe the evolution of the high-energetic partons to a multitude of particles with lower energy.

Kinematic observables can be defined, such that they are less sensitive to the soft- and collinear emissions involved in this transition. Most prominently final state particles are clustered into *jets* based on their angular separation and momenta, which reflect to some extent the parton level kinematics.

Parton-shower Monte Carlo (MC) generators can be used to simulate the quark-gluon splittings of the high energy partons until they reach a certain energy threshold $\Lambda_{\text{QCD}} \sim 1$ GeV. Examples for state-of-the-art parton shower algorithms are PYTHIA [35], SHERPA [36] and HERWIG [37]. The parton shower step is followed by a hadronisation step converting the quarks and gluons into colourless

¹This includes not only up-and down quarks, but also gluons and all other kinds of quarks and anti-quarks

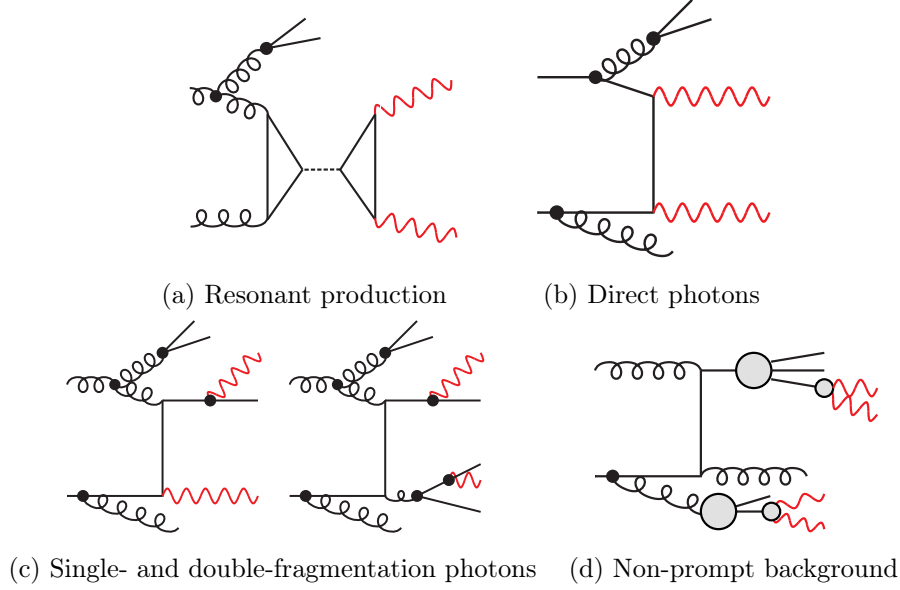


Figure 2.3.: Schematics of theoretical photon-pair production mechanisms. Quarks are represented by straight lines, gluons by curly lines, photons by red wavy lines and a spin-0 heavy particle (e.g. the SM Higgs boson) by the dashed line. The black dots represent resummed bremsstrahlung, e.g. from a fragmentation function or parton shower. The grey circles represent the fragmentation of a quark or gluon into a hadron. Mechanisms for prompt photon production are depicted in (a)-(c), whereas (d) illustrates the non-prompt background from hadron decays. Adapted from [38].

hadrons based on heuristic models.

As an alternative to the numeric parton-shower approach, the contributions from soft and collinear emission can also be resummed analytically by an expansion in the corresponding logarithmically enhanced terms. These analytically resummed calculation are only available for certain observables.

2.3. Photon-pair production in hadron collisions

The production of pairs of prompt photons was one of the final states instrumental to the discovery of the Higgs boson [9, 10] and is therefore an essential part of the LHC physics program. Prompt photons are defined as not originating from a hadron decay. Resonant production of a heavy particle like the Higgs boson and the subsequent decay into a pair of prompt photons as depicted in Fig. 2.3(a) contributes only very little to the overall prompt diphoton² production, which is dominated by the continuous mechanisms depicted in Figs. 2.3(b) and 2.3(c). Precise knowledge of this irreducible background to resonant production underpins the background estimation in Higgs measurements and heavy resonance searches, which is one of the core motivations of the measurement of continuous diphoton production presented in this thesis. Just as importantly, the results of the measurement

²Diphoton and photon pair are synonyms.

can be used to scrutinize various predictions for the dominant QCD contributions of photon-pair production which will be outlined in the following. Validated predictions for the QCD initiated photon-pair production are also a significant step towards measuring the electroweak photon-pair production in vector-boson scattering topologies [39], which could be e.g. sensitive to anomalous gauge couplings indicating beyond SM (BSM) physics.

Photons are ubiquitously produced inside of QCD jets by the decay of neutrals meson which is illustrated in Fig. 2.3(d). The contributions of these non-prompt photons represent the main experimental background for the measurement of prompt photon-pair production in this thesis and are subtracted using a data-driven approach.

The leading-order process for prompt diphoton production in hadron-hadron collisions is quark-antiquark annihilation $q\bar{q} \rightarrow \gamma\gamma$ which is contained in Fig. 2.3(b) with additional soft-gluon emissions as described e.g. by a parton-shower algorithm. In the fiducial phase space of inclusive diphoton production $pp \rightarrow \gamma\gamma + X$ studied in this thesis the contribution of this purely electromagnetic leading-order (LO) process is relatively small compared to the gluon-initiated channels $gg \rightarrow q\gamma\gamma$ opening up at next-to-leading order (NLO), e.g. due to the much larger gluon PDFs. These configurations with a photon radiated by a quark are referred to as fragmentation or brems-component (cf. Fig. 2.3(c)) and especially contribute to events with a highly energetic jet accompanied by a photon of lower energy. The collinear emission of photons creates additional divergences in perturbative calculations. There are multiple options to treat these mixed QCD and QED divergences [40]. The fragmentation component can be analytically resummed, which is implemented in DIPHOX [41] at NLO. The photon emissions can also be simulated in the parton shower [42, 43] like implemented in the PYTHIA [44] samples used for the diphoton measurement (cf. Section 7.2.1), where LO QCD processes are combined with photons from the parton shower.

Another option is to avoid the divergences by performing the perturbative calculations for photons, which are isolated from additional activity in their vicinity on parton-level [45]. This so-called *smooth-cone* or *Frixione* isolation criterion is described in Ref. [45]. It is defined as a function of the angular separation $R_{i\gamma}$ of additional partons to the photon and their transverse momentum $p_{T,i}$:

$$\sum_i p_{T,i} \theta(\delta - R_{i\gamma}) \leq \mathcal{X}(\delta) \quad \text{for all} \quad \delta \leq \delta_0. \quad (2.5)$$

Only partons with a separation $R_{i\gamma} < \delta_0$ enter in the calculation. The function $\mathcal{X}(\delta)$:

$$\mathcal{X}(\delta) = p_{T,\gamma} \epsilon_\gamma \left(\frac{1 - \cos \delta}{1 - \cos \delta_0} \right)^n, \quad (2.6)$$

depends smoothly on the radius of the isolation region δ , applying a stricter criterion on the summed momenta closer to the photon. The criterion is defined as a fraction ϵ_γ of the transverse momentum of the photon $p_{T,\gamma}$.

There are fixed-order calculations up to next-to-NLO (NNLO) for the production of pairs of isolated photons [46–50]. Another implementation of the fragmentation component in a parton shower approach is used for the nominal signal samples of the diphoton measurement (cf. Section 7.2.1) in this thesis. For these $pp \rightarrow \gamma\gamma + 0$ or 1 jet at NLO calculations and $pp \rightarrow \gamma\gamma + 2$ or 3 jets at LO calculations for isolated photons are merged with the SHERPA parton shower generator using the

MEPS@NLO prescription [51, 52].

The transverse momentum of the photon-pair system $p_{T,\gamma\gamma}$ is equivalent to the recoil of the additional QCD activity in the event and is sensitive to different phenomena for low and high values. Low values of $p_{T,\gamma\gamma}$ are sensitive to soft wide-angle QCD radiation, which can not be described by fixed-order calculations. To describe this region, resummed calculation are necessary, which can be implemented numerically with parton-shower MC generators. Alternatively, there are also first analytically resummed calculations for the $p_{T,\gamma\gamma}$ spectrum at N³-leading logarithm and NNLO in α_s [53, 54]. High values of $p_{T,\gamma\gamma}$ indicate additional highly energetic jets, which are not contained in the LO calculation $q\bar{q} \rightarrow \gamma\gamma$ which predicts a fixed value of $p_{T,\gamma\gamma} = 0$. This means only starting from NLO the calculations yield non-trivial result for $p_{T,\gamma\gamma}$. Therefore the NLO calculations are effectively LO and the NNLO calculations are NLO for $p_{T,\gamma\gamma}$, but there are first genuine $\gamma\gamma$ +jet calculations at NNLO [55] which are valid for high transverse momenta of the jet.

2.4. Previous measurements

The first measurements of photon-pair production in hadron collisions were established by experiments at the CERN intersecting storage rings in proton-proton collisions at $\sqrt{s} = 63$ GeV [56, 57]. First evidence was found by the NA3 experiment [58], which was a fixed-target experiment with collisions of an incident beam of $p = 200$ GeV charged pions from the CERN Super Proton-Synchrotron (SPS) with a stationary carbon target. This result was followed by the first observation of the process by the WA70 experiment [59], which was also a fixed-target experiment at the SPS provided with a π^- beam of 280 GeV incident momentum.

For all existing measurements of pairs of prompt photons in hadron collisions the backgrounds from neutral mesons (mostly π^0) decaying into a pair of photons $h^0 \rightarrow \gamma\gamma$ is the dominant background. In the earlier measurements [56–59] the background from $h^0 \rightarrow \gamma\gamma$ decays is mainly rejected and estimated based on creating e.g. π^0 candidates by matching multiple photon showers and calculating their invariant mass and energy asymmetry, comparing the result to the π^0 hypotheses. In the relatively low $1 \text{ GeV} < p_T < 4 \text{ GeV}$ momentum regime of these early analysis the individual photons of the hadron decay can usually be resolved and background events with one of the photons out of the geometric acceptance of the detector are important.

Later, photon-pair production was also measured in proton-antiproton collisions at the Super Proton-Antiproton Synchrotron ($S\bar{p}\bar{p}$ S) by the UA1 [60] and UA2 [61] experiment at up to $\sqrt{s} = 630$ GeV and at the Fermilab Tevatron by the CDF experiment [62] at $\sqrt{s} = 1.8$ TeV.

The main difference of these measurements with respect to the previous ones is the higher transverse momentum range $10 \text{ GeV} < p_T < 20 \text{ GeV}$ of the photons and the introduction of isolation criteria to reject and estimate the $h^0 \rightarrow \gamma\gamma$ background, which is necessary because the background photons merge more often into one cluster of energy deposits in the calorimeter in this higher p_T -regime. The isolation values are defined as the sum of the charged-track momenta or calorimeter energies in a region around the photon candidate. The photons from hadron decays occur usually accompanied by other hadrons within a collimated jet of particles and can therefore be rejected to a large extends by a requirement on the isolation energy. This restricts also the sensitivity of the measured signal to isolated prompt photons, because possible non-isolated prompt photons are rejected. The restriction to isolated prompt-photons is also common to all following measurements and simplifies the comparison

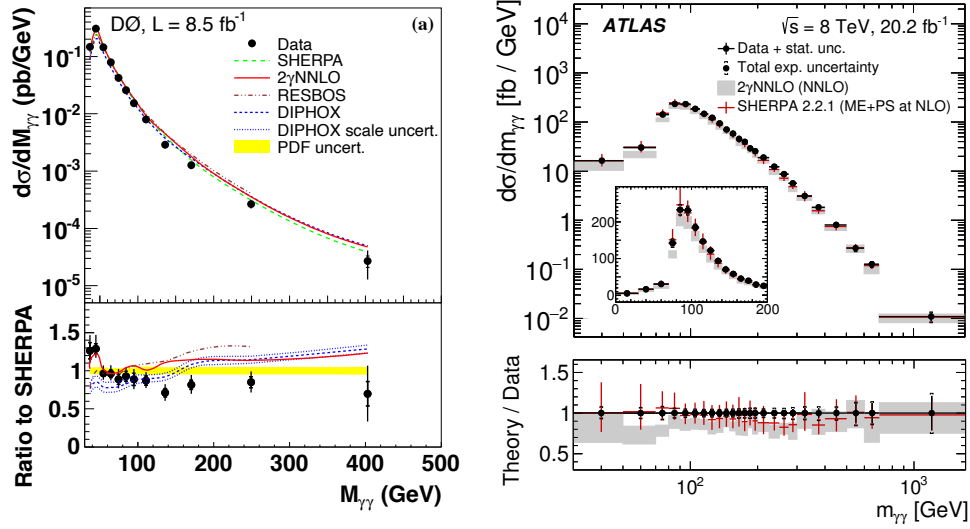


Figure 2.4.: Differential cross section of prompt isolated diphoton production as a function of the invariant mass $m_{\gamma\gamma}$ measured by D0 in proton–antiproton collisions at $\sqrt{s} = 1.92$ TeV (left) [64] and by ATLAS in proton–proton collisions at $\sqrt{s} = 8$ TeV (right) [69] compared to different theory predictions.

to fixed-order calculations which also tend to apply isolation criteria as described above. Up to this point the measurements are statistically limited due to the low integrated luminosities of up to around 10 pb^{-1} and the high background fractions.

The most recent measurements were performed in the Tevatron Run-2 proton–antiproton collisions at $\sqrt{s} = 1.92$ TeV by CDF [63] and D0 [64]; and in the LHC Run-1 proton–proton collisions by CMS [65, 66] and ATLAS [67, 68] at $\sqrt{s} = 7$ TeV, and at $\sqrt{s} = 8$ TeV by ATLAS [69]. The large datasets with integrated luminosities of up to 20 fb^{-1} and unprecedented collision energies enabled precise differential cross-section measurements including photons with a momentum of up to a few hundred GeV providing valuable information about the range of validity and the accuracy of different theory predictions. The measurements are performed as a function of different kinematic observables like the invariant mass $m_{\gamma\gamma}$ or the transverse momentum $p_{T,\gamma\gamma}$ of the photon-pair system, probing different phenomena. The measured invariant mass spectrum of the D0 measurement and the ATLAS measurement at 8 TeV are shown in Fig. 2.4. Especially in the highly abundant regions at intermediate $m_{\gamma\gamma}$ the precision of the measurements is limited by systematic uncertainties related e.g. to the photon selection efficiencies.

Chapter 3.

The ATLAS Detector at the Large Hadron Collider

The Large Hadron Collider (LHC) [70, 71] is the largest particle accelerator in the world. It was build to investigate particle physics at the high energy frontier, enabling the discovery of the Higgs boson, searches for BSM physics and a wide range of SM measurements. The LHC was preceded by the Large Electron-Positron Collider (LEP) which was housed in the same tunnel. In contrast to LEP the LHC does not accelerate and collide electrons and positrons, but the much heavier particles like protons or heavy ions. The acceleration of heavy particles has the benefit of much reduced bremsstrahlung losses¹, but comes at the cost of an only probabilistically known initial state of the elementary partons constituting the protons and a plethora of multi-jet background events.

The LHC has a circumference of 26.7 km and is located at the European Organization for Nuclear Research (CERN) on the Franco-Swiss border near Geneva. The LHC is installed in a tunnel between 45 to 170 m below the surface and is part of the large CERN accelerator complex (see Fig. 3.1), which includes several other accelerators used, among other applications, to create, shape and pre-accelerate bunches of protons or heavy ions before they are injected into the two beam pipes of the LHC for their final acceleration. The protons are accelerated in superconducting RF cavities. The trajectory of the two counterrotating beams is steered by the LHC magnet system producing magnetic flux densities above 8 T using NbTi superconductors cooled down below 2 K with superfluid helium. The beams are crossed at four interaction points where the four large detectors ALICE [73], CMS [74], LHCb [75] and ATLAS [76] are installed.

The general-purpose detectors ATLAS and CMS are designed to be sensitive to a wide range of interesting physics processes, e.g. involving the production of electrons, muons, b -jets, hadronic τ -decays or photons with up to TeV scale energies despite the challenging conditions of many simultaneous interactions occurring at MHz frequencies. The design of ATLAS and CMS was strongly motivated by the different predicted decay channels of the Higgs boson whose fractions depend on the Higgs mass, which was unknown at that time.

¹The limiting factor for the energy achievable with a circular electron-positron collider are energy losses due to bremsstrahlung, which are reduced by a factor of $(m_e/m_p)^4 \approx 10^{-13}$ for protons.

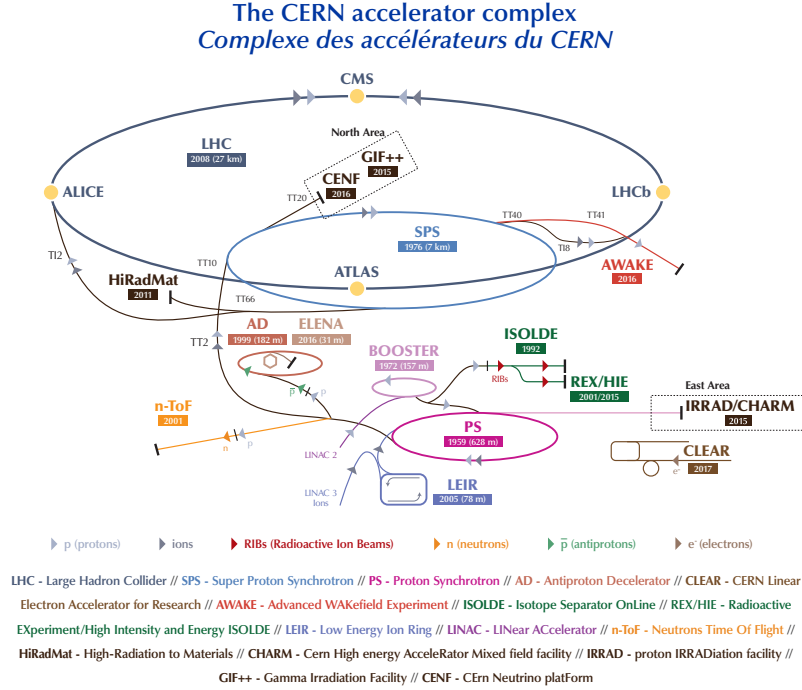


Figure 3.1.: The CERN accelerator complex in 2018 during the LHC Run-2 [72].

3.1. The Run-2 of the LHC

The data analysed in this thesis was recorded by ATLAS in the proton-proton collisions runs of the LHC in the years 2015-2018. This was Run-2 of the LHC [77] which increased the centre-of-mass energy from $\sqrt{s} = 8 \text{ TeV}$ to $\sqrt{s} = 13 \text{ TeV}$ with respect to the end of Run-1 in 2012. Furthermore the spacing between the proton bunches in the beams was decreased from 50 ns to 25 ns. Up to 2556 bunches per ring, each bunch containing more than 10^{11} protons, were rotated in the LHC simultaneously achieving unprecedented² luminosities of up to $L = 2.14 \times 10^{34} \text{ cm}^{-2}\text{s}^{-1}$ in 2018. The integrated luminosity $\mathcal{L}$ of the collisions provided by the LHC is, besides the centre-of-mass energy, the key metric of its success, because it determines the number of expected events N of a physics process based on the cross section σ of the process:

$$N = \sigma \cdot \int L(t) dt = \sigma \cdot \mathcal{L}. \quad (3.1)$$

The LHC delivered an integrated luminosity of $\mathcal{L} = 156 \text{ fb}^{-1}$ to the ATLAS detector of which $\mathcal{L} = 139 \text{ fb}^{-1}$ are good for physics measurements (see Fig. 3.2).

The increase of the centre-of-mass energy yields an increase of roughly a factor of 2 in the photon-pair production cross section with respect to the previous ATLAS analysis of the Run-1 data at 8

²this record was surpassed by the SuperKEKB electron-positron collider in 2020.

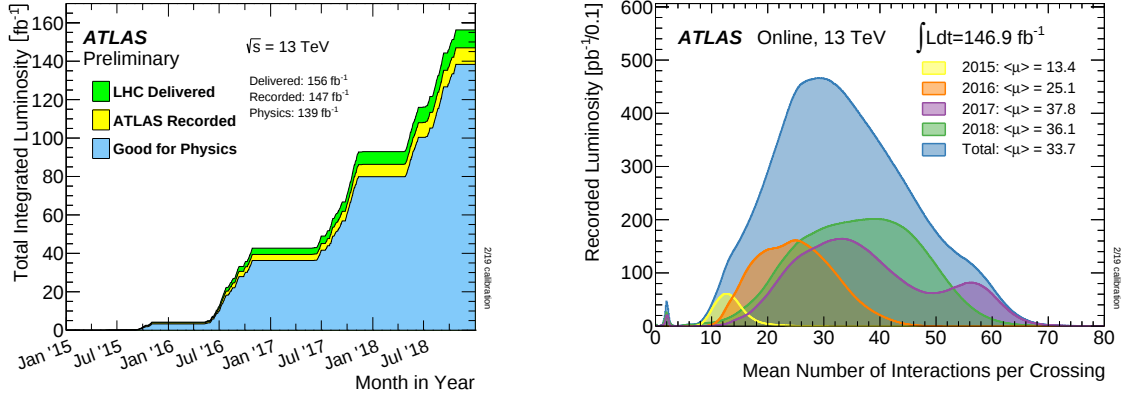


Figure 3.2.: Integrated luminosity delivered by the LHC during Run-2 in the years 2015-2018 (left) and mean number of interactions per bunch crossing for each year (right) [78].

TeV [69], which measured photon-pair production in a very similar fiducial phase space (e.g. same threshold values on the transverse energies of the photons). Together with the factor of 6 higher integrated luminosity with respect to the 20.2 fb^{-1} of Run-1 data at 8 TeV, the Run-2 data provides a factor of 12 larger dataset with an extended kinematic range of photon-pair production.

The high luminosities are only achievable in connection with multiple inelastic scattering events occurring in the same bunch crossing for the limited bunch crossing frequency of $f \lesssim 30$ MHz. The interactions additional to the one of interest, e.g. photon-pair production, are mostly adding noise to the event and are referred to as *pileup*. The mean number of interactions per bunch crossing is connected to the instantaneous luminosity L and the cross section for inelastic scattering σ_{inel} by:

$$\mu = \frac{L \cdot \sigma_{\text{inel}}}{f}. \quad (3.2)$$

The inelastic proton-proton cross section has been measured by multiple experiments at different centre-of-mass energies. A good overview is included in Ref. [79] which presents the measurement at $\sqrt{s} = 13$ TeV with the TOTEM experiment [80]. The inelastic cross-section at $\sqrt{s} = 13$ TeV is around 80 mb which is only approximately 5% higher than the value at $\sqrt{s} = 8$ TeV showing the mild logarithmic dependency of σ_{inel} on $\sqrt{s}$. The maximum values of the mean interactions per bunch crossing corresponding to the peak luminosity are around 60 in 2018 (see Fig. 3.2). The bulk of the distribution is below the peak values, because the luminosity is not constant over one run of the LHC, but decays mostly due to the beam losses from collisions. In 2017 there were runs with especially high pileup conditions building up the peak around 58 in Fig. 3.2. They were connected to a special bunch filling scheme *8b4e* [81], where 8 filled bunch spaces are followed by 4 empty ones, which had to be adopted to overcome beam losses in a specific LHC section due to contaminations of the vacuum [82]. This led to a reduced number of bunches of 1916. In order to achieve the high instantaneous luminosities necessary to reach the expectations on the integrated luminosities other beam parameters were optimized. This led to very high pileup conditions which impose a challenge to the experiments. These high pileup conditions in 2017, but also in Run-2 in general, are an opportunity to study and

mitigate the influence of pileup. This gives important insights for the even higher luminosities and pileup (up to $\mu \sim 200$) anticipated for the high luminosity LHC [83].

3.2. The ATLAS Detector

The ATLAS detector [84] measures the energies and momenta of the particles produced in the LHC collision events and enables particle identification. The detector consists of multiple subsystems arranged in multiple layers around the interaction point. The detector is around 40 m long and 25 m high and located in a cavern around 100 m below the surface at one of the interaction points of the LHC under the CERN main Meyrin site. An overview of the ATLAS detector is depicted in Fig. 3.3. A short overview over the different subdetectors mostly summarizing information from [84] with an emphasis on the parts relevant for photon measurements is given in the following in Sections 3.2.1 to 3.2.4.

The ATLAS coordinate system is a right-handed coordinate system. The origin of the coordinate system is in the interaction point. The x -axis points from the origin towards the center of the LHC, the y -axis is pointing upwards and the z -axis is parallel to the beam-axis (pointing such that the system is right handed).

Directions are measured in terms of the azimuthal angle ϕ in the transverse x - y -plane and the polar angle θ with respect to the beam axis. The pseudo-rapidity $\eta = -\ln \tan(\theta/2)$ is usually used instead of the polar angle, because pseudo-rapidity differences $\Delta\eta$ are conserved by Lorentz boosts along the z -axis for massless particles.

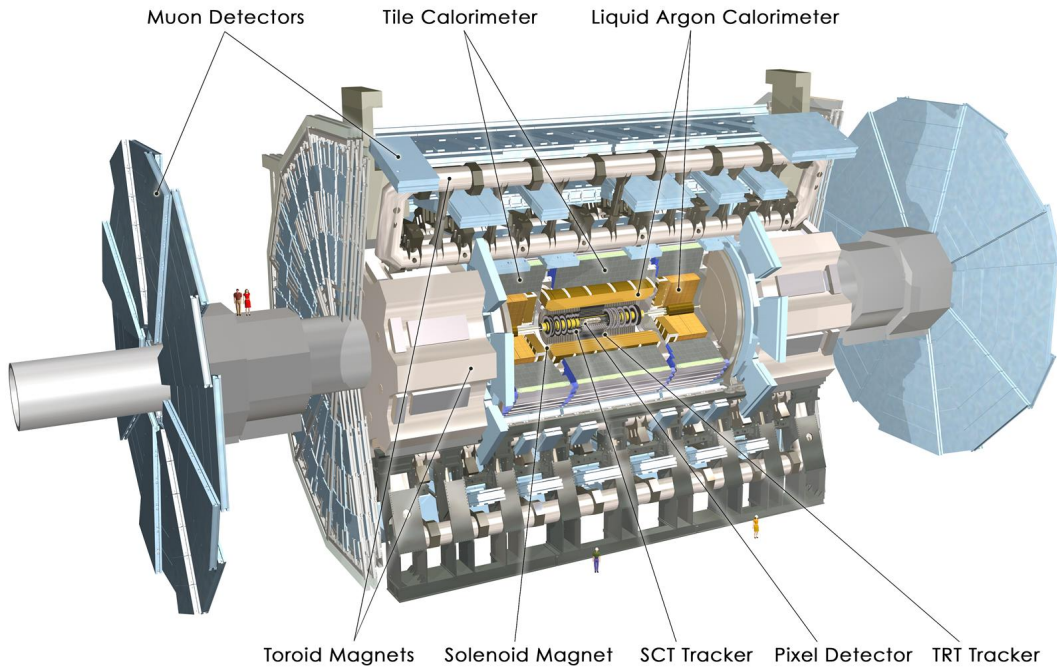


Figure 3.3.: Computer generated image of the ATLAS detector [85].

3.2.1. Inner Detector

The inner detector covers the region $|\eta| < 2.5$ and is approximately 6 m long and 2 m in diameter. The inner detector is used to measure the trajectory of charged particles. It is permeated by a 2 T magnetic field of a superconducting solenoid surrounding the inner detector. The magnetic field bends the path of charged particles and therefore the sign of the charge of the particles and the momentum of the particles can be inferred from their trajectories.

The inner detector consists of three components. The pixel tracker, the silicon microstrip tracker (SCT) and the transition radiation tracker (TRT) (see Section 3.2). The pixel tracker provides very precise locations of the particle hits in 92.4 million small $50 \times 400 \mu\text{m}^2$ or $50 \times 250 \mu\text{m}^2$ size pixels of the silicon detector. A particle usually traverses 4 layers of pixels of the pixel tracker. The pixel detector was upgraded with respect to Run-1 by adding the insertable B-Layer (IBL) [86], which is a new innermost pixel layer. The pixel tracker is surrounded by the SCT which is based on silicon strips layered with small angular offsets to reconstruct a 3D position from two strips passed consecutively. It provides usually around 4 additional space-points of a particle trajectory. The last sub-detector a particle with $|\eta| < 2.0$ passes is the TRT which consists of 351000 drift tubes with a diameter of 4 mm filled with a gas mixture with a large fraction of Xenon. In regions with large losses of the gas mixture due to leaks Argon is used instead of Xenon, because of the high cost of Xenon [87]. The tubes are interleaved with plastic fibres or foils causing transition radiation for particles with large Lorentz boost γ . The transition radiation is absorbed by the Xenon or Argon triggering a large ionization signal. This signature is used to distinguish tracks of light highly boosted electrons from tracks of heavier particles like pions. The tubes are arranged parallel to the beam-pipe in the central ($|z| < 780$ mm) region and radially otherwise. The tubes have a length of 37 mm or 144 mm, therefore the TRT mostly provides projective two dimensional positional information orthogonal to the tubes and a large number of typically 36 hits per particle.

Ideally particles would lose energy mainly through ionizing hits in the active volume of the inner detector and therefore not losing much of their energy and not creating any secondary highly energetic particles before entering the calorimeter systems. To achieve this the material budget in the inner detector was kept as low as possible. The material budget in terms of energy loss of electrons due to bremsstrahlung is quantified by the radiation length X_0 ³, the distance an electron travels before it lost on average 63% of its energy due to bremsstrahlung.

One of the main signatures of photons are their missing hits in the inner detector. Highly energetic $E_\gamma > 10$ GeV photons interact with matter almost exclusively by pair production of electron-positron pairs [88]. If this occurs in the volume of the inner detector a photon is referred to as converted. The interaction length of pair production is directly proportional to the radiation length X_0 and the probability for an photon to be converted after a distance x_c smaller than x can be approximated as given in Eq. (3.3) [88].

$$P(x_c < x) \approx 1 - e^{-\frac{7}{9} \frac{x}{X_0}}. \quad (3.3)$$

The material distribution in terms of radiation lengths X_0 is shown in Fig. 3.4. The main contributions of the different sub-detectors are given by the cables, cooling, electronics and support structures necessarily included in their volume and not by the active detector material. According to Eq. (3.3) after around $9/7 \ln(2) X_0 \approx 0.89 X_0$ radiation lengths 50% of the photons are converted to

³The radiation length X_0 determines the energy loss per path length $dE/dx = -E/X_0$ of an electron with energy E .

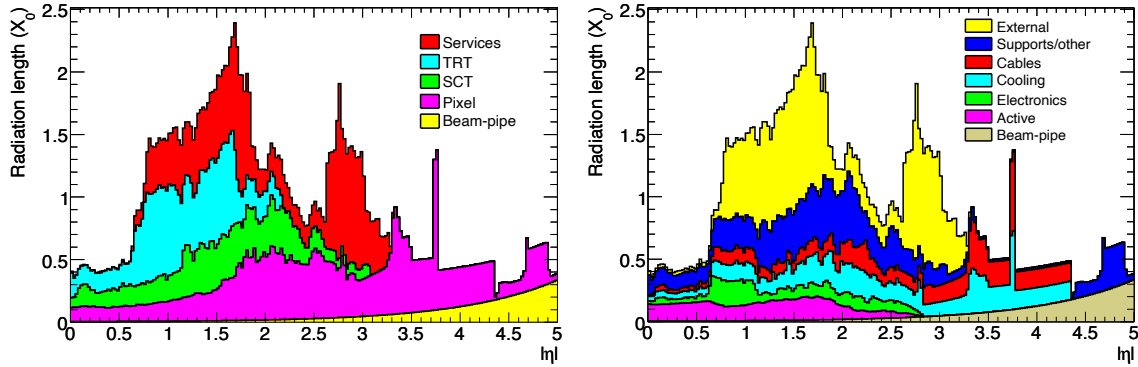


Figure 3.4.: Material distribution of the different parts of the inner detector in terms of radiation length X_0 as a function of $|\eta|$ averaged over ϕ . The material is grouped by sub-detector in which it is included (left) and by function (right) [76]. The changes to the material from the addition of the IBL are not included [86]. The material of the IBL amounts to around $0.02 X_0$ around $|\eta| = 0$ and goes up to $0.2 X_0$ at $|\eta| = 2.8$.

electron-photon pairs. Comparing to Fig. 3.4 this means that for large parts of the detector most of the photons convert in the inner detector material, although this happens often only late, in the TRT or in the external material. To correctly reconstruct and identify as many photons as possible dedicated reconstruction algorithms (cf. Chapter 4) are applied, which take differences between converted and unconverted photons into account.

The inner detector of ATLAS will be replaced before the runs of the high luminosity LHC [83]. The new inner detector [89] will cover a larger rapidity-range up to $|\eta| = 4.0$ which will enable photon identification beyond what is possible with the current setup ($|\eta| < 2.5$). In addition the new tracker will be purely silicon based and will not contain a TRT. This will reduce the material and therefore also the fraction of converted photons.

3.2.2. Electromagnetic Calorimeter

The electromagnetic (EM) calorimeter is the second subsystem a particle traverses and is part of the liquid argon (LAr) calorimeter (cf. Fig. 3.3). The EM calorimeter consists of a barrel module covering $|\eta| < 1.475$ and two endcaps covering $1.375 < |\eta| < 3.2$ in the forward-and backward regions. It is designed to measure the energy of electrons⁴ and photons. One of the guiding design targets for the EM calorimeter was a good energy resolution and identification for photons enabling the discovery of a relatively low mass $m_h < 125$ GeV Higgs boson⁵.

The EM calorimeter is a sampling calorimeter, which means it consists of alternating absorption and detection layers. The absorption layer consists of lead, in which photons are likely to undergo pair production and electrons are likely to radiate bremsstrahlung, creating secondary electrons and

⁴If not explicitly specified otherwise electrons and positrons are both included when referring to electrons.

⁵Already at slightly lower Higgs masses $m_h \sim 120$ GeV the channel $h \rightarrow \gamma\gamma$ was considered the main discovery channel, because other important discovery channels like $h \rightarrow ZZ^*$ are strongly suppressed compared to higher m_h scenarios.

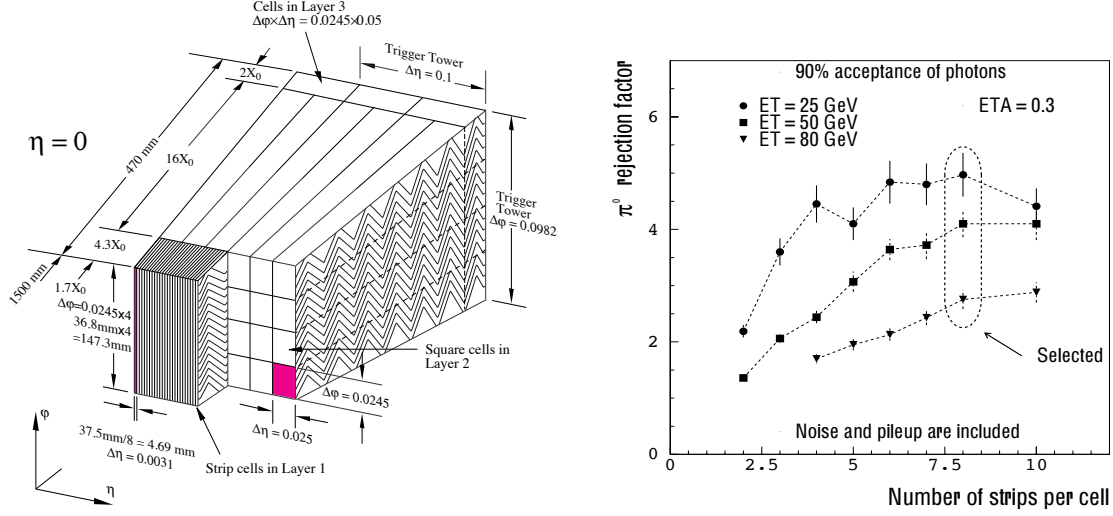


Figure 3.5.: Granularity of the ATLAS LAr-Calorimeter around $\eta = 0$ (left) [76] and simulation study of the dependency of the background rejection of single π^0 events as a function of the granularity of the first layer (strip layer) of the calorimeter (right) [90].

photons. Similarly, these secondary particles can create additional electrons and photons in the subsequent absorption layers. This avalanche of electrons and photons is referred to as EM shower.

The detection layers in between the absorption layers are filled with liquid argon and have copper-board electrodes enclosed in polyimide in the centre. The energy deposited in the detection layers is reconstructed from the current of the electrons and argon ions drifting to the electrodes.

The absorption and detection layers are folded into an accordion structure and a pattern is etched onto the electrodes, such that the calorimeter signal can be readout separately in different $\eta \times \phi$ regions in three longitudinal layers. The accordion structure and the longitudinal and lateral granularity of the EM calorimeter is depicted in Fig. 3.5. The accordion structure has the benefit of a high uniformity in ϕ -direction, because no gaps in ϕ are needed inside of the calorimeter for the readout.

One of the main backgrounds to prompt photon production is given by neutral mesons (mostly π^0 or η) decaying into a pair of collimated photons with a very low angular separation, such that their EM showers in the calorimeter are overlapping. The very fine $\Delta\eta = 0.025/8$ granularity of the first layer of the EM calorimeters was optimized to enable discrimination between the shower of neutral meson decays and prompt photons (cf. Fig. 3.5). Shower variables quantifying the lateral shape in the first layer of the calorimeter are an important input for the photon identification (cf. Section 4.4).

The comparatively large size of $\Delta\phi \approx 0.1$ in the azimuthal direction of the cells in the first layer is partially compensated by the smaller $\Delta\phi \approx 0.0245$ granularity of the following middle layer of the calorimeter, which is the largest layer of the LAr calorimeter. Also the magnetic field of the solenoid magnet enclosing the inner detector is smearing the shower in ϕ -direction, especially for converted photons, and therefore $\Delta\phi$ -granularity provides less stringent π^0/γ -discrimination power compared to η -granularity.

The consecutive middle and back layer of the EM calorimeter enable a precise percent level $\Delta E/E$

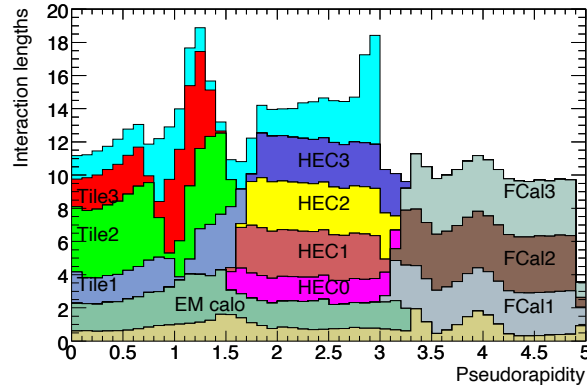


Figure 3.6.: Amount of material in the different subsystems of the ATLAS detector before the muon spectrometer in terms of nuclear interactions lengths. The material in front of the EM calorimeter is shown in light brown and the material behind the hadronic calorimeters is shown in light blue [76].

photon-energy measurement (cf. Section 4.3) and provide information about longitudinal shower development also used for the photon identification to discriminate against background from hadrons (cf. Section 4.4).

The energy loss through bremsstrahlung is strongly suppressed for heavier particles than the electron like muons and charged hadrons. Muons are losing small fractions of their energy through ionization. Hadrons are in addition able to interact via the strong interaction with the atomic nuclei of the detector material. These interactions are in general much rarer than bremsstrahlung for a corresponding electron. Analogous to the radiation length X_0 the nuclear interaction length λ is defined, which quantifies the length after which a nuclear interaction creating e.g. secondary hadrons occurs.

For a usual trajectory the material in the EM calorimeter corresponds to more than 20 radiation lengths X_0 , therefore the electromagnetic shower of electrons and photons is usually fully contained in the EM calorimeter. But the material in the EM calorimeter corresponds to only around 2-4 nuclear interaction lengths λ . This means although hadrons usually have their first nuclear interactions in the EM calorimeter only a fraction of their energy is deposited and most of it is leaving the EM calorimeter in terms of secondary hadrons originating the hadronic shower in the consecutive hadronic calorimeter.

3.2.3. Hadronic Calorimeter

The hadronic calorimeter consists of the tile calorimeter covering $|\eta| < 1.7$ surrounding the liquid argon calorimeters (cf. Fig. 3.3), the LAr hadronic end caps (HEC) ($1.5 < |\eta| < 3.2$), located at the back of the EM end caps, and the LAr forward calorimeters (FCal) ($3.1 < |\eta| < 4.9$) in the centre of the endcaps.

The three subsystems are sampling calorimeters. The tile calorimeter uses steel as absorber material and scintillating tiles as detection material. The hadronic end caps and the forward calorimeter use

liquid argon as detection material and copper and tungsten as absorber.

The hadronic calorimeters are designed to confine the propagation of hadrons. This is achieved by using large amounts of absorber material in terms of nuclear interactions lengths λ (cf. Fig. 3.6) triggering nuclear interactions of the hadrons with the material which yields secondary hadrons with lower energy cascading into subsequent nuclear interactions.

Similar to the EM calorimeter, the information of the hadronic calorimeter is read out from different cells providing longitudinal and lateral information about the shower enabling precise energy determination of QCD jets. The tile calorimeter and the HEC have three layers and a minimal lateral granularity of $\Delta\eta \times \Delta\phi = 0.1 \times 0.1$. In the context of this thesis QCD jets are not directly analysed, instead the superior energy resolution of the photon reconstruction in the EM calorimeter is used to infer information also sensitive to the QCD activity in the events e.g. through transverse momentum conservation. The information of the hadronic calorimeter is important for the photon identification and isolation. The ratio of energy in the EM calorimeter to the energy in the hadronic calorimeter is a powerful discriminant to distinguish isolated photons from jets (cf. Sections 4.4 and 4.5).

3.2.4. Muon Spectrometer

The muon system is the outer-most subdetector of ATLAS and is usually only reached by muons, because of their low bremsstrahlung-energy losses due to their high mass. The muon system contributes the largest fraction to the volume of ATLAS (cf. Fig. 3.3). It consists of trigger chambers, precision-tracking chambers and a system of large toroid magnets. The hits in the muon-tracking chambers are used in combination with the inner detector information to reconstruct the trajectory of muons and to precisely measure their momentum [91].

A more detailed summary is spared, because in this work muons are only used to tag radiative $Z \rightarrow \mu\mu\gamma$ events for the comparison of photon selection efficiencies in data and simulation in Section 6.2.

3.2.5. Trigger

Because of the bunch crossing frequency of 40 MHz it is not possible to permanently store the detector output for each bunch crossing, which would amount to a data rate of $\sim 100 \text{ TBs}^{-1}$. It is the purpose of the trigger system [92] to select events at a rate for which the data can be stored and processed. This is done by selecting events with signatures of interest, which occur at a low rate (e.g. the cross-section of $\sigma_{\gamma\gamma}^{\text{fid}} \sim 30 \text{ pb}$ for photon-pair production studied in this work corresponds to an event rate of about 0.6 Hz at the design instantaneous luminosity of $1 \times 10^{34} \text{ cm}^{-2}\text{s}^{-1}$). The time optimized decision of the trigger which is a crucial part of the data taking are referred to as *online* algorithms and the precision optimized software reconstruction algorithms which are used to process the permanently stored data are referred to as *offline*.

The trigger selection is organized in multiple levels. The first Level-1 (L1) trigger is implemented in custom hardware, which calculates a decision for each bunch-crossing within a short timespan of a few μs for which the detector readout is buffered on sub-detector specific front-end electronics. It selects events at a rate of up to 100 kHz which are subsequently transferred and temporarily stored in the ATLAS Read-Out System.

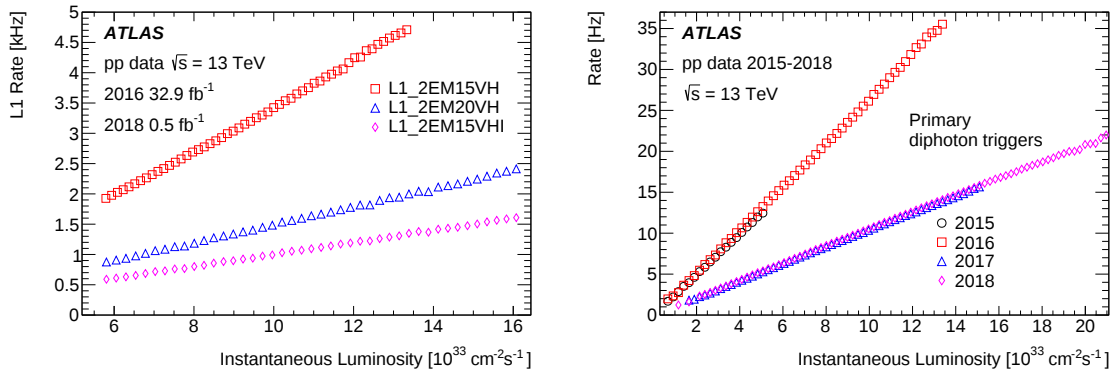


Figure 3.7.: Trigger rate for the primary Level-1 photon-pair trigger (left) as a function of the instantaneous luminosity measured in 2016 and 2018. The red boxes show the rate for the trigger used in 2015-2016 with a requirement of $E_T > 15 \text{ GeV}$ and the triangles for the trigger used in 2017-2018. The diamonds illustrate the influence of an additional isolation cut. Trigger rate for the primary HLT photon-pair trigger (right) in the different data taking years. A stricter identification criterion was applied in 2017 and 2018 compared to 2015-2016 to cope with higher instantaneous luminosities [93].

The L1 trigger decision selecting events with photons or electrons [93] is purely based on information from the calorimeters. The signals are summed in $\eta \times \phi = 0.1 \times 0.1$ regions separately for the EM and for the hadronic calorimeter referred to as trigger towers. The L1 EM trigger objects are formed by windows of 2×2 trigger towers exceeding a programmable threshold. In addition a requirement on the maximal transverse energy⁶ in the hadronic calorimeter can be applied. For the measurement of photon-pairs described in Chapter 7 a L1 trigger is used which requires two EM trigger objects exceeding a transverse energy of $E_T > 15 \text{ GeV}$ in 2015 and 2016 and of $E_T > 20 \text{ GeV}$ in 2017 and 2018. If the transverse energy of the trigger objects is below 50 GeV there is also a threshold on the energy in the hadronic trigger towers at the back of the EM trigger towers of 1 to 2 GeV depending on the transverse energy of the trigger object. These L1 photon-pair triggers select events at a rate of 1 to 3 kHz (cf. Fig. 3.7).

If a L1 trigger selects an event it is further processed by the software based high level trigger (HLT) which runs on a CPU farm. The HLT can access the full granularity of the detector information by processing a specific region-of-interest identified by the L1 trigger, or by reconstructing the complete event. For this the HLT applies reconstruction and analysis software similar to what is used offline and applies event selections based on the reconstructed objects like electrons or photons. These selections reduce the event rate from the 100 kHz of all L1 triggers to 1 kHz which amounts to a data rate of 1 to 2 GBs^{-1} for which the data of the events is transferred to the CERN Tier-0 computing centre and permanently stored.

The HLT algorithm for the selection of photons [93] is split into two steps. The first fast reconstruction step uses calorimeter information in the region-of-interest of a corresponding L1 trigger to calculate three shower shape variables emulating some of the variables used in the offline selection

⁶The transverse energy is defined based on the energy E and pseudo-rapidity η of the object as $E_T = E \cosh \eta$.

(cf. Section 4.4). For the candidates passing the requirements on these shower shape variables the second precision step is executed. The precision step uses cell information from a slightly larger region and applies energy calibration and identification algorithms closely matching the offline algorithms (cf. Sections 4.3 and 4.4). For the photon-pair measurement presented in this thesis a photon-pair trigger is used for which the (sub)-leading⁷ HLT photon trigger needs to exceed a transverse energy of $E_T^\gamma > (25)35 \text{ GeV}$. For 2015 and 2016 a *loose* identification criterion is applied for both photon triggers which was restricted to *medium* in 2017 and 2018 to cope with higher instantaneous luminosities. The trigger rate for this primary HLT photon-pair trigger was around 10 to 30 Hz in Run-2 (cf. Fig. 3.7).

3.2.6. Processing of data and simulated samples

The event generation, simulation, reconstruction and user analysis are processed decentralized on the world wide LHC computing grid (referred to as *grid*) [94].

The event generation step in ATLAS utilizes the broad variety of available MC generators. The sample production and validation is coordinated centrally [95].

The starting point for the simulation are the particle content and kinematics of a final state of a collision e.g. as created by a MC event generator. The ATLAS Simulation Software [96] uses a detailed model describing the detector geometry and material composition to simulate the energy deposits of the particles in the detector with the GEANT4 framework [97]. The energy deposits of the event are overlayed with the energy deposit from separate pileup samples which are generated with PYTHIA 8 [44] with the ‘A3’ tune [98] for Run-2. The total energy deposits are digitized, simulating the response of the detector electronics and the L1 trigger and saved in a data format similar to that of data with the addition of truth information.

This means the same reconstruction software can be applied to simulated samples and real data. This allows for a precise quantitative evaluation of the performance of the reconstruction algorithms with respect to the truth information of the event. This is e.g. the prerequisite for correcting the data for detector inefficiencies and resolution effects referred to as *unfolding* and discussed in detail for the photon-pair production measurement in Section 7.6.

The event reconstruction and analysis code is part of the ATLAS ATHENA framework [99]. It applies different algorithms to reconstruct particle candidates for e.g. electrons, photons, muons, jets and hadronic tau decays. An overview over some relevant parts for photons is given in Chapter 4. The output of the reconstruction is saved in Analysis Object Data (AOD) files. The AOD data samples for one data-taking year have a size of around 1 to 3 PB. To reduce the amount of data an individual analysis needs to access, the AODs are centrally processed into multiple smaller derived (D)AOD formats tailored to the needs of individual physics analysis e.g. targeting different signatures. This is achieved by event selections, by reducing the number of objects (e.g. photon candidates) and by removing some of the information stored for certain objects. The processing step AOD to DAOD is also utilized to apply updated reconstruction algorithms. The individual DAOD samples have a size of usually less than 100 TB and are processed by individual users usually still utilizing the grid.

For the photon-pair measurement the DAODs are processed into small ROOT [100] n-tuple files which have a size of a few GB for data and up to a few hundred GB for simulated samples, which include over one hundred systematic variations.

⁷in terms of transverse energy.

Corrections to the simulated samples are applied in the last step from DAOD to n-tuple. The corrections are based on dedicated measurements comparing the detector performance between simulation and real data. These measurements are coordinated by the combined performance (CP) groups of the ATLAS collaboration which are also responsible of maintaining and developing the respective reconstruction and analysis algorithms. The CP groups release recommendations to the whole ATLAS collaboration about the specific signature the CP group is dedicated to (e.g. electrons and photons in the e/γ -group). The performance studies which are performed in the context of this thesis are discussed in Chapters 4 and 5 with the results from Chapter 5 entering into the central e/γ recommendations and supporting the choice of the new pileup overlay used for Run-3 and the Run-2 reprocessing.

Chapter 4.

Photon reconstruction in ATLAS

In this chapter the reconstruction of photon candidates with the ATLAS detector is discussed. In Section 4.1 the reconstruction of important inputs to the photon reconstruction like the tracks of charged particles and clusters of calorimeter energy deposits are discussed. Section 4.2 describes the creation of photon candidates and the reconstruction of photon conversions as well as the electron-photon ambiguity resolution. In Section 4.3 the determination of the photon energy is summarized. Section 4.4 describes the discrimination of genuine photons from background candidates, based on the shower shape in the calorimeter and Section 4.5 gives an overview of the measurement of the photon isolation energy.

4.1. Low-level inputs

4.1.1. Inner-detector tracks

The inner-detector tracks are reconstructed from the hits in the pixel detector, SCT and TRT (cf. Section 3.2.1). The track reconstruction [101] is based on two complementary approaches. The inside-out approach starting from signatures in the silicon detectors and the outside-in approach starting from the TRT. Objects referred to as *spacepoints* are build from the hits in the Pixel and SCT detector which contain information about the position of the hit and its uncertainty. The spacepoints serve as input to the track reconstruction.

The inside-out approach uses clusters of spacepoints compatible with a trajectory as a starting step. A Kalman filter [102] approach is then used to iteratively add spacepoints based on the extrapolated expected trajectory reconstructed from the previous set of spacepoints and its uncertainty. The new spacepoint is then updating the trajectory and its uncertainty. The expectations of the Kalman filter include changes to the trajectory in the material due to ionisation losses. The track candidates undergo an ambiguity resolution retaining only the best track in cases where tracks share multiple spacepoints. The remaining tracks are extrapolated to the TRT and the corresponding TRT hits are added.

The outside-in approach is of special relevance for the reconstruction of converted photons, because depending on the radius R at which the pair production occurs, there might be no or not enough hits in the silicon detectors to seed the track. In addition the large radiative energy losses of the electron and positron can cause a failure of the extrapolation of the silicon track to the TRT, because the

expected energy loss in the Kalman filter of the nominal track reconstruction takes only ionization losses into account. This also motivates refitting the tracks with an alternative energy-loss hypothesis for the tracks of converted photons as discussed in Section 4.2.

For the outside-in approach tracks are seeded by the hits in the TRT which do not provide information parallel to the tubes. This means only two dimensional projective information of the hits is available. Due to the magnetic field each single hit is compatible with a range of trajectories parametrized by their ϕ -direction and their momentum p . To identify TRT track candidates, the following procedure is used. A two dimensional histogram is prepared binned in ϕ and p of hypothetical trajectories. For each hit an entry is added to all bins of the histogram associated to a hypothetical trajectory compatible with the hit. Finally, track candidates are identified based on the maxima of the histogram.

4.1.2. Calorimeter clusters

Calorimeter clusters are a combination of multiple cells with the purpose of capturing the energy deposits optimally of a single particle and suppressing noise from e.g. pileup. The photon reconstruction [103] relies on topological clusters [104] which are formed based on the energies of the cells E_{cell} and their expected noise level σ_{cell} . The energies E_{cell} are reconstructed based on an optimal Filter applied to the digitized pulse shapes of the signal from the cell and conversion factors determined in electronic calibration runs and testbeam studies [105, 106]. The noise level σ_{cell} of a cell is the combination of electronic noise $\sigma_{\text{el.}}$ and pileup noise σ_{pileup} :

$$\sigma_{\text{cell}} = \sqrt{\sigma_{\text{el.}}^2 + \sigma_{\text{pileup}}^2}. \quad (4.1)$$

The pileup noise is created by the ambient spray of low energetic particles from additional interactions of the current, previous and following bunch-crossings. Previous and following bunch crossings enter, because the drift time of the electrons in the LAr calorimeters is up to $\tau \approx 450$ ns and therefore the pulse shape of each cell is influenced by additional bunch crossings which occur every 25 ns, this is referred to as *out-of-time* pileup. The electrical noise $\sigma_{\text{el.}}$ can be measured and the pileup noise level σ_{pileup} is set to the expected noise in each cell for the average number of interactions per crossing $\langle\mu\rangle$ for the run in simulated samples. To use a consistent value in the offline analysis and for the trigger this value is fixed before the actual data taking based on the expected $\langle\mu\rangle$.

The topological clustering is seeded by cells with energy deposits with a significance ς :

$$\varsigma = \frac{E_{\text{cell}}}{\sigma_{\text{cell}}} \quad (4.2)$$

of greater than $|\varsigma| > 4$. Adjacent cells are added to this proto-cluster if their significance is greater than $|\varsigma| > 2$. After all connected cells with $|\varsigma| > 2$ are added a last layer of cells with no requirement on the significance is added. To separate deposits of multiple collimate particles of which the significant cells overlap, clusters are split if they have multiple local maxima with at least 4 neighbouring cells with energies smaller than 500 MeV less than maxima.

For Run-1 and early Run-2 analyses the photon reconstruction was still based on fixed $\eta \times \phi$ -sized rectangular clusters [107, 108]. The new topological cluster based approach [103] improves the energy

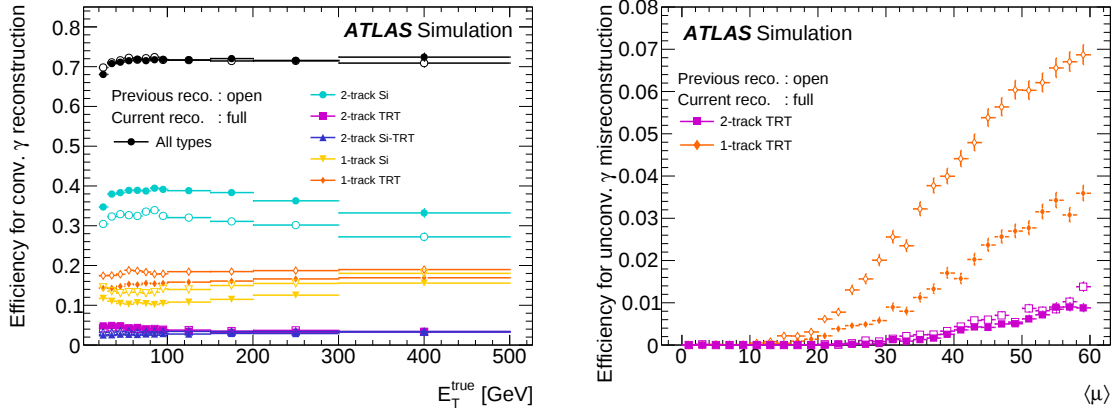


Figure 4.1.: Fraction of true converted photons (left) with a matched conversion vertex. The black markers indicate the overall conversion reconstruction efficiency, the coloured markers represent different classes of conversion vertices with one or two tracks with hits in the silicon (Si) layers or the TRT (TRT) or both (Si-TRT). Fraction of true unconverted photons (right) miss-reconstructed with one or two TRT conversion tracks as a function of the average number of pileup interactions $\langle\mu\rangle$ in the event [103].

resolution (cf. Section 4.3).

4.2. Reconstruction

Because of the similarities of the electromagnetic showers created by electrons and photons (e/γ) in the calorimeter, the e/γ -reconstruction [103] share some of their steps. Topological clusters with a fraction of more than $f_{\text{EM}} > 0.5$ of their energy in the electromagnetic calorimeters are used as seeds for the e/γ -reconstruction. Track candidates from the nominal track reconstruction (cf. Section 4.1.1) in the region of a calorimeter cluster, which satisfies loose requirements on its lateral and transverse shape, are used as input for the e/γ -reconstruction. These tracks are refitted taking into account the high expected radiative energy losses of electrons in the inner detector allowing up to 30% energy loss at each material crossing. Photon-conversion vertices are reconstructed from track pairs originating from the same point and being consistent with a massless particle. In addition conversion vertices are reconstructed from single tracks which are missing the inner silicon hits on their trajectory. To ensure a high fraction of genuine electron tracks as input to the conversion vertex reconstruction requirements on the transition radiation signature of the tracks in the TRT are applied.

Conversion-vertex candidates and refitted tracks are matched to the topological clusters to form photon and electron candidates. A cluster with a matched track is an electron candidate, a cluster with a conversion vertex is a converted photon and a cluster without track or vertex is an unconverted photon. An electron and photon candidate can be created from a single cluster and the ambiguity is partially resolved as described in Section 4.2.1 below.

The expected efficiency to find a conversion vertex for a true converted photon from simulated samples is around 70% (cf. Fig. 4.1). True unconverted photons mis-reconstructed as converted occur

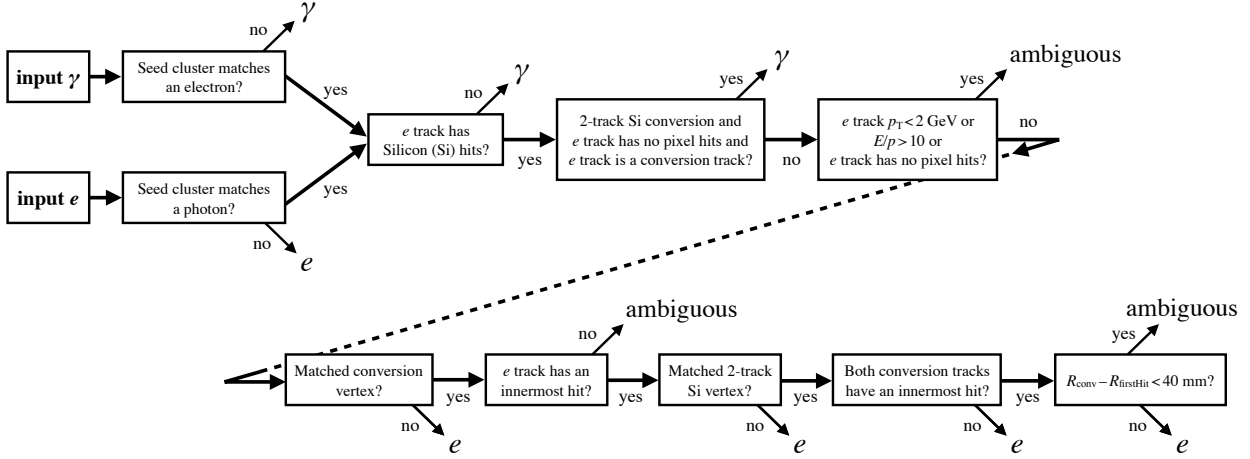


Figure 4.2.: Treatment of ambiguous cases where an electron and a photon candidate are created for the same cluster [103].

e.g. if a pileup track is matched to the cluster. Especially TRT tracks in high pileup conditions are prone to be imitated by pileup particles, because of the limited granularity of the TRT tubes parallel to the tube direction (cf. Fig. 4.1).

Photon conversions in front of the calorimeter and the radiative energy losses of the subsequent electrons can create separate *satellite* topological clusters in the calorimeter. These clusters are mostly separated in the ϕ -direction, because of the orientation of the magnetic field in the inner detector. The satellite clusters are added to the seed cluster to recover the energy. First all clusters in a $\Delta\eta \times \Delta\phi = 0.075 \times 0.125$ -vicinity of the seed cluster are added. For converted photons with a conversion vertex with two tracks with hits in the silicon layers clusters are added if one of the tracks matches to them. In the last step the supercluster formed by the seed cluster and added satellites is cropped to contain only cells in the EM calorimeters and to have a maximal width of 0.075 (0.125) in η in the barrel (endcap) to limit the sensitivity to pileup noise.

4.2.1. Electron-photon ambiguity resolution

In many cases there is both an electron candidate and a photon candidate created for one calorimeter cluster. For cases where the cluster can be assigned with high certainty to be coming from either photon or electron only the respective object is saved and the other option is neglected. For cases where the arbitration is not clear both objects are saved and they are marked as *ambiguous*. The different steps in the categorization are depicted in Fig. 4.2.

The cuts in the first row are checking if the track of the electron candidate is compatible with a photon conversion, e.g. missing hits in the silicon layers, and are removing the electron candidate while keeping the photon (γ) or labelling the electron and photon candidate as ‘ambiguous’. The cuts in the second row check the conversion vertex of the photon candidate. If it does not have a conversion vertex the photon candidate is removed and only the electron candidate is stored (e). The remaining cuts either identify ambiguous cases or remove the photon candidate if the quality of the reconstructed photon conversion vertex is insufficient.

Although the algorithm is optimized to have a high efficiency by retaining both objects in ambiguous cases, slight inefficiencies occur and candidates from genuine photons are removed and only the reconstructed electron objects are stored. Especially the requirement of the conversion vertex removes some genuine photons, which are reconstructed as unconverted. This can happen, if the photon converts very early with only one high energy track, or if the quality of the track is good enough to create an electron object, but not sufficient to reconstruct a conversion vertex. The efficiency of the ambiguity resolution for genuine photons and its modelling in simulation is studied in Section 6.2 and is only around 95%.

4.3. Energy calibration

The energy of the photon candidates is estimated based on the energy of the supercluster. A multivariate regression is trained on simulated samples to correct for the energy losses of the photon outside of the cluster, e.g. in front of the calorimeter [106]. The regression uses e.g. the η -position of the cluster and the longitudinal shower development in terms of the energy ratio E_1/E_2 between the energy deposited in the first and second layer of the calorimeter as input. The relative energy resolution is usually below $\Delta E/E < 2\%$ for photons with $E_{T,\gamma} > 30$ GeV which are relevant for the photon pair measurement.

Using superclusters instead of the previously used fixed size cluster approach improves the energy resolution, because the topological clusters are able to capture a larger fraction of the energy. The energy resolution as a function of the average interactions per bunch crossing $\langle\mu\rangle$ is depicted in Fig. 4.3. For very high pileup conditions the improvements in terms of energy resolution of the supercluster approach vanish. This indicates that the dynamical expansion of the clusters make it also more susceptible to pileup noise. This could possibly be inhibited by limiting the size in ϕ or by using dynamical pileup noise thresholds for the topological cluster formation instead of the fixed value.

Besides the multivariate energy reconstruction, which is derived purely simulation based, multiple data-driven calibration procedures are deployed to ensure matching energy scale and resolution in simulated samples and real data. Only a short overview of the full procedure described in [106] is given here.

The relative energy scales of different layers of the calorimeter are adjusted in data to match the ones in simulation to make the simulation based energy reconstruction more reliable for data. This interlayer calibration is based on muon energy deposits in $Z \rightarrow \mu\mu$ events in data and simulation. Muons are used, because their energy deposits in the calorimeter are insensitive to energy deposits in front of the calorimeter. After the application of the multivariate energy reconstruction the photon candidate energies in data are corrected for non-uniformities of the energy response. The non-uniformities are measured based on the ratio of the electron track momentum in $Z \rightarrow ee$ events to the corresponding energy measured in the calorimeter. The position of the $Z \rightarrow ee$ mass peak is used to derive small residual energy scale corrections in data. The width of the peak is used to derive corrections to the energy resolution in simulation. Because of similarities of the EM shower of electrons and photons the corrections derived in $Z \rightarrow ee$ events are also applicable to photons. The validity of this assumption is checked based on the three-body mass in $Z \rightarrow ee\gamma$ and $Z \rightarrow \mu\mu\gamma$ events (cf. Fig. 4.3).

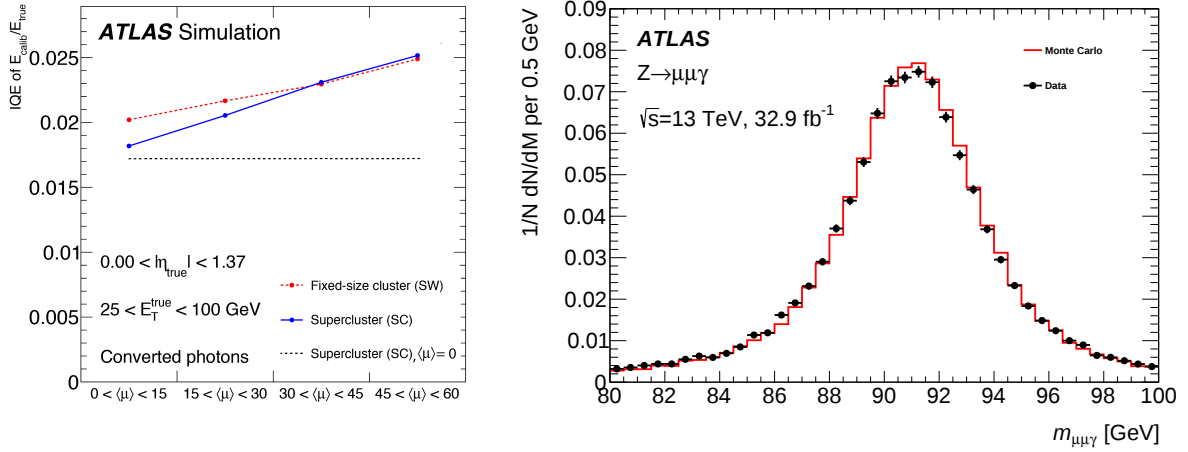


Figure 4.3.: Energy resolution (left) of the photon energy measurement in simulated samples in terms of the inter quartile range IQR, which is defined as the range between the 25% and 75% quartile of the energy response $E_{\text{calib}}/E_{\text{true}}$ distribution divided by a normalization constant of 1.349 such that the range would correspond to a $\pm 1 \sigma$ interval for a gaussian distribution [103]. Comparison of the distribution of the invariant mass (right) in $Z \rightarrow \mu\mu\gamma$ events between data and simulation after the energy calibration [106].

4.4. Photon identification

The photon identification [103] is based on the shape of the electromagnetic shower created by the photon in the calorimeter. Multiple identification variables are calculated which quantify the longitudinal and lateral shape of the shower. Cuts on these variables are used to distinguish photon candidates created by genuine photons from photon candidates from background processes. Genuine or prompt photons are defined as photons not originating from a hadron decay. The main source of background are hadronic jets including a neutral meson decaying into a pair of collimated photons.

The identification variables are summarized in Table 4.1 and can be grouped into three different categories:

- variables describing the hadronic leakage, which are defined as the ratio of the energy in the electromagnetic calorimeter to the energy in the hadronic calorimeter,
- variables quantifying the lateral shower shape in the middle layer of the electromagnetic calorimeter,
- variables using information in the first narrow strip layer of the calorimeter.

Requirements on the first two categories of variables are good to reject most of the background from hadronic jets, which usually consist of many collimated particles including e.g. charged pions $\pi^\pm$ which deposit a significant fraction of their energy in the hadronic calorimeter. The requirements on these first two categories are combined into the *Loose'5* working point of the photon identification, which has a high efficiency for genuine photons, but is already rejecting large fractions of the background.

Category	Description	Name	<i>Loose'5</i>	<i>Loose'2</i>	<i>Tight</i>
Hadronic leakage	Ratio of E_T in the first sampling layer of the hadronic calorimeter to E_T of the EM cluster (used over the range $ \eta < 0.8$ or $ \eta > 1.37$)	R_{had_1}	✓	✓	✓
	Ratio of the E_T in the hadronic calorimeter to E_T of the Em cluster (used over the range $0.8 < \eta < 1.37$)	R_{had}	✓	✓	✓
EM Middle Layer	Ratio of $3 \times 7 \eta \times \phi$ to 7×7 cell energies	R_η	✓	✓	✓
	Lateral width of the shower	$w_{\eta 2}$	✓	✓	✓
	Ratio of $3 \times 3 \eta \times \phi$ to 3×7 cell energies	R_ϕ	✓	✓	✓
EM Strip Layer	Total lateral shower width	w_{stot}		✓	✓
	Ratio of the energy difference associated with the largest and second largest energy deposits to the sum of these energies	E_{ratio}		✓	✓
	Difference between the energy associated with the second maximum in the strip layer and the energy reconstructed in the strip with the minimum value found between the first and second maxima	ΔE		✓	✓
	Energy outside the core of the three central strips but within seven strips divided by energy within the three central strips	F_{side}			✓
	Shower width calculated from three strips around the strip with maximum energy deposit	w_{s3}			✓

Table 4.1.: Description of photon identification variables and definition of various identification criteria which take into account different subsets of the variables [103, 109].

If the overlapping electromagnetic showers of a neutral meson decay in a jet are separated enough from the other particles in the jet or carry a large fraction of the energy of the jet they can also create a photon candidate passing the *Loose'5* requirements. The last category of identification variables uses the information of the narrow strips in the first layer of the calorimeter, which is in many cases granular enough to resolve separate energy maxima of the two collimated photons. The variables quantify these separate energy maxima and the width of the shower in the first layer. The requirements on this set of variables are used in addition to the *Loose'5* ones to define the *Tight* identification criterion.

Even the *Tight* criterion can be passed by background e.g. if the angular separation of the photons from the hadron decay aligns with the ϕ direction, where the granularity of the first layer is only $\Delta\phi = 0.1$. The background from jets is especially large at low transverse momentum of the photon candidates and is estimated based on data control regions in the photon pair measurement (cf. Section 7.5). The control regions are enriched in background by requiring the photon candidates to fail the *Tight* identification, but to pass the requirements of the *Loose'2* requirement, which includes requirements on three of the strip layer shower shape variables in addition to the *Loose'5* requirements (cf. Table 4.1). The cuts for all working points are optimized based on simulated samples of signal and background in order to maximise the signal efficiency and background rejection. The requirements are optimized separately for photons reconstructed as converted or unconverted. This leads to looser cut values for converted photons for which the EM shower tends to be wider.

The background estimation and the correction of the detector level results for selection inefficiency require reliable estimates of the identification efficiencies of genuine photons. This is achieved in two steps.

In the first step the photon identification variables are compared between data and simulation in radiative $Z \rightarrow ll\gamma$ events. Tight lepton (here electron or muon) identification and a requirement on the three-body mass $m_{ll\gamma}$ are used to select a pure sample of genuine photons without identification requirements on the photon candidate. An optimal shift to the distribution of the identification variables in the simulated sample is derived, such that they recreate the distributions in data as close as possible.

In the second step the photon identification efficiencies are compared between data and simulated samples after the shifts of the first step are applied. Three different processes covering different transverse momentum regimes of the photon candidates are used to investigate the efficiencies. The first process are again radiative $Z \rightarrow ll\gamma$ events which contain photons with relatively low transverse momentum. The second process are the electrons in $Z \rightarrow ee$ events exploiting the similarities between photon and electron showers at the cost of an additional uncertainty related to the extrapolation from electrons to photons. The third process most relevant at high transverse momentum, where the fraction of background photons is low, are single photon events. This process extends the measurement into the TeV regime. The photon efficiencies in simulated samples are corrected based on weights derived from the ratio of the efficiency measured in data to the efficiency measured in simulation which are referred to as *scale factors* in this context. The shifts and efficiency corrections are measured as a function of the rapidity η and transverse momentum of the photons.

A selection of the results of the efficiency measurements is depicted in Fig. 4.4. For $p_{T,\gamma} > 30$ GeV the efficiencies range between 80 to 99% and the ratios of the efficiencies of data to simulation are compatible with one within the uncertainties of the measurements.

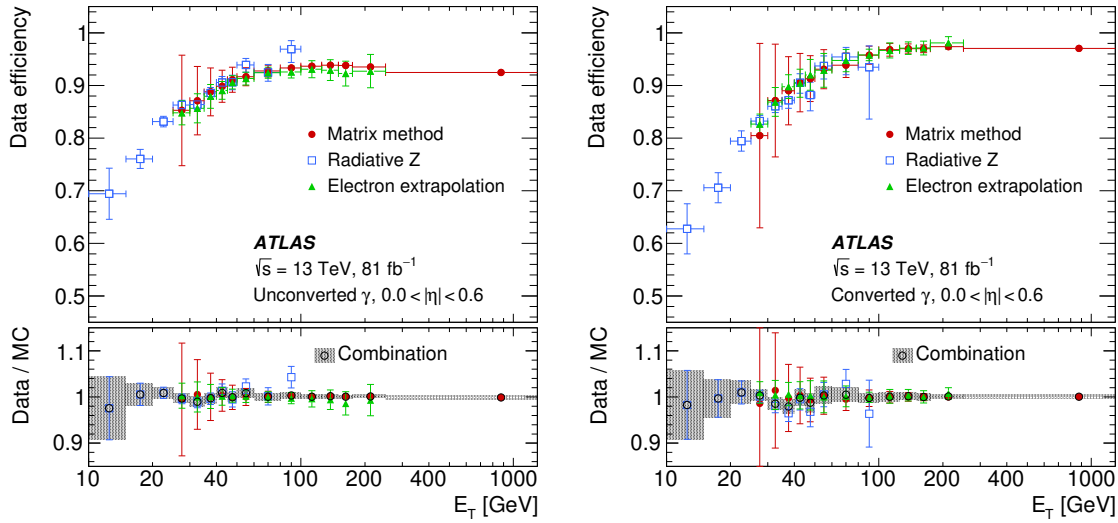


Figure 4.4.: Efficiency of the tight photon identification requirements measured in radiative Z (blue), $Z \rightarrow ee$ (green) and single photon (red) events in data (top) and the ratio to the value in simulation (bottom) for unconverted photons (left) and converted photons (right) [103].

4.5. Isolation

The photon isolation [103] is an additional property mostly independent from the identification requirements and can be used to further discriminate prompt photons against background. It is a measure of the additional activity in a wider area around the photon candidate excluding the signatures of the photon candidate itself. Two options to reconstruct isolation energies are widely used. One is based on the inner detector tracks (*tracking isolation*) and the other is based on topological calorimeter clusters (*calorimetric isolation*) in a cone around the photon candidate.

The tracking isolation p_T^{coneXX} is defined as the sum of the transverse momenta p_T of tracks in a cone of $\Delta R < 0.XX$ around the photon direction. The tracks associated to a converted photon are excluded and only tracks with $p_T > 1$ GeV enter. Furthermore tracks which are separated by more than $|\Delta z_0| \sin \theta > 3$ mm from the primary vertex of the event are removed to suppress the influence of pileup particles.

The calorimetric isolation has the benefit of including the energy of neutral particles and of particles which do not pass the p_T threshold of the tracking isolation, but is also much more susceptible to pileup. The calorimetric isolation is calculated in multiple steps. The raw isolation $E_{T,\text{raw}}^{\text{coneXX}}$ is defined as the sum of the transverse energies of all topological clusters in a cone of a certain radius $\Delta R < 0.XX$ around the photon direction.

The transverse energy deposited in the rectangular window of 5×7 cells in $\eta \times \phi$ around the photon $E_{T,\text{core}}$ is subtracted from the raw transverse isolation energy. The average transverse energy leaking out of this core region into the isolation cone $E_{T,\text{leakage}}$ is studied in MC samples, parametrized as a function of p_T and η of the photon and subtracted.

Furthermore effects of pileup are corrected for on an event-by-event based estimation of the ambient

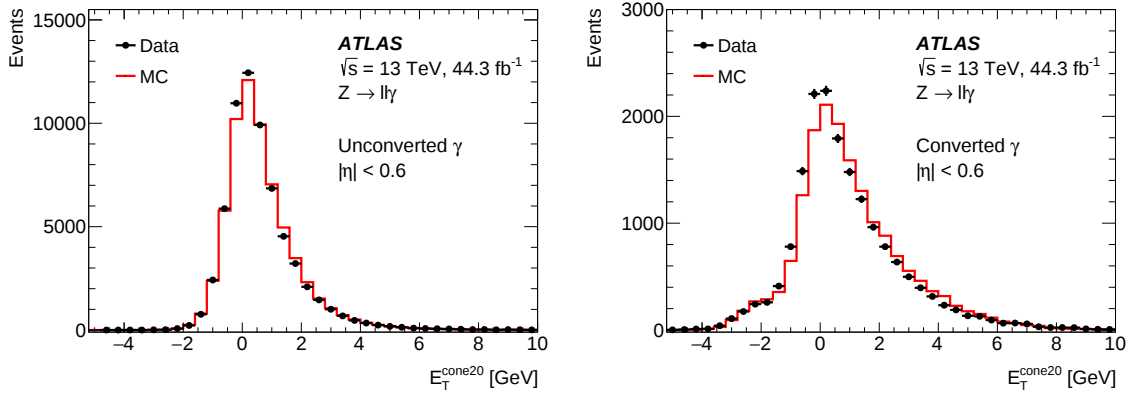


Figure 4.5.: Distribution of the calorimetric photon isolation E_T^{cone20} in $Z \rightarrow l\bar{l}\gamma$ events in data and MC for unconverted (left) and converted (right) photons [103].

transverse momentum density [110, 111], which is for simplicity referred to as energy density in the following. The energy density ρ is defined as the median of the individual jet transverse momentum densities of the event:

$$\rho = \text{median}_{i \in \{0, \dots, N_{\text{jet}}\}} \left\{ \frac{p_{T,i}^{\text{jet}}}{A_i^{\text{jet}}} \right\}. \quad (4.3)$$

The jet transverse momentum density is the transverse momentum of the jet $p_{T,i}^{\text{jet}}$, divided by its area A_i^{jet} . The jets used for the calculation are created from the momenta of the calorimetric clusters with the k_t -algorithm [112] with a radius parameter of $R = 0.5$. The area of the jets A_i^{jet} is estimated based on the Voronoi area algorithm as implemented in FASTJET [113]. For a k_t -jet this is the area in which a soft particle added to the event would be clustered into the jet. The area not covered by any jets (e.g. because there are no calorimetric clusters) is considered to be filled with jets with zero transverse momentum and they are included into the median calculation. This means the energy density can be zero, if only a few jets are reconstructed [113].

The energy density is determined independently for jets in the central region $|\eta| < 1.5$ and in the forward region $1.5 < |\eta| < 3$. The corresponding energy density values are referred to as central energy density and forward energy density. The pileup correction to the photon isolation is then calculated with the energy density of the respective η -region the η of the photon candidate lies in:

$$E_{T,\text{pileup}}(\eta) = \rho(\eta) \cdot (\pi \Delta R^2 - A_{\text{core}})$$

with the core area of the photon A_{core} and the radius of the isolation cone ΔR . The fully corrected isolation energy is then calculated as:

$$E_T^{\text{coneXX}} = E_{T,\text{raw}}^{\text{coneXX}} - E_{T,\text{core}} - E_{T,\text{leakage}}(\eta, p_T) - E_{T,\text{pileup}}(\eta).$$

Similar to the corrections for the photon identification variables, shifts for the calorimetric isolation

variables are derived to correct the distributions in simulation to recreate the ones in data. They are derived from single photon and $Z \rightarrow l\gamma$ events in bins of η , p_T of the photons and separately for converted and unconverted photons.

The tracking and calorimetric isolation variables are calculated in a similar way for electrons and muons with slight adjustments on the subtraction of the contribution of the electron or muon to the isolation.

An example of the distribution of the calorimetric isolation for photons in data and simulation is depicted in Fig. 4.5. The distribution is centred around zero for genuine photons. The width of the distribution is driven by the amount of pileup in the events.

Chapter 5.

Pileup dependency of calorimetric isolation variables

To achieve very high precision measurements in the environment of increasing pileup it is crucial to subtract effects of pileup as much as possible and to have a correct model of the residual pileup effects in simulation.

In this chapter the pileup dependency of the calorimetric isolation is investigated in $Z \rightarrow ee$ events. The goal is to capture only the pileup dependency of the isolation energy around the electron which should then also generalize to other isolated objects like e.g. photons.

The data and MC samples are introduced in Sections 5.1 and 5.2. The $Z \rightarrow ee$ event selection is described in Section 5.3 and the details of the isolation definitions used throughout the chapter are discussed in Section 5.4. In Section 5.5 a parametrization of the median of the energy in different isolation regions around the electron is derived as a function of the pseudo-rapidity η , the area of the isolation region A and the transverse energy density ρ . The results are used to derive an improved pileup subtraction which is continuous in η , increasing the stability of the calorimetric isolation variables as a function of pileup and η compared to the current two ρ -bin approach. A similar approach is used in Section 5.6 to correct the pileup dependency of the calorimetric isolation in simulation. Section 5.7 compares the noise added to the calorimetric isolation by pileup in data and simulation with different pileup overlay models.

5.1. Data samples

The full pp collision data taken by ATLAS from 2015 to 2018 during the LHC Run-2 is used. Only data with stable beam and detector conditions [114] is considered, which corresponds to an integrated luminosity of 139 fb^{-1} . Some of the studies only use the data of specific years, in which case this is explicitly stated.

5.2. MC samples

The POWHEG BOX v1 MC generator [115–118] was used for the simulation of the hard-scattering processes of Z boson production and the decay in the electron channel. The NLO calculation was

matched to PYTHIA 8.186 [44] for the modelling of the parton shower, hadronisation, and underlying event, with parameters set according to the AZNLO tune [119].

5.2.1. Pileup overlay

For the studies in Sections 5.5 and 5.6 the nominal ATLAS pileup overlay for the MC samples is used, which overlays the simulated primary-scattering event with inelastic proton–proton (pp) events generated with PYTHIA 8.186 [44] using the NNPDF2.3LO set of PDFs [120] and the A3 set of tuned parameters [98].

To study the influence of the modelling of the pileup overlay on the width of the calorimetric isolation distribution in Section 5.7 alternative setups are used for the pileup overlay.

- The PYTHIA 8 **Monash** tune [121] is used. The nominal A3 tune is based on this tune, but gives a better description of the charged particle multiplicity compared to data [98]. It is mostly used as a reference to study the influence of the overestimation of the charged particle multiplicity.
- **EPOS** [122] is used, which is a generator developed in the context of heavy ion collisions and is also applied for cosmic ray simulations. In Ref. [123] EPOS is studied in the context of proton–proton collisions and shows good agreement in the charged particle multiplicities especially at low p_T .
- A combination of **EPOS+A3** is used utilizing the good description of PYTHIA 8 at high p_T and the benefits of EPOS at low p_T .

5.2.2. Pileup reweighting

The distribution $g_{MC}(\mu)$ of the number of interactions per bunch crossing μ in the MC samples is reweighted to match the distributions in data $g_{data}(\mu)$. The reweighting function $w(\mu)$ can be adjusted such that the MC distribution recreates the data distribution scaled by a factor $f_{\mu-scale}$:

$$w(\mu)g_{MC}(\mu) = g_{data}(f_{\mu-scale} \cdot \mu)/f_{\mu-scale}. \quad (5.1)$$

This means the average $\langle\mu\rangle$ in MC is scaled down by $1/f_{\mu-scale}$ after the reweighting. Nominally a factor of $f_{\mu-scale} = 1.03 \pm 0.04$ is used in ATLAS to improve agreement between data and simulation in the visible inelastic pp cross-section [124]. The pileup reweighting is varied in Section 5.7 studying the pileup noise of the isolation distribution. The μ -distributions in data and MC after the reweighting are depicted in Fig. 5.1.

5.3. Event Selection

The event and object selection is designed to get a sample of pure unbiased electrons from $Z \rightarrow ee$ events in data. In this context unbiased means no requirement can be applied on the property under investigation which in this case is the isolation of the electron. This is achieved with a tag-and-probe strategy, applying strict requirements on one of the electrons (tag) and at least no isolation requirements on the other electron (probe) which is studied.

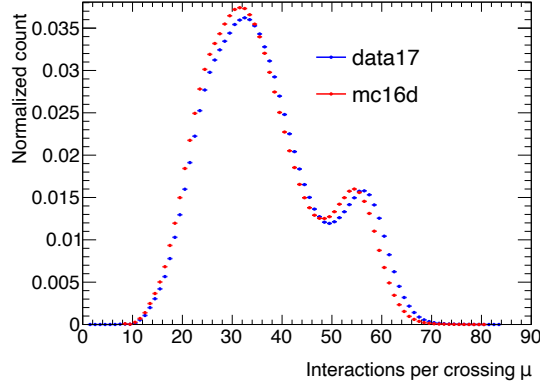


Figure 5.1.: Comparison of the distribution of numbers of interactions per bunch crossing μ in data taken in 2017 (blue) and the corresponding mc16d MC samples (red) after the pileup reweighting with the nominal factor $1/f_{\mu-scale} = 1/1.03$ is applied.

The electron reconstruction and energy calibration follows mostly the same procedure as described in Chapter 4 for photons. A multivariate projective likelihood discrimination is used for the electron identification, which uses variables based on information of the electron track in addition to the photon identification variables [103].

Events are selected for which all detector components were working nominally, at least two electron candidates are reconstructed and at least one of the two single electron triggers [93] described in the following is fired.

The first HLT trigger option (HLT_e26_lhtight_nod0_ivarloose) is fired by electrons with $E_T > 26$ GeV fulfilling the tight likelihood working point and satisfy the following isolation criteria. The scalar sum of the p_T of tracks within a variable-size cone around the electron, must be less than 10% of the electron p_T , excluding tracks originating from the lepton itself. The track isolation cone radius for electrons $\Delta R = \sqrt{(\Delta\eta)^2 + (\Delta\phi)^2}$ is given by the smaller of $\Delta R = 10 \text{ GeV}/p_T$ and $\Delta R = 0.2$.

For the second option (HLT_e60_lhmedium_nod0) the isolation criteria is dropped and the identification working point is loosened to the medium working point whereas the energy requirement is restricted to $E_T > 60$ GeV.

Tag-and probe pairs are built from electron combinations in the events. The trigger must have a matching direction to the tag electron. Furthermore strict identification requirements are imposed on the tag electron and on the invariant mass of the tag-and probe pair to increase the purity of $Z \rightarrow ee$ events in the selection. At the same time the requirements on the probe electron are kept looser.

The tag electron has to pass the following selection criteria:

- must have a matching direction to one of the fired electron triggers
- tight identification
- outside of crack $|\eta| < 1.37$ or $|\eta| > 1.52$
- must be central $|\eta| < 2.47$

- minimal transverse momentum $p_T > 25$ GeV

The following selection is imposed on the probe electrons:

- not more than one jet with $p_T > 20$ GeV in a cone of $\Delta R < 0.4$ around the probe
- tight identification
- angular distance to tag $\Delta R > 0.4$
- both electrons are required to have opposite charge
- invariant mass of tag-and probe system $86.2 \text{ GeV} < m_{ee} < 96.2 \text{ GeV}$

The selection is applied in the same way to MC and data. For MC the electrons are in addition required to match to true electrons from a Z decay. A comparison of m_{ee} , p_T^{probe} and η^{probe} between data and MC is depicted in Fig. 5.2. The high purity shown by the good agreement motivates the negligence of small background effects for the following studies. The selected sample provides excellent statistics with around 58 million probe electrons selected in the full Run-2 data.

5.4. Supercluster based core subtraction

The electron isolation is defined in the same way as for photons in Section 4.5. This definition contains the subtraction of the energy in a fixed-size window around the electron candidate and a subsequent parametrized leakage correction as a function of η and p_T of the candidate.

Alternatively with the new topological-cluster based e/γ -reconstruction (cf. Chapter 4) the associated topological clusters combined into the e/γ supercluster can be used to subtract the energy contribution of the electron or photon to the isolation region more faithfully. Because of the dynamical expansion of the topological clustering they contain a larger fraction of the electron or photon energy and the energy leaking into the isolation region is reduced. For the studies in the following sections the supercluster based core subtraction is used to reduce the sensitivity to the electron in the centre.

The supercluster based core subtraction can lead to a reduced background rejection of the isolation, because the subtracted energy for a background candidates can be also larger compared with the fixed-size-window subtraction, especially if the wider shower of the background candidate causes the topological clusters to expand to a larger volume than for an electron or photon candidate. This caveat is the reason for currently not using the supercluster based subtraction as the default. Constraining the maximal size of the supercluster in ϕ direction could improve this.

5.5. Improved data-driven pileup subtraction

The current parametrization of the pileup subtraction was described in Section 4.5 and is given by $A \times \rho$, where ρ is derived in two bins of η . The new subtraction is only using the central energy density derived for the central bin as a proxy for the pileup activity in the event and introduces a new factor $\zeta(\eta)$ which describes the η -dependency of the pileup contribution to the isolation energies. In the following Section 5.5.1 this approach is motivated and in Section 5.5.2 the data-driven derivation of $\zeta(\eta)$ is described.

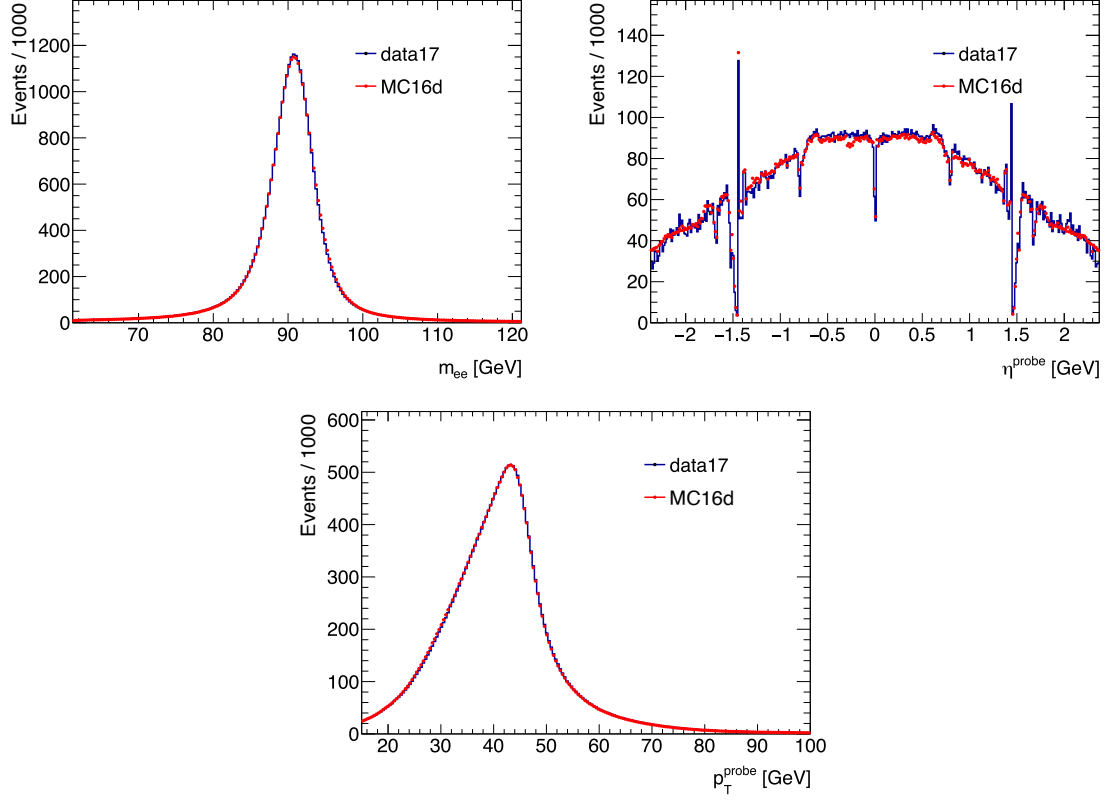


Figure 5.2.: Distribution of the invariant mass of the electron-positron system m_{ee} (left) the pseudorapidity of the probe electron η^{probe} (middle) and its transverse momentum p_T^{probe} (right). For the mass distribution the mass cut is not applied. The distributions are shown for data taken in 2017 in blue and for the corresponding MC in red. The MC histograms are normalized to data.

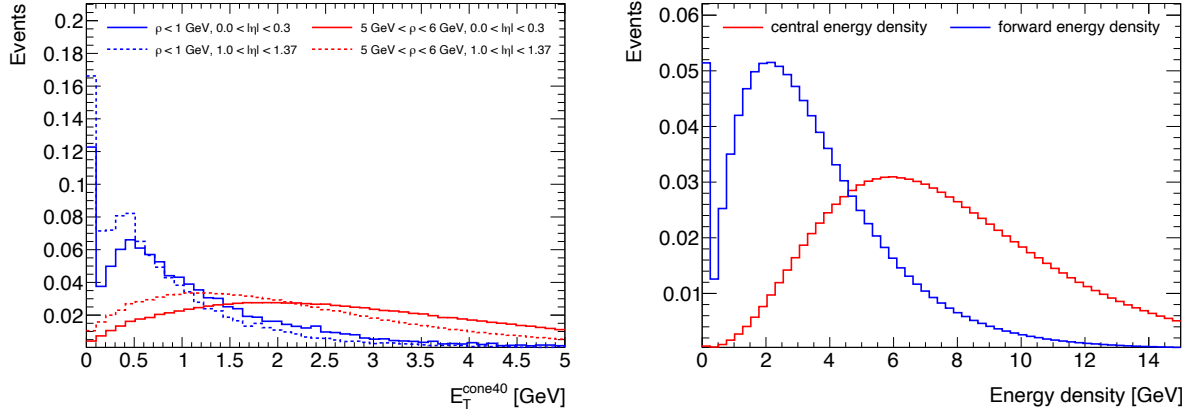


Figure 5.3.: Distributions in full Run-2 data passing the $Z \rightarrow ee$ selection are depicted. The left plot shows the calorimetric isolation E_T^{cone40} without pileup subtraction and with the supercluster based core subtraction (right) for events with low values $\rho < 1$ GeV (blue) and medium values $5 \text{ GeV} < \rho < 6 \text{ GeV}$ (red) of the central energy density. The histograms with solid lines show the isolation distribution for electrons in a central η -region ($|\eta| < 0.3$) and the dashed lines for a more forward region ($1.0 < |\eta| < 1.37$). The right plot shows the central (blue) and forward (red) energy density.

5.5.1. Motivation

The new pileup subtraction is motivated by looking at the calorimetric isolation variables without pileup correction and comparing the distributions in different $|\eta|$ and ρ bins, which is depicted in Fig. 5.3 on the left. In events with low energy densities ($\rho < 1$ GeV) the distributions have a discrete peak at zero. This occurs if no calorimetric cluster is inside the isolation region in addition to the clusters associated to the electron. For events with a higher energy density ($5 \text{ GeV} < \rho < 6 \text{ GeV}$) this occurs only in a small fraction of events and the distribution is wider and has a higher mean value compared to the low energy density selection. The distributions of electrons with a high $|\eta|$ value are peaked at lower values of E_T^{cone40} compared to the distribution with the same energy density selection, but selecting more central electrons. Both selected $|\eta|$ -regions for which the isolation distribution is depicted in Fig. 5.3 are in the region $|\eta| < 1.5$, which means the nominal pileup subtraction values are the same for both distributions, although the mean value of the distributions is clearly different. This motivates an η -dependency of the pileup correction beyond the two η -bins of the current one.

Using only the central energy density is motivated by the comparison of the distributions in Fig. 5.3. The forward energy density distribution has a discrete peak at zero, this can occur as explained in Section 4.5, if a larger fraction of the area in the detector is empty. In these events the nominal pileup subtraction of the isolation energy is zero and therefore most likely underestimating the true pileup contribution.

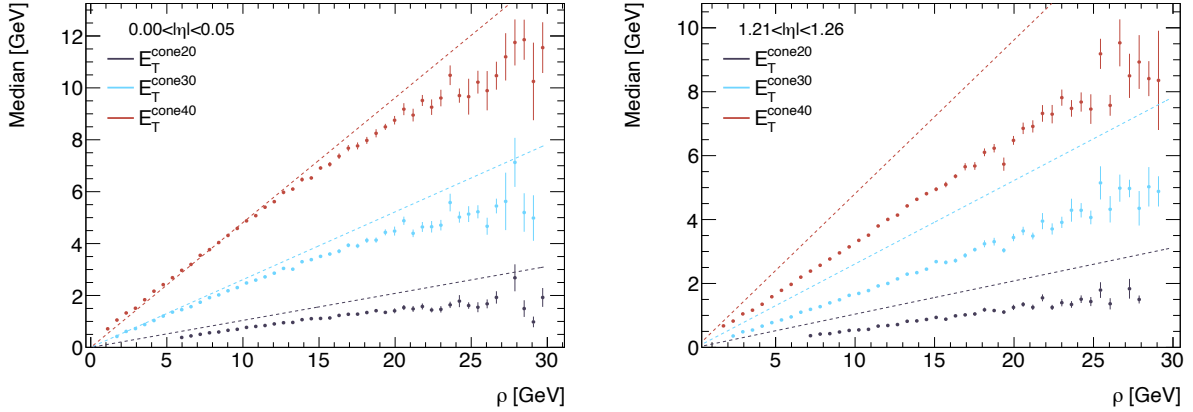


Figure 5.4.: Comparison of the median isolation values (points) with the current pileup subtraction scheme (dashed lines). The different colours indicate the different isolation variables E_T^{cone40} (red), E_T^{cone30} (blue), E_T^{cone20} (grey). The left hand plot shows the results for electrons in $|\eta| < 0.05$ and the right hand plot for electrons in $1.21 < |\eta| < 1.26$. Probe electrons of $40 \text{ GeV} < p_T < 45 \text{ GeV}$ are used.

5.5.2. Pileup subtraction as a function of η

The improved pileup subtraction is derived in data based on a measurement of the median of the isolation distribution as a function of η of the probe electrons and the central energy density ρ of the event in data. The median values of isolation variables with different cone sizes are depicted for two $|\eta|$ -regions of the probe electron in Fig. 5.4. The values are compared to the current pileup correction scheme. Whereas fairly good agreement can be observed in the very central $|\eta| < 0.05$ region the agreement is degraded for $1.21 < |\eta| < 1.26$. The measured median values show a non-linear saturating dependency in the region of $\rho > 30 \text{ GeV}$ and the extrapolation to $\rho = 0 \text{ GeV}$ does not yield median=0, which means there are regions where the linear pileup subtraction is not optimal.

The new pileup subtraction:

$$\Delta^{\text{pileup}} = A\rho\zeta(\eta), \quad (5.2)$$

introduces an additional factor $\zeta(\eta)$, which corresponds to a changing slope $\frac{\Delta^{\text{median}}}{\Delta\rho}$ as a function of $|\eta|$. The $\zeta(\eta)$ function is supposed to model the smoothly decreasing transverse energy density from pileup to larger η and to account for inhomogeneities of the pileup acceptance of the detector (e.g. lower cluster reconstruction efficiency in the transition region between the barrel and end-cap calorimeters $1.37 < |\eta| < 1.52$ referred to as *crack*). Especially because of these detector effects it is beneficial to adjust the $\zeta(\eta)$ for different isolation area definitions. For example a small circular cone of an electron near the crack has a large fraction of its area inside the crack region. Whereas a larger cone around the same electron has a much smaller fraction of its area inside the crack. Therefore the $\zeta(\eta)$ should be larger for the larger cone. To accommodate this based on one set of parameters f_i for

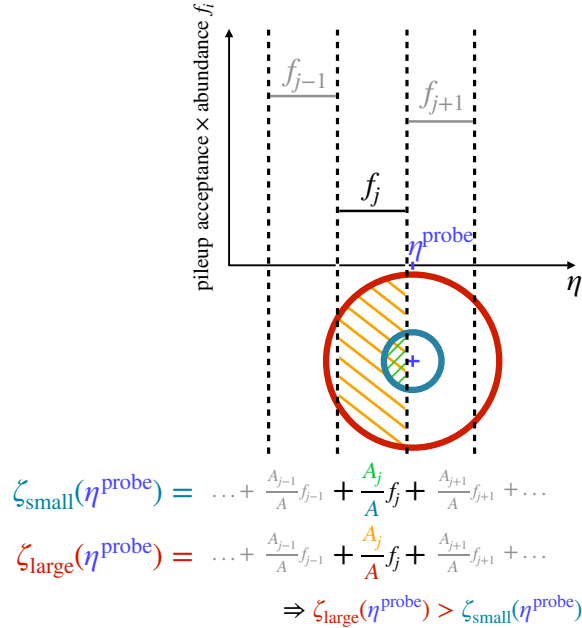


Figure 5.5.: Exemplary sketch comparing the calculation of $\zeta_{\text{shape}}(\eta)$ of a large and small radius cone near a bin with small detector pileup acceptance.

arbitrary isolation area shapes the $\zeta_{\text{shape}}(\eta)$ -functions for Eq. (5.2) are calculated as follows:

$$\zeta_{\text{shape}}(\eta) = \sum_{i=0}^{n_\eta} \frac{A_i}{A} f_i. \quad (5.3)$$

The sum runs over a number n_η of η -bins. It is assumed that the f_i are constant in each of these bins. They describe the average pileup abundance and acceptance in their respective η -bin. The variable A is the complete area of the shape of the isolation region and A_i is the area in the i -th η -bin. An example for the calculation of the $\zeta_{\text{shape}}(\eta)$ is illustrated in Fig. 5.5. The f_i -factors are defined in 23 equal-spaced bins between $|\eta| = 0$ and $|\eta| = 2.8$.

The f_i are extracted from the data by fitting the median values m of $E_{\text{T}}^{\text{cone40}} - E_{\text{T}}^{\text{cone30}}$ and $E_{\text{T}}^{\text{cone30}} - E_{\text{T}}^{\text{cone20}}$ as a function of ρ of the event and $|\eta^{\text{probe}}|$ of the probe electron. The $E_{\text{T}}^{\text{cone40}} - E_{\text{T}}^{\text{cone30}}$ and $E_{\text{T}}^{\text{cone30}} - E_{\text{T}}^{\text{cone20}}$ isolation variables correspond to annulus shaped isolation regions, which are used to reduce sensitivity to the electron in the centre. Disjunct areas are chosen to avoid double counting. The data is split into fine bins of $|\eta^{\text{probe}}|$ and ρ and the median values of the isolation variables are derived in each bin. 47 equal size bins between $|\eta^{\text{probe}}| = 0$ and $|\eta^{\text{probe}}| = 2.37$ and 49 bins between $\rho = 0.2$ GeV and $\rho = 30$ GeV are used. This means a total of 2303 median values per isolation variable are calculated and used to derive the parametrization.

The following fit model is used to perform a χ^2 minimization with respect to all median points of the different isolation regions, $|\eta^{\text{probe}}|$ -bins and ρ -bins simultaneously:

$$m_{\text{shape}}(\rho, \eta) = A\rho\zeta_{\text{shape}}(\eta) + c_{\text{shape}}(\eta) \quad (5.4)$$

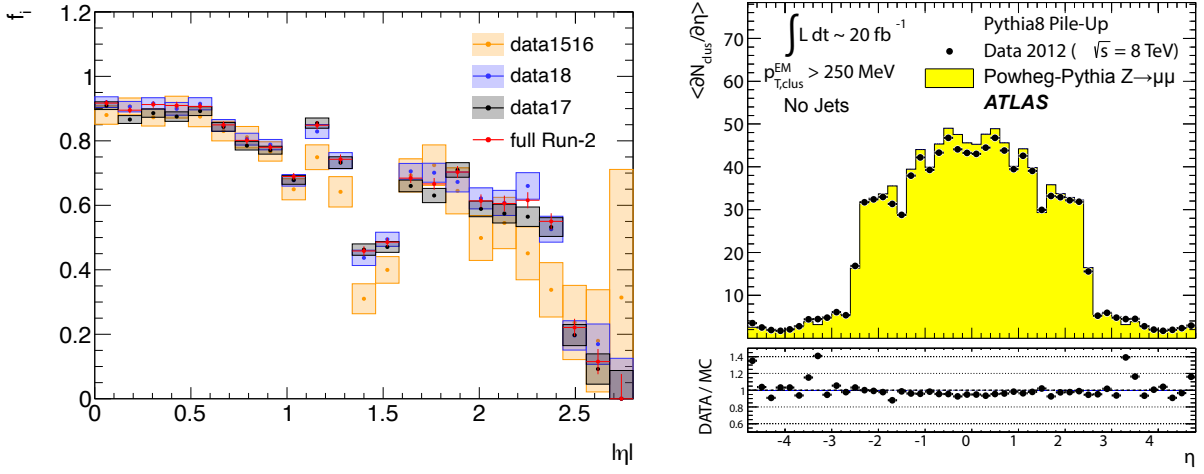


Figure 5.6.: The left plot shows the results for the f_i -parameters for each $|\eta^{\text{model}}|$ bin from the fit with full Run-2 data using the median values of $E_T^{\text{cone40}} - E_T^{\text{cone30}}$ and $E_T^{\text{cone30}} - E_T^{\text{cone20}}$. The right hand plot shows the average number of topological clusters from pileup with $p_T > 250$ MeV in different η -bins in data and MC from [104].

where $c_{\text{shape}}(\eta)$ is a individual constant term for each isolation variable and each $|\eta^{\text{probe}}|$ bin. Although these constant terms are needed for the fit, they are not included in the correction (see Eq. 5.3), because they do not describe a pileup dependency of the isolation. The constant terms describe small offsets of the isolation distribution in different η -regions which could e.g. be related to the subtraction of the energy of the electron. To exclude regions of non-linearity, events with low $\rho < 3$ GeV and high $\rho > 25$ GeV energy densities are excluded. In addition points where the median falls below $m < 750$ MeV are excluded. Furthermore electrons in the transition bin $1.46 < |\eta^{\text{probe}}| < 1.51$ are neglected for the fit and only electrons with $40 \text{ GeV} < p_T < 45 \text{ GeV}$ are used. The fit is performed for the full Run-2 dataset and also individually for 2015+2016, 2017 and 2018.

The resulting optimal f_i -parameters of the fit to the different datasets are summarized in Fig. 5.6. As expected f_i is decreasing as a function of $|\eta|$. The sharp drop in the crack region $1.37 < |\eta| < 1.52$ shows the capability of the fit to derive detector effects depending on the η of a individual cluster from variables calculated by summing over clusters in a large isolation area. Because the energy density is calculated with $k_t(R = 0.5)$ -jets in the $|\eta| < 1.5$ region it could be expected that the f_i in the central region would average to $\bar{f}_i \approx 1$ with higher values towards $|\eta| = 0$ and lower values towards $|\eta| = 1.5$. This is not the case the f_i average to around 80%. This indicates that the energy density of k_t -jets is not an optimal proxy for the energy density in the fixed sized cones of the isolation variables. The k_t -jets are by definition centred around a region of energy deposits, while the isolation cones are random with respect to the pileup events. Furthermore the area of k_t -jets in the presence of soft homogeneously distributed radiation (e.g. from pileup) is found to be smaller than πR^2 [111], because the soft radiation occupies some of the area at the edges of a hard jet creating additional soft jets. In contrast the area of the isolation regions is fixed and therefore independent of the radiation pattern of the event.

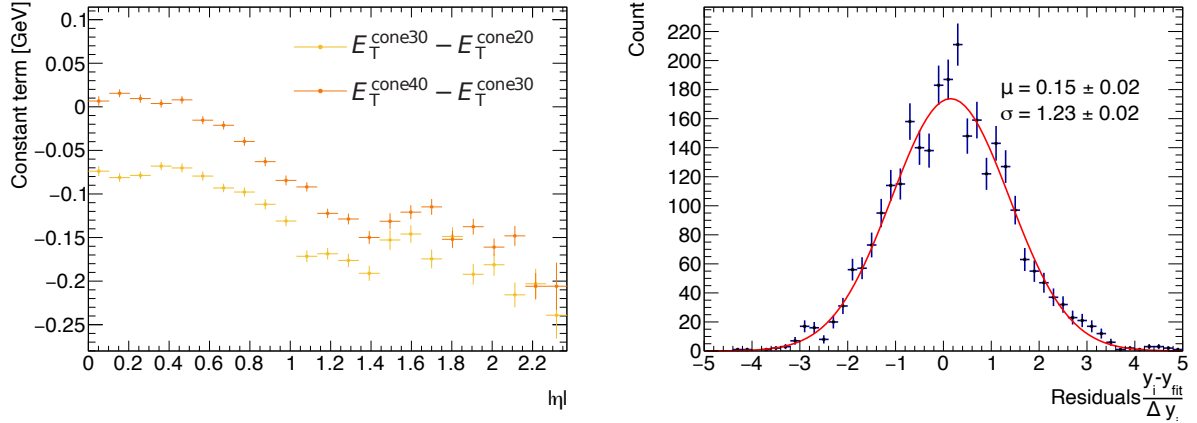


Figure 5.7.: Fit result for the constant $c_{\text{shape}}(\eta)$ parameters of the model (left). Residuals of the fit model (right), which are defined as the difference between the fit model and the data values divided by the uncertainty.

The sharp drop of the f_i factors for $\eta > 2.4$ is also expected. In this region the granularity of the detector gets much larger. Topological clusters are seeded by energy depositions which are significantly greater than the noise threshold. Because of the larger cells this threshold is higher and therefore more difficult to reach for the soft energy depositions from pileup. This effect is also visible in the right hand plot of Fig. 5.6 from [104], where the number of topological clusters has a sharp drop around $\eta = 2.5$.

In general the results for the f_i -parameters agree well within statistical uncertainties between the different years of the data taking. Slight deviations are visible for the values derived in data 2015+2016 in the four η -bins between $1.15 < |\eta| < 1.65$ where all f_i values are around 10 to 25% lower than the respective values in 2017 or 2018. This region is mostly relevant for the isolation region of candidates in the crack region $1.37 < |\eta| < 1.52$ and it was decided to use the same correction for all years for simplicity.

The results for the constant terms $c_{\text{shape}}(\eta)$ of the fits to the full Run-2 dataset are depicted in Fig. 5.7 (left). The values are relatively low $|c| < 200$ MeV which shows that the extrapolation to low energy density events gives a reasonable result. The constant terms do not enter into the new pileup subtraction (cf. Eq. (5.3)), because the goal is to only subtract the ρ dependent part.

The residuals of the fit are depicted in Fig. 5.7 on the right. They are approximately following a Gaussian distribution. Ideally this Gaussian distribution should have a standard deviation of $\sigma = 1$ and a vanishing expectation value $\mu = 0$. The small deviations from these values indicate that the model is not perfectly describing all points. Including a non-linear term could improve the modelling at high ρ . The standard deviation of $\sigma > 1$ could also indicate an underestimation of the statistical uncertainty of the median values. In Fig. 5.8 the fit results are compared with the data points in two η -regions showing the overall good agreement of the model with the data.

The results of the f_i are used to calculate the $\zeta_{\text{shape}}(\eta)$ functions for E_T^{cone20} , E_T^{cone30} and E_T^{cone40} using Eq. (5.3). The core of the isolation regions is subtracted from these isolation variables and therefore also not susceptible to pileup effects. This is incorporated into the shape of the isolation

5.5. Improved data-driven pileup subtraction

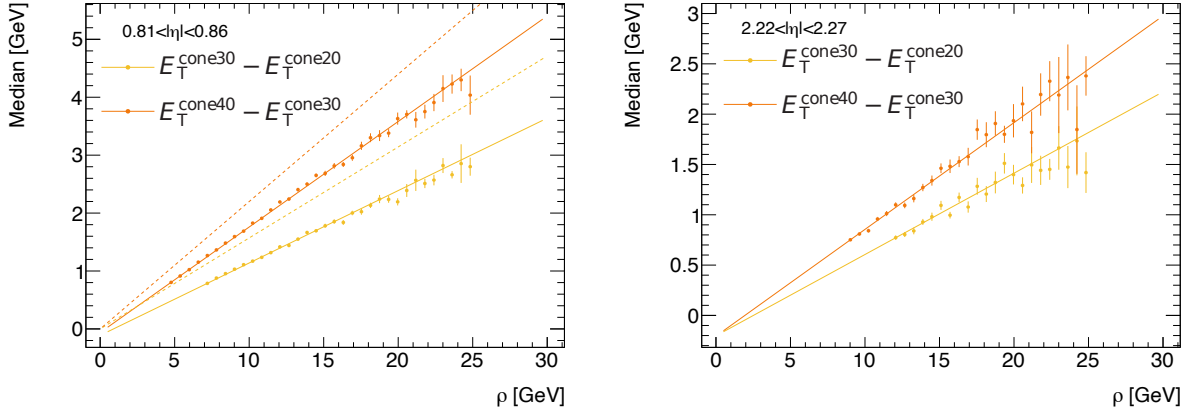


Figure 5.8.: Comparison of the fit results (solid lines) for the parametrization of the median isolation energy for $E_T^{\text{cone40}} - E_T^{\text{cone30}}$ (orange) and $E_T^{\text{cone30}} - E_T^{\text{cone20}}$ (yellow) for probe electrons in a central region ($0.81 < \eta < 0.86$) (left) and a forward region ($2.22 < \eta < 2.27$). The dashed lines in the left plot indicate the old pileup correction calculated as the product of the central energy density with the area.

region by defining them as annulus shaped with a small inner radius, such that the excluded area corresponds to a 5×7 window of cells in the middle layer of the EM calorimeter. This approximation could be improved upon by using the shape of the electron supercluster, if the supercluster based core subtraction is used or the shape of the window of cells subtracted in the default core subtraction. In general the influence of the core subtraction is small, because the area of the isolation cone is much larger than the area of the core.

The results for $\zeta_{\text{shape}}(\eta)$ are depicted in Fig. 5.9. The coloured bands indicate the statistical errors of the fit parameters f_i propagated to $\zeta_{\text{shape}}(\eta)$:

$$\Delta\zeta_{\text{shape}}(\eta) = \sqrt{\sum_{i,j} \frac{A_i A_j}{A^2} \text{cov}(f_i, f_j)}. \quad (5.5)$$

The different cone sizes show a very similar pileup dependency as a function of $|\eta|$. The largest differences are observed near the crack region and are in the order of 5 – 10 %.

5.5.3. Signal performance

To evaluate the performance of the new pileup subtraction it is applied to the different isolation variables and the results are compared with the current subtraction scheme. Two plots with results for E_T^{cone40} are depicted in Fig. 5.10. In both the central $0 < \eta < 0.1$ and more forward $1.15 < \eta < 1.37$ region the new correction yields an improved narrower peak. In addition the peak position is more stable as a function of η for the new correction, while for the old correction the distribution is clearly shifted towards negative values in the more forward region.

The selection efficiency for electrons are compared for a cut of $E_T^{\text{cone40}} < 3.5$ GeV using the new

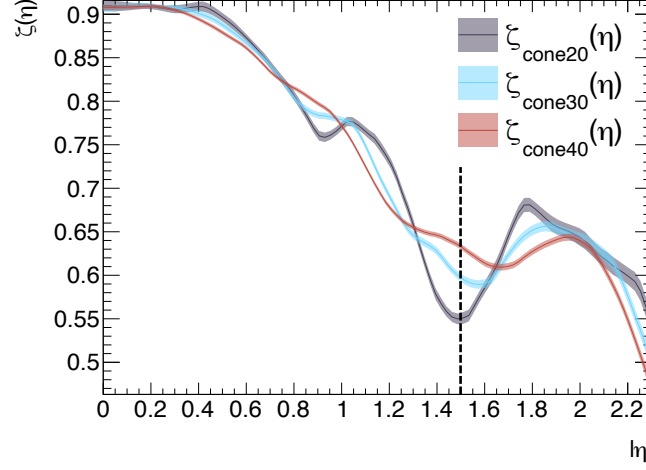


Figure 5.9.: Fit result propagated to the $\zeta_{\text{shape}}(\eta)$ of E_T^{cone20} (grey), E_T^{cone30} (blue) and E_T^{cone40} (red). The old pileup subtraction corresponds to using $\zeta(\eta) = 1$ for $|\eta| < 1.5$.

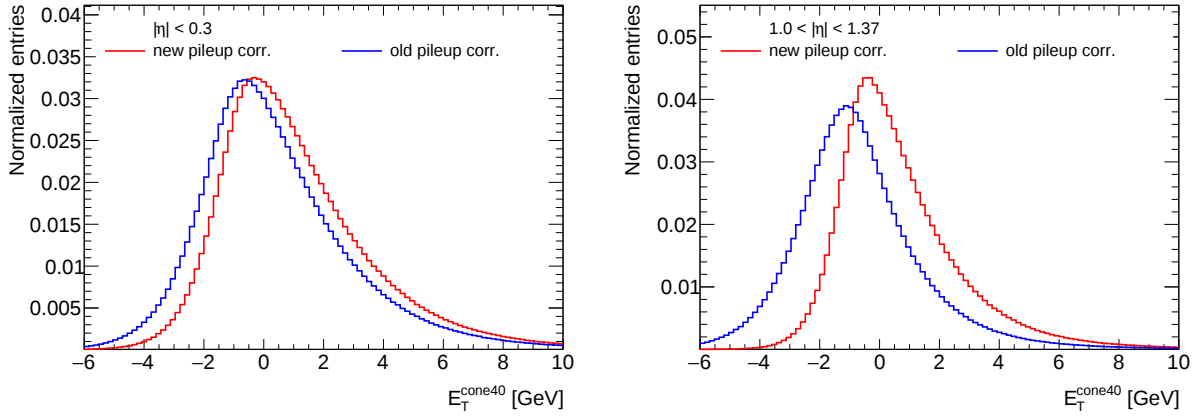


Figure 5.10.: Comparison of the distribution of E_T^{cone20} using the new (red) and old (blue) parametrized pileup subtraction for probe electrons with $0 < \eta < 0.3$ (left) and $1.0 < \eta < 1.37$ (right) of the probe electron.

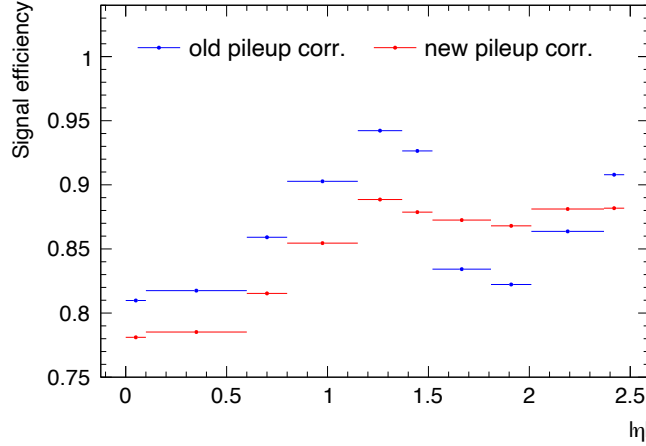


Figure 5.11.: Signal efficiency for a cut of $E_T^{\text{cone40}} < 3.5$ GeV for electrons in 2018 data passing the $Z \rightarrow ee$ selection as a function of η with the new (red) and old (blue) pileup subtraction.

and the old pileup subtraction. The values are derived in 2018 data from events passing the $Z \rightarrow ee$ selection. The overall efficiency is not relevant for the comparison as it can be changed by a different threshold value. Usually the threshold values used by ATLAS analysis are fixed and not changed as a function of $|\eta|$, which means the stability of the efficiency as a function of $|\eta|$ is important. The efficiencies are compared as a function of $|\eta|$ in Fig. 5.11. The efficiency values with the new correction are more stable compared to the values with the old correction. The new efficiency values vary from 78% in the centre to 88% in the most forward region more or less monotonically increasing. The old efficiency values also have their minimum in the central region with a value around 81%, but have their maximum around $|\eta| = 1.25$ with 95% and are again dropping to low values for $|\eta| > 1.5$.

For a fixed isolation cut value a rising efficiency as a function of $|\eta|$ is expected, because the noise from pileup is decreasing towards higher $|\eta|$ which is reducing the width of the isolation distribution. The large jump in the isolation efficiency with the old pileup correction at $|\eta| = 1.5$ is created by the two-bin approach with only the switch from the central to the forward energy density. This is avoided by using the smooth $\zeta(\eta)$ functions and only the more reliable central energy density for the new correction.

The signal efficiency is lower for the new pileup correction in the central $|\eta| < 1.5$ region, because the $\zeta(\eta)$ values are smaller than one and therefore a smaller value is subtracted. For $|\eta| > 1.5$ the efficiency values with the new pileup subtraction can get larger than the values with the old correction, because the central energy density is used for the new subtraction, while the forward one is used for the old correction in this region. A meaningful comparison of the signal efficiencies needs to take into account the background rejection which is done in the next section.

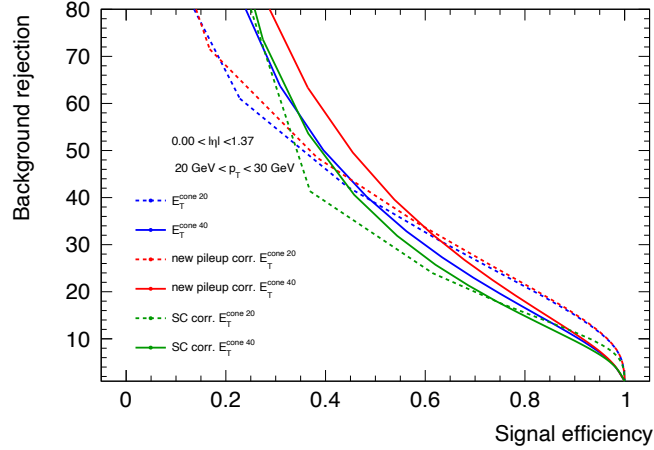


Figure 5.12.: Background rejection versus signal efficiency for cuts in different isolation variables. The blue lines correspond to variables with the fixed size core subtraction and the old pileup subtraction, the green lines use the supercluster based subtraction and the red lines variables with the fixed size core subtraction and the new pileup subtraction. The dashed lines are created with isolation variables with a small $\Delta R < 0.2$ cone size and the solid lines with a large cone size $\Delta R < 0.4$.

5.5.4. Background rejection

The performance of the pileup correction is evaluated in terms of signal efficiency versus background rejection¹ for arbitrary cuts on the isolation variables. The background rejection is calculated in a data control region enriched in background. For this only the trigger matching is required for the tag electron, but no further offline identification is applied. The Z -mass window cuts are inverted and the probe electron is required to fail a loose electron identification criterion.

The background rejection and signal efficiencies are evaluated for multiple cut values of different isolation variable definitions and the results are depicted in Fig. 5.12. The Figure shows that the supercluster based subtraction of the core is deteriorating the background rejection as explained in Section 5.4. The new pileup correction is applied on isolation variables with the fixed core subtraction and the parametrized leakage correction. This is done to compare the new and old pileup subtraction on the optimal setup of the core subtraction in terms of background rejection.

For the variables with a large cone size of $\Delta R < 0.4$ the pileup subtraction yields a small but significant improvement in terms of background rejection versus signal efficiency. The improvements for the small $\Delta R < 0.2$ cone size are mostly negligible. For both the new and the old pileup correction the small cone size outperforms the large cone size at the relevant signal efficiencies above 50%. Although the larger cone size should capture more additional activity, e.g. in the vicinity of a background candidate, it is also more susceptible to pileup noise. The crossing point of the curves of the large and the small cone size is shifted towards a higher signal efficiency of 60% for the new pileup correction making the larger cone size more viable. This can be important for measurements

¹The background rejection is defined as the inverse of the background efficiency.

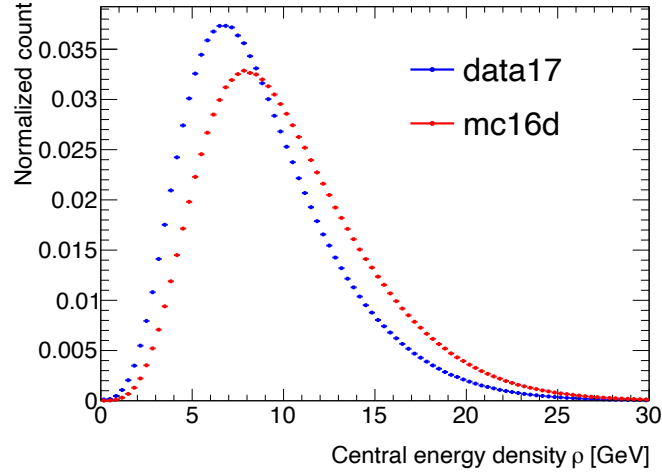


Figure 5.13.: Comparison of the central energy density ρ between 2017 $Z \rightarrow ee$ data and corresponding MC samples.

where the choice of the isolation region is not only driven by background rejection considerations, but also for the definition of the fiducial phase space, e.g. fiducial cross section measurements of isolated photons with isolation criteria with different cone sizes. The plot shows the results for electrons with $0 < |\eta| < 1.37$ and $20 \text{ GeV} < p_T < 30 \text{ GeV}$. The trends are the same in other $|\eta|$ and p_T regions.

The pileup subtraction could be further improved by introducing additional proxies for the pileup activity in the event like the number of reconstructed primary vertices or the number of interactions per bunch crossing based on the instantaneous luminosity. A machine learning based multivariate regression technique utilizing e.g. boosted decision trees could be used to estimate the not pileup corrected isolation variables based on these proxy variables and the η of the electron candidate. The estimate would then be subtracted. A main disadvantage would be that the parameters of the machine learning algorithms are not as interpretable as the parameters of the fit.

5.6. Pileup-dependent correction of isolation variables in simulation

The studies presented in the previous Section 5.5 were purely data driven studies of the pileup dependency of the isolation variables. In this section similar studies are performed in simulated samples and the results are compared between data and MC to study possible mismatches.

Fig. 5.13 shows the distribution of the central energy density in $Z \rightarrow ee$ data and MC, which is an important input to the calculation of the isolation variables as discussed before. The MC clearly overestimates the energy density from pileup in the event. If the pileup subtraction works properly this does not necessarily imply that the average isolation energies are miss-modelled. Here it is studied whether the $\zeta(\eta)$ derived in data in the previous Section 5.5 are the same for MC, which would indicate differences in the proportionality of the isolation energy with the central energy density between data and MC.

To achieve this the median values of the isolation before pileup subtraction is extracted for the

MC $Z \rightarrow ee$ samples in the same way as done for data previously. Instead of fitting the MC median points directly the difference between data and MC median values is fitted as follows:

$$\Delta m_{\text{shape}}^{\text{data-MC}}(\rho, \eta) = A\rho\Delta\zeta_{\text{shape}}^{\text{data-MC}}(\eta) + \Delta c^{\text{data-MC}} \quad (5.6)$$

with:

$$\Delta\zeta_{\text{shape}}^{\text{data-MC}}(\eta) = \sum_{i_{\eta\text{bin}}} \frac{A_{i_{\eta\text{bin}}}}{A} \Delta f_i. \quad (5.7)$$

The free parameters of the fit are the difference between the f_i factors in data and MC Δf_i and the constant term difference $\Delta c^{\text{data-MC}}$. Again all points for $E_T^{\text{cone40}} - E_T^{\text{cone30}}$ and $E_T^{\text{cone30}} - E_T^{\text{cone20}}$ are fitted simultaneously.

The results of the fit are summarized in Fig. 5.14. The difference of the median in data and MC has a negative slope as a function of energy density which is larger for the larger isolation area. This means pileup is a driving factor for the difference between data and MC. The slope of the median value as a function of energy density is higher for MC than for data.

To correct this effect the difference is added as a correction to MC. The distribution of the residuals is closer to a normal distribution than for the fit of the median in data in Section 5.5, which indicates that some of the non-linear effects cancel looking at the difference between data and MC. One constant parameter is used for all η -regions while different values for different η -regions were needed for the fit to data. The constant value is $\Delta c^{\text{data-MC}} = 17 \pm 5$ MeV and is neglected for the correction applied to MC (cf. Eq. (5.8)), because it is small and there are dedicated central measurements of the shift of the isolation distribution which are derived after the pileup-dependent shift is applied.

$$\text{corr}_{\text{shape}}(A, \rho, \eta) = A\rho\Delta\zeta_{\text{shape}}^{\text{data-MC}}(\eta) \quad (5.8)$$

This pileup dependent data-driven correction is relatively small, e.g. for E_T^{cone40} of an electron at $\eta = 0.4$ in an event with $\rho = 10$ GeV it is approximately 300 MeV.

To check the performance of this correction it is applied and the data and MC distribution are compared directly. The distributions of E_T^{cone20} and E_T^{cone40} for a central $|\eta|$ bin are shown in Fig. 5.15. The main difference visible between MC and data distributions is the width, which will be discussed in more detail in Section 5.7. The reason for this is the higher abundance of high energy density events in MC compared to data (see Fig. 5.13). This problem is not solved by applying the ρ -dependent correction, although it is slightly narrowing the distribution. The main improvement is visible at the right tails of the distribution. There MC and data match much better when applying the correction. This is the region where all common isolation cuts are applied.

5.7. Pileup noise studies

In the previous Sections 5.5 and 5.6 the position of the isolation distribution was studied as a function of pileup and compared between data and MC. In this section the width of the distribution is studied, which is influenced by the pileup noise.

The pileup dependency of the width of the isolation distribution is studied by calculating the

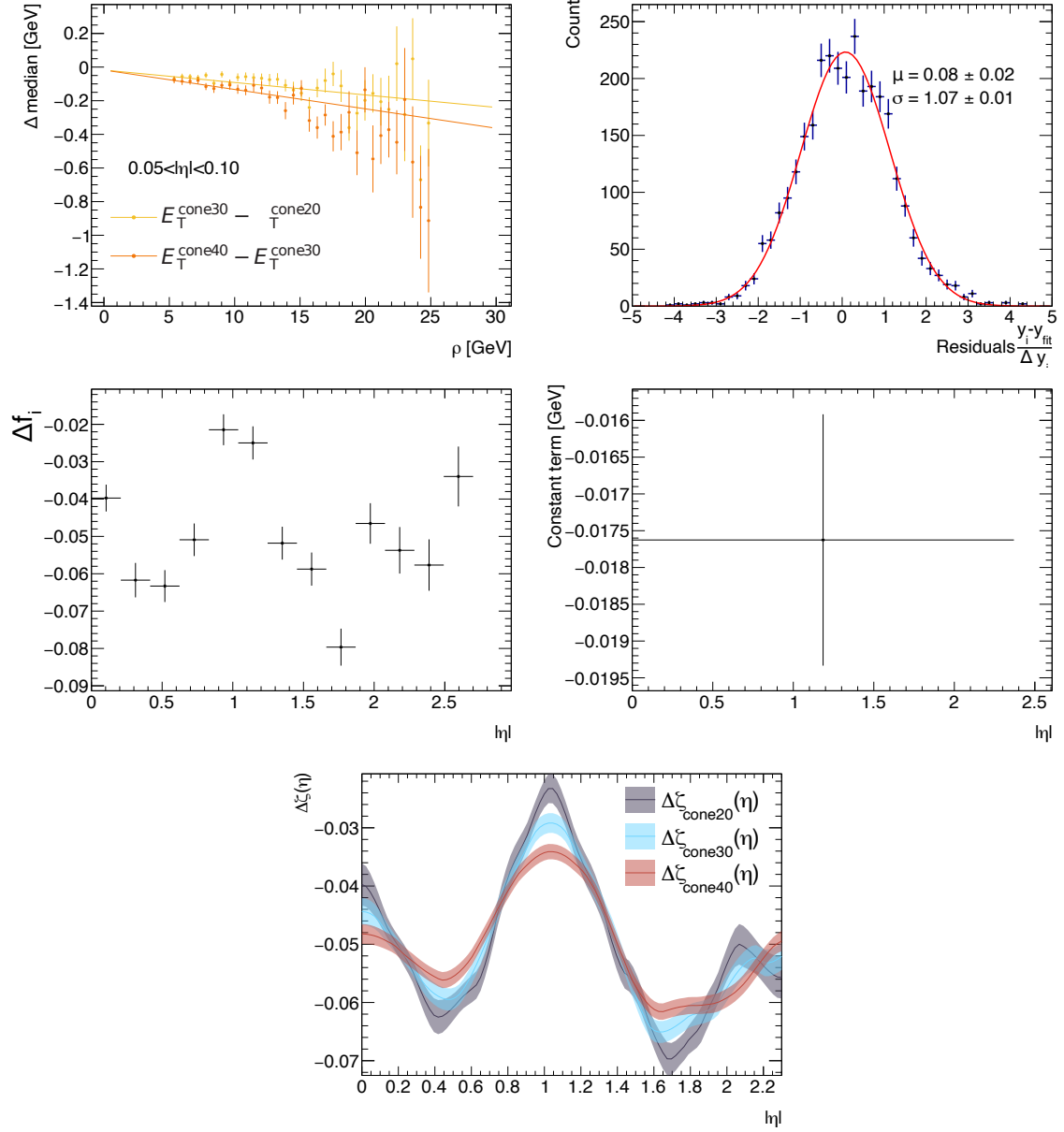


Figure 5.14.: Median isolation difference for $E_T^{\text{cone40}} - E_T^{\text{cone30}}$ and $E_T^{\text{cone30}} - E_T^{\text{cone20}}$ between full Run-2 data and MC in $0.05 < |\eta| < 0.10$ as a function of the energy density (top left). Residuals of all points used for the fit (top right). Slope parameters Δf_i (middle left) and constant term $\Delta c^{\text{data-MC}}$ (middle right) extracted by the fit. Correction for the pileup correction function $\Delta \xi_{\text{shape}}^{\text{data-MC}}(\eta)$ for MC (bottom).

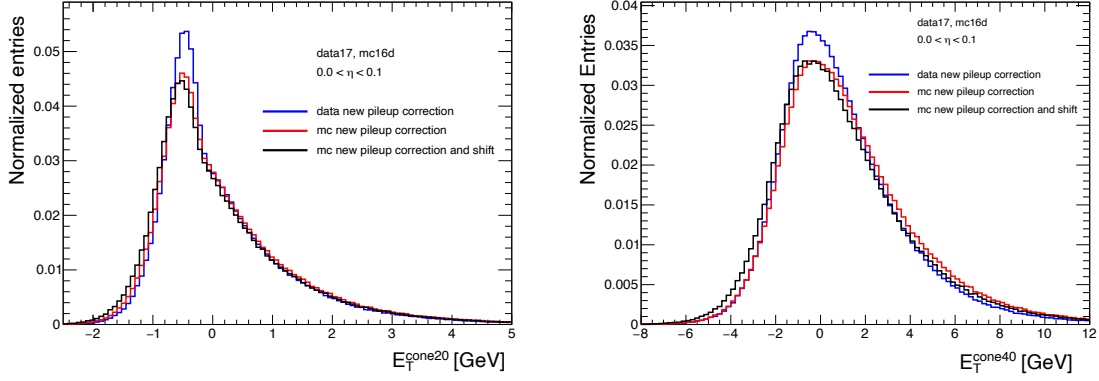


Figure 5.15.: Comparison of the distribution of $E_T^{\text{cone}20}$ (left) and $E_T^{\text{cone}40}$ (right) in data (blue) and MC using the new pileup correction for $0 < \eta < 0.1$ of the probe electron. For the black line in addition to the new pileup correction also the pileup dependent data-driven correction is applied to MC.

variance of the distribution in bins of number of interactions per bunch crossing μ and $|\eta|$ of the probe electron. The variance $\sigma^2(\mu)$ of the isolation distribution is given by:

$$\sigma^2(\mu) = \sigma_{\text{el}}^2 + \sigma_{\text{pu}}^2 \mu \quad (5.9)$$

with a constant term σ_{el}^2 from electronic noise and the noise per pileup interaction σ_{pu}^2 . The values of σ_{pu}^2 are derived by fitting a linear function as depicted in Fig. 5.16. The fit function is shifted into the centre of the μ values to reduce the correlation between the constant and the linear term. For this study 2018 data passing the $Z \rightarrow ee$ selection described in Section 5.3 is used for which corresponding MC samples with different pileup overlays (cf. Section 5.2.1) are available.

The results for $E_T^{\text{cone}40}$ with the new pileup correction and pileup-dependent correction for simulation (cf. Sections 5.5 and 5.6) are summarized in Fig. 5.16. The pileup noise contribution to the isolation distribution σ_{pu}^2 is larger in MC than in data for all pileup overlays and in all $|\eta|$ regions. Extrapolating the pileup noise $\sigma^2(\mu)$ to $\mu = 0$ yields in general roughly compatible values between data and MC. Therefore, the data and MC differences of the width of the isolation distribution are driven mainly by pileup. The ratio between the MC and data pileup noise $\sigma_{\text{pu,MC}}^2 / \sigma_{\text{pu,data}}^2$ does not show significant trends as a function of $|\eta|$ with the limited statistics of the special MC samples with different pileup overlays. The values of $\sigma_{\text{pu,MC}}^2 / \sigma_{\text{pu,data}}^2$ yield compatible values using an isolation variable with a smaller cone size like $E_T^{\text{cone}20}$, but the statistical uncertainties for the estimated noise values are higher for smaller cone sizes, because they are less sensitive to pileup.

A constant function is fit to the values of $\sigma_{\text{pu,MC}}^2 / \sigma_{\text{pu,data}}^2$ in the different $|\eta|$ regions for a comparison between the different overlays with reduced uncertainty. For the nominal Pythia A3 the pileup noise $\sigma_{\text{pu,MC}}^2$ is 1.244 ± 0.020 times higher than the data pileup noise. This is an improvement with respect to the Monash tune ($\sigma_{\text{pu,MC}}^2 / \sigma_{\text{pu,data}}^2 = 1.346 \pm 0.022$) on which the A3 tune is based. The samples using the EPOS generator or EPOS+A3 give similar results and improve the ratio to around 1.15. This insight has influenced the decision for using EPOS+A3 as new nominal pileup overlay simulation

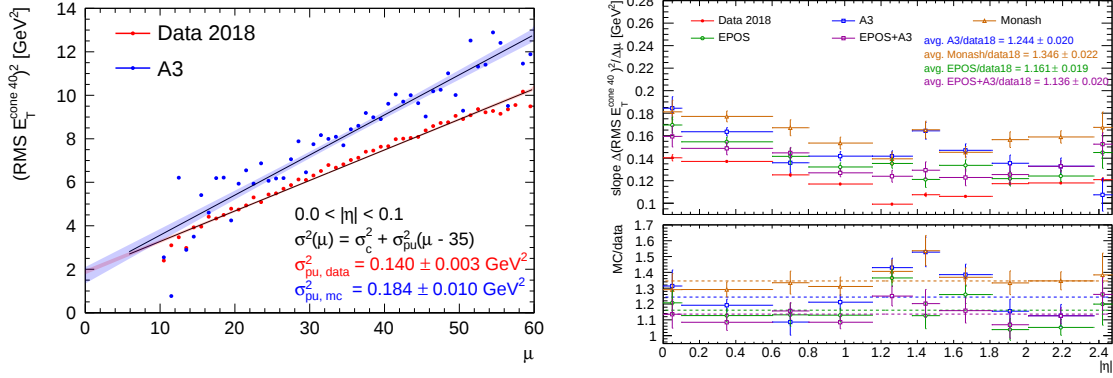


Figure 5.16.: Variance of the distribution of E_T^{cone40} (left) as a function of the interactions per bunch crossing in $Z \rightarrow ee$ data and MC. The $Z \rightarrow ee$ MC is using the nominal Pythia A3 pileup overlay. A linear function is fit to the values. The right plot shows the slope of the linear function fitted to MC samples with different pileup overlays and to data, in multiple $|\eta|$ -bins of the probe electron.

for the Run-3 MC samples.

Using the old pileup subtraction and neglecting the pileup-dependent shift for simulation increases the ratio of $\sigma_{\text{pu, MC}}^2 / \sigma_{\text{pu, data}}^2$ by around 10% deteriorating the agreement between data and MC.

The agreement of the calorimetric isolation distribution between data and simulation can be restored utilizing the pileup reweighting (cf. Section 5.2.2), but scaling down the distribution of the number of interactions per bunch-crossing in MC with an alternative $f_{\mu\text{-scale}} = \sigma_{\text{pu, MC}}^2 / \sigma_{\text{pu, data}}^2$. The effect of the pileup reweighting is shown in Fig. 5.17. The distribution of E_T^{cone40} in the MC sample with alternative pileup reweighting matches well with the distribution in data, especially for high isolation variable values which are most relevant for the efficiency of commonly used isolation cuts.

The alternative pileup reweighting can not be applied universally, because there are other observables e.g. based on tracking information which show good agreement with the nominal pileup reweighting. The approach applied for the photon-pair measurement is to use the alternative pileup reweighting to derive the calorimetric isolation quantities like isolation efficiencies and to use the nominal reweighting for everything else. Additionally an uncertainty is assigned using different pileup reweighting configurations for the calculation of the isolation efficiencies.

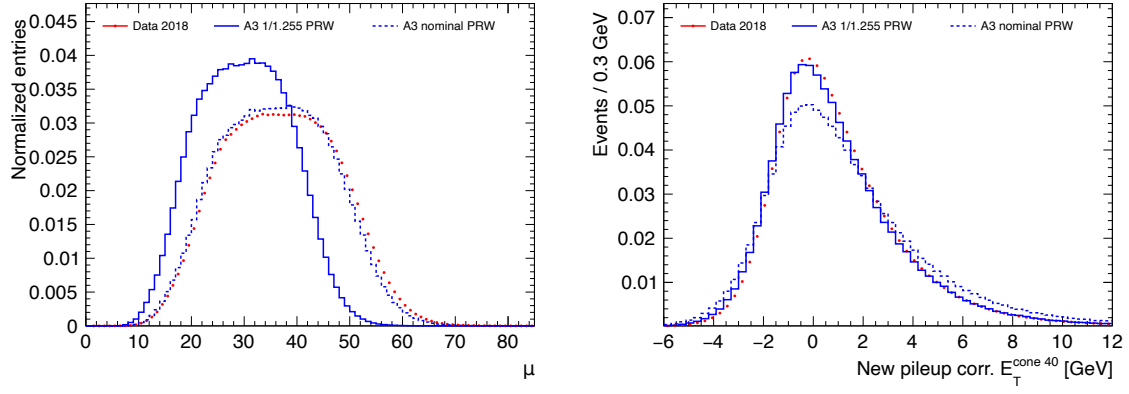


Figure 5.17.: The left plot illustrates the pileup reweighting scaling down the MC pileup profile by $\sigma_{\text{pu,MC}}^2 / \sigma_{\text{pu,data}}^2 = 1.255 \pm 0.020$ (dashed line) for the sample with nominal A3 pileup overlay. The right plot shows the effect on the distribution of E_T^{cone40} with new pileup corrections.

Chapter 6.

Photon efficiency measurement using radiative $Z \rightarrow \mu\mu\gamma$ events

The main motivation for the studies in this section is the slight discrepancy seen between the result of the photon-pair cross section measurement between different years which will be explained in detail in Section 7.7.5. A difference in the photon selection efficiencies in different years which is not reflected in MC could explain this difference. Although there are existing measurement utilizing $Z \rightarrow \ell\ell\gamma$ to measure photon selection efficiencies as e.g. described in Section 4.4, a few aspects are not part of these measurements and the corresponding central ATLAS recommendations, which justifies the studies in this chapter:

- The recommended efficiency corrections are provided inclusively for the full Run-2 dataset and not for the individual years.
- The efficiency corrections are derived independently for photons reconstructed as converted and unconverted, but the fraction of photons reconstructed as converted is not corrected in the simulation, which could slightly bias the efficiencies.
- At the time of this thesis no ATLAS recommendations for the efficiency of the photon-electron ambiguity resolution (cf. Section 4.2.1) are available and ATLAS measurements with photons assume that it is well modelled in simulation. This is usually reasoned by the high efficiency of the ambiguity resolution. The efficiency of the photon-electron ambiguity resolution for genuine photons is referred to as photon reconstruction efficiency in the following, although the efficiency on the creation and selection of a topological cluster are not included. The topological cluster related efficiencies are expected to be above 99% for photons with $E_T > 30$ GeV [103].

The reconstruction efficiency can be measured in data with $Z \rightarrow \mu\mu\gamma$ events. The number of miss-reconstructed photons is calculated from events with an electron candidate without a photon candidate nearby and a three-body mass $m_{\mu\mu e}$ near the Z mass. The number of these miss-reconstructed events $N_{\mu\mu e}$ is then compared to the number of correctly reconstructed events $N_{\mu\mu\gamma}$ to calculate the reconstruction efficiency $\varepsilon_{\text{reco}}$:

$$\varepsilon_{\text{reco}} = \frac{N_{\mu\mu\gamma}}{N_{\mu\mu e} + N_{\mu\mu\gamma}} \quad (6.1)$$

No identification requirements can be applied on the electron or photon candidate, because the differences of the electron and photon identification criteria, and of correctly and incorrectly reconstructed photons would bias the efficiency. Therefore the estimation of background events, where the photon or electron candidate is created by a jet in a $Z \rightarrow \mu\mu$ +jet event is crucial.

6.1. Data and MC samples

Similar to the studies in Chapter 5 the full LHC Run-2 pp collision data is used. Data events are selected based on an ‘or’ of the unprescaled muon and di-muon triggers with the lowest p_T threshold [125]. The reference signal sample of the $Z\gamma$ final states was simulated with the SHERPA 2.2.4 [36] generator. Matrix elements at LO accuracy in QCD for up to three additional parton emissions were matched and merged with the SHERPA parton shower based on Catani–Seymour dipole factorisation [126, 127] using the MEPS@LO prescription [51, 52, 128, 129].

6.2. Event selection

Events with two muon candidates with $p_T^\mu > 10$ GeV and $|\eta^\mu| < 2.5$ passing the *medium* identification criterion and a loose isolation requirement are selected [130]. The samples are processed with the same framework as for the central radiative $Z \rightarrow \mu\mu\gamma$ identification and isolation efficiency measurements [103] and the event selection is also based on the one used for the existing measurements.

The photon candidates are only required to be separated by at least $\Delta R > 0.2$ from the two muons, but no additional identification or isolation cuts are used and the candidate with the highest p_T is selected.

The electron candidates are selected if there is no photon candidate reconstructed in a cone of $\Delta R < 0.2$ around them and again the candidate with the highest p_T is used.

The mass of the two-muon system $m_{\mu\mu}$ and the mass of the three body system of the muons and the photon or electron candidate $m_{\mu\mu\gamma}$ are used for a further selection and to estimate the background.

A two dimensional mass requirement in the $m_{\mu\mu}$ versus $m_{\mu\mu\gamma}$ is used to select events with a final state radiation topology, where the $m_{\mu\mu\gamma}$ is close to the Z -mass:

$$m_{\mu\mu} < 182 \text{ GeV} - m_{\mu\mu\gamma}. \quad (6.2)$$

This requirement is the inverse of the one used to select initial state radiation topologies in the ATLAS $Z\gamma$ cross section measurement [131]. There the initial state radiation topology is studied, because it represents the irreducible background to $H \rightarrow Z\gamma$ production and serves as a precise benchmark process for perturbative QCD predictions. Here the final state radiation topology is preferable, because it has a higher signal purity and the $m_{\mu\mu\gamma}$ shape can be described by a parametric function which simplifies the background estimation.

The distribution of $m_{\mu\mu}$ versus $m_{\mu\mu\gamma}$ in the selected data events and the requirement are illustrated in Fig. 6.1 separately for events with a photon candidate and with only an electron candidate.

The events are split into categories of $|\eta|$ and p_T of the photon or electron candidate (cf. Section 6.2).

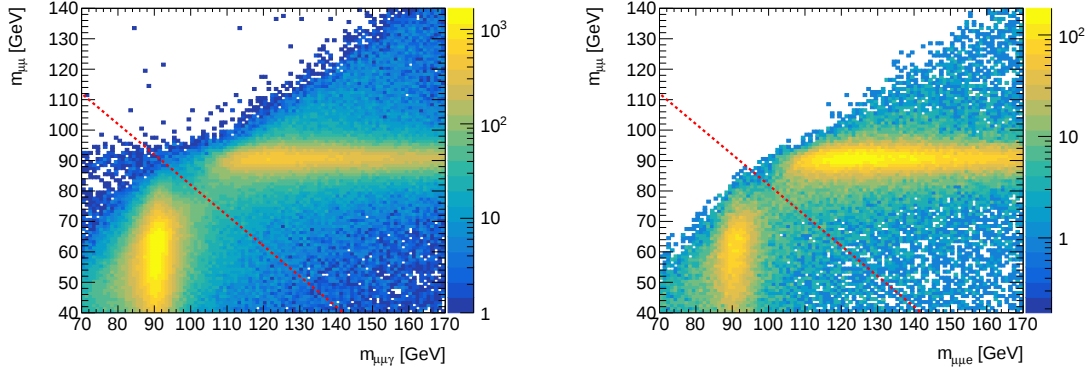


Figure 6.1.: Three-body mass $m_{\mu\mu\gamma(e)}$ versus two-body mass $m_{\mu\mu}$ for Run-2 data events with two muons and a photon candidate (left) and an electron candidate with no photon candidate nearby (right). Events with mass combinations below the red dashed line are selected.

$$p_T^{\gamma(e)} \in \{[20, 25], [25, 30], [30, 35], [35, 40], [40, 60], [60, 80]\} \text{ GeV} \quad (6.3)$$

$$|\eta^{\gamma(e)}| \in \{[0., 0.6], [0.6, 0.82], [0.82, 1.15], [1.15, 1.37], [1.52, 1.81], [1.81, 2.37]\} \quad (6.4)$$

Each bin is further split into different control regions based on isolation criteria, identification criteria and the reconstructed photon conversion type. This is done to extract information about the photon identification efficiencies and reconstructed conversion fraction. Furthermore this creates regions with a high background fraction which are useful to determine the shape of the $m_{\mu\mu\gamma}$ distribution for the background.

The photon candidates are split into 16 disjunct categories based on the Cartesian product of the following categories:

$$\begin{aligned} & [\text{converted}, \text{unconverted}] \\ & \times [E_T^{\text{cone20}} < 0.05 \cdot p_T^\gamma, E_T^{\text{cone20}} > 0.05 \cdot p_T^\gamma] \\ & \times [\text{not } Loose'5, Loose'5 \text{ but not } Loose'2, Loose'2 \text{ but not } Tight, Tight] \end{aligned}$$

The requirements included in the different identification criteria are described in Section 4.4. The electron events are only split into two regions: $E_T^{\text{cone20}} \leq 0.05 \cdot p_T^\gamma$. The isolation cut $E_T^{\text{cone20}} < 0.05 \cdot p_T^\gamma$ is the same as used for the photon-pair measurement.

6.3. Fit model

The distribution of signal or background events for each category c_i and for values of $m_{\mu\mu\gamma}$ is described by the product:

$$g(m_{\mu\mu\gamma}, c_i) = h(m_{\mu\mu\gamma})k(c_i) \quad (6.5)$$

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18								
T	L'2	L	IL	T	L'2	L	IL	T	L'2	L	IL	T	L'2	L	IL										
isolated				not isolated				isolated				not isolated				i.	li.								
converted								unconverted																	
reco. γ																el.									

Figure 6.2.: Numbering scheme of the different categories used for the fit. The second row indicates the photon different identification categories: *Tight* (T), *Loose'2* but not *Tight* (L'2), *Loose'5* but not *Loose'2* (L) and not *Loose'5* (!L).

of the probability density function $h(m_{\mu\mu\gamma})$ for the mass and the probability $k(c_i)$ for each category. This means it is assumed that the mass shape is independent of the category.

The distribution of all events is described as the sum of the signal and background events:

$$g_{\text{total}}(m_{\mu\mu\gamma}, c_i) = f_{\text{sig}} g_{\text{sig}}(m_{\mu\mu\gamma}, c_i) + (1 - f_{\text{sig}}) g_{\text{bkg}}(m_{\mu\mu\gamma}) \quad (6.6)$$

The probability for each category $k(c_i)$ is described in terms of efficiencies ε and correlation correction parameters R in Eq. (6.7). The numbering of the categories is described in Fig. 6.2. The parametrization has similarities to the model used in the background estimation of the photon-pair measurement and was inspired by it (cf. Section 7.5).

The model has 17 free parameter $\vec{\theta}$ to describe the event fractions in the 18 categories. This means no assumption are made and the model is fully flexible to fit to any distribution. The parameters are: the reconstruction efficiency $\varepsilon_{\text{reco}}$, the fraction of photons reconstructed as converted f_c , the identification efficiencies of the consecutive identification cuts¹ $\varepsilon_L^{c(\text{uc})}$, $\varepsilon_{L'2}^{c(\text{uc})}$ and $\varepsilon_T^{c(\text{uc})}$ for converted (unconverted) photons, the isolation efficiencies for converted or unconverted photons or electrons $\varepsilon_{\text{iso}}^{c/\text{uc}/e}$ and isolation-identification correlation correction factors $R_{!L \rightarrow L}^{c,(\text{uc})}$, $R_{L \rightarrow L'2}^{c,(\text{uc})}$, $R_{L'2 \rightarrow T}^{c,(\text{uc})}$. The R factors take into account, that the isolation efficiencies can be lower for photons not passing a certain identification criterion and for each of the consecutive identification criteria and for each conversion type one factor is included. Therefore the isolation efficiencies $\varepsilon_{\text{iso}}^{c(\text{uc})}$ are the values for photons passing the tight identification.

¹This means the efficiency with respect to photons passing the previous looser identification criterion already.

$$k(c_i; \vec{\theta}) = \left\{ \begin{array}{ll} \varepsilon_{\text{reco}} & f_c \quad (1 - \varepsilon_L^c) \quad R_{\text{IL} \rightarrow \text{L}}^c \quad R_{\text{L} \rightarrow \text{L}'/2}^c \quad R_{\text{L}'/2 \rightarrow \text{T}}^c \quad \varepsilon_{\text{iso}}^c \quad \text{for } i = 1 \\ \varepsilon_{\text{reco}} & f_c \quad \varepsilon_L^c \quad (1 - \varepsilon_{\text{L}'/2}^c) \quad R_{\text{L} \rightarrow \text{L}'/2}^c \quad R_{\text{L}'/2 \rightarrow \text{T}}^c \quad \varepsilon_{\text{iso}}^c \quad \text{for } i = 2 \\ \varepsilon_{\text{reco}} & f_c \quad \varepsilon_L^c \quad \varepsilon_{\text{L}'/2}^c \quad (1 - \varepsilon_{\text{T}}^c) \quad R_{\text{L}'/2 \rightarrow \text{T}}^c \quad \varepsilon_{\text{iso}}^c \quad \text{for } i = 3 \\ \varepsilon_{\text{reco}} & f_c \quad \varepsilon_L^c \quad \varepsilon_{\text{L}'/2}^c \quad \varepsilon_{\text{T}}^c \quad \varepsilon_{\text{iso}}^c \quad \text{for } i = 4 \\ \varepsilon_{\text{reco}} & f_c \quad (1 - \varepsilon_L^c) \quad (1 - R_{\text{IL} \rightarrow \text{L}}^c) \quad R_{\text{L} \rightarrow \text{L}'/2}^c \quad R_{\text{L}'/2 \rightarrow \text{T}}^c \quad \varepsilon_{\text{iso}}^c \quad \text{for } i = 5 \\ \varepsilon_{\text{reco}} & f_c \quad \varepsilon_L^c \quad (1 - \varepsilon_{\text{L}'/2}^c) \quad (1 - R_{\text{L} \rightarrow \text{L}'/2}^c) \quad R_{\text{L}'/2 \rightarrow \text{T}}^c \quad \varepsilon_{\text{iso}}^c \quad \text{for } i = 6 \\ \varepsilon_{\text{reco}} & f_c \quad \varepsilon_L^c \quad \varepsilon_{\text{L}'/2}^c \quad (1 - \varepsilon_{\text{T}}^c) \quad (1 - R_{\text{L}'/2 \rightarrow \text{T}}^c) \quad \varepsilon_{\text{iso}}^c \quad \text{for } i = 7 \\ \varepsilon_{\text{reco}} & f_c \quad \varepsilon_L^c \quad \varepsilon_{\text{L}'/2}^c \quad \varepsilon_{\text{T}}^c \quad (1 - \varepsilon_{\text{iso}}^c) \quad \text{for } i = 8 \\ \varepsilon_{\text{reco}} & (1 - f_c) \quad (1 - \varepsilon_L^{\text{uc}}) \quad R_{\text{IL} \rightarrow \text{L}}^{\text{uc}} \quad R_{\text{L} \rightarrow \text{L}'/2}^{\text{uc}} \quad R_{\text{L}'/2 \rightarrow \text{T}}^{\text{uc}} \quad \varepsilon_{\text{iso}}^{\text{uc}} \quad \text{for } i = 9 \\ \varepsilon_{\text{reco}} & (1 - f_c) \quad \varepsilon_L^{\text{uc}} \quad (1 - \varepsilon_{\text{L}'/2}^{\text{uc}}) \quad R_{\text{L} \rightarrow \text{L}'/2}^{\text{uc}} \quad R_{\text{L}'/2 \rightarrow \text{T}}^{\text{uc}} \quad \varepsilon_{\text{iso}}^{\text{uc}} \quad \text{for } i = 10 \\ \varepsilon_{\text{reco}} & (1 - f_c) \quad \varepsilon_L^{\text{uc}} \quad \varepsilon_{\text{L}'/2}^{\text{uc}} \quad (1 - \varepsilon_{\text{T}}^{\text{uc}}) \quad R_{\text{L}'/2 \rightarrow \text{T}}^{\text{uc}} \quad \varepsilon_{\text{iso}}^{\text{uc}} \quad \text{for } i = 11 \\ \varepsilon_{\text{reco}} & (1 - f_c) \quad \varepsilon_L^{\text{uc}} \quad \varepsilon_{\text{L}'/2}^{\text{uc}} \quad \varepsilon_{\text{T}}^{\text{uc}} \quad \varepsilon_{\text{iso}}^{\text{uc}} \quad \text{for } i = 12 \\ \varepsilon_{\text{reco}} & (1 - f_c) \quad (1 - \varepsilon_L^{\text{uc}}) \quad (1 - R_{\text{IL} \rightarrow \text{L}}^{\text{uc}}) \quad R_{\text{L} \rightarrow \text{L}'/2}^{\text{uc}} \quad R_{\text{L}'/2 \rightarrow \text{T}}^{\text{uc}} \quad \varepsilon_{\text{iso}}^{\text{uc}} \quad \text{for } i = 13 \\ \varepsilon_{\text{reco}} & (1 - f_c) \quad \varepsilon_L^{\text{uc}} \quad (1 - \varepsilon_{\text{L}'/2}^{\text{uc}}) \quad (1 - R_{\text{L} \rightarrow \text{L}'/2}^{\text{uc}}) \quad R_{\text{L}'/2 \rightarrow \text{T}}^{\text{uc}} \quad \varepsilon_{\text{iso}}^{\text{uc}} \quad \text{for } i = 14 \\ \varepsilon_{\text{reco}} & (1 - f_c) \quad \varepsilon_L^{\text{uc}} \quad \varepsilon_{\text{L}'/2}^{\text{uc}} \quad (1 - \varepsilon_{\text{T}}^{\text{uc}}) \quad (1 - R_{\text{L}'/2 \rightarrow \text{T}}^{\text{uc}}) \quad \varepsilon_{\text{iso}}^{\text{uc}} \quad \text{for } i = 15 \\ \varepsilon_{\text{reco}} & (1 - f_c) \quad \varepsilon_L^{\text{uc}} \quad \varepsilon_{\text{L}'/2}^{\text{uc}} \quad \varepsilon_{\text{T}}^{\text{uc}} \quad (1 - \varepsilon_{\text{iso}}^{\text{uc}}) \quad \text{for } i = 16 \\ (1 - \varepsilon_{\text{reco}}) & & & & & \varepsilon_{\text{iso}}^e \quad \text{for } i = 17 \\ (1 - \varepsilon_{\text{reco}}) & & & & & \varepsilon_{\text{iso}}^e \quad \text{for } i = 18 \end{array} \right. \quad (6.7)$$

The signal mass distribution $h_{\text{sig}}(m_{\mu\mu\gamma})$ is described with a double sided crystal ball function:

$$h_{\text{sig}}(m_{\mu\mu\gamma}; \mu, \sigma, \alpha_l, \alpha_r, n_l, n_r) = \begin{cases} A_L \cdot \left(B_L - \frac{m_{\mu\mu\gamma} - \mu}{\sigma} \right)^{-n_l}, & \text{for } \frac{m_{\mu\mu\gamma} - \mu}{\sigma} < -\alpha_l \\ \exp \left(-\frac{1}{2} \cdot \left[\frac{m_{\mu\mu\gamma} - \mu}{\sigma} \right]^2 \right), & \text{for } -\alpha_l \leq \frac{m_{\mu\mu\gamma} - \mu}{\sigma} \leq \alpha_r \\ A_R \cdot \left(B_R + \frac{m_{\mu\mu\gamma} - \mu}{\sigma} \right)^{-n_r}, & \text{otherwise.} \end{cases} \quad (6.8)$$

The function has a Gaussian core with position μ and standard deviation σ , which turns into a power law for $m_{\mu\mu\gamma} - \mu < -\alpha_l\sigma$ or $m_{\mu\mu\gamma} - \mu > \alpha_r\sigma$ with different powers n_l and n_r for the left and right tail. The parameters $\mu, \sigma, \alpha_l, \alpha_r, n_l$ and n_r are free in the fit. The coefficients A_L, A_R, B_L and B_R depend on the free parameters and ensure the normalization and continuity of the distribution. The implementation of the function in ROOT is used [100].

The background shape is also described by a wide peak. The decreasing distribution in the tails towards high $m_{\mu\mu\gamma}$ is driven by the 2D mass cut. A double sided asymmetric crystal ball function is used to describe the background shape:

$$h_{\text{bkg}}(m_{\mu\mu\gamma}; \mu, \sigma_l, \sigma_r, \alpha_l, n_l, \alpha_r, n_r) = \begin{cases} A_L \cdot \left(B_L - \frac{m_{\mu\mu\gamma} - \mu}{\sigma_l}\right)^{-n_l}, & \text{for } \frac{m_{\mu\mu\gamma} - \mu}{\sigma_l} < -\alpha_l \\ \exp\left(-\frac{1}{2} \cdot \left[\frac{m_{\mu\mu\gamma} - \mu}{\sigma_l}\right]^2\right), & \text{for } -\alpha_l < \frac{m_{\mu\mu\gamma} - \mu}{\sigma_l} < 0 \\ \exp\left(-\frac{1}{2} \cdot \left[\frac{m_{\mu\mu\gamma} - \mu}{\sigma_r}\right]^2\right), & \text{for } 0 < \frac{m_{\mu\mu\gamma} - \mu}{\sigma_r} < \alpha_r \\ A_R \cdot \left(B_R + \frac{m_{\mu\mu\gamma} - \mu}{\sigma_r}\right)^{-n_r}, & \text{otherwise.} \end{cases} \quad (6.9)$$

It is similar to the crystal ball function used for the signal mass shape, but has a bifurcated Gaussian in the central region, which has different standard deviations σ_l and σ_r for the left and right tails.

An unbinned maximum likelihood fit of all parameters of the model $\vec{\theta}$ to the n_{evt} measured ($m_{\mu\mu\gamma}, c_i$) values is performed by minimizing the negative log likelihood:

$$\vec{\theta}_{\text{opt}} = \underset{\vec{\theta}}{\text{argmin}} \left[-L(\vec{\theta} | m_{\mu\mu\gamma}^0, c_i^0, \dots, m_{\mu\mu\gamma}^{n_{\text{evt}}}, c_i^{n_{\text{evt}}}) \right] = \underset{\vec{\theta}}{\text{argmin}} \left[-\sum_{j=0}^{n_{\text{evt}}} \log g(m_{\mu\mu\gamma}^j, c_i^j | \vec{\theta}) \right]. \quad (6.10)$$

The statistical uncertainties and correlations of the parameters are estimated based on the inverse Hessian matrix of the log likelihood:

$$\text{cov}(\theta_i, \theta_j) = -\left(\mathcal{H}^{-1}(\vec{\theta}_{\text{opt}})\right)_{ij} = -\left(\left[\frac{\partial^2 L}{\partial \theta_k \partial \theta_l}\right]_{\vec{\theta}=\vec{\theta}_{\text{opt}}}^{-1}\right)_{ij}. \quad (6.11)$$

The minimization and estimation of the Hessian matrix is performed using the implementation in **RooFit** [132] utilizing **Minuit** [133].

The result of the fit in one p_T and $|\eta|$ region for full Run-2 data is depicted in Fig. 6.3 as a function of $m_{\mu\mu\gamma}$ and the categories. A projection in the number of signal and background events per category is depicted in Fig. 6.4. The model gives a reasonable description of the data. The non isolated regions where the photon candidates do not pass the *Loose5* identification and the non isolated electron candidate region have a very high background fraction and are useful for the extraction of the background shape. All other regions have a large fraction of signal characterized by the sharp peak at the Z -mass. Most of the signal events are in the regions passing the *Tight* identification illustrating the high identification efficiencies. The background rejection is in the order of 10^3 if reconstruction, identification and isolation are included in the consideration. Already the selections of the reconstruction, related to the photon-electron ambiguity using the information of tracks and conversion vertices associated to the photon candidate, are able to reject a large fraction of around 65% of the background. Although the reconstruction efficiency in this p_T and $|\eta|$ -region is high with $\varepsilon_{\text{reco}} = (97.22 \pm 0.26)\%$ it is significantly below 1 which is illustrated by the clearly visible Z -peak in the isolated electron category.

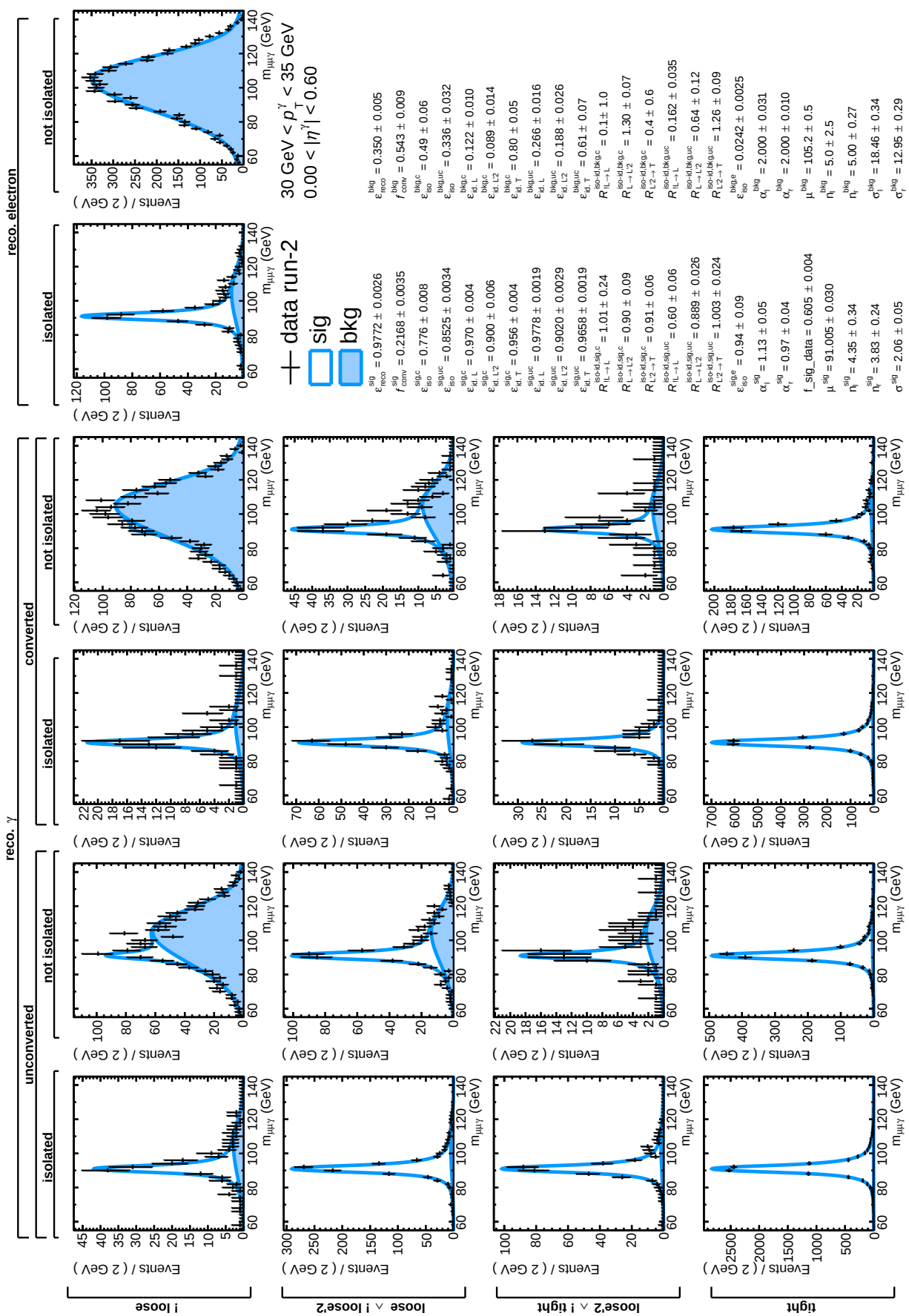


Figure 6.3.: Fit of the invariant mass $m_{\mu\mu\gamma}$ of data events passing the $Z \rightarrow \mu\mu\gamma$ selection in different disjunct categories based on the identification, isolation and reconstructed type of the object. The results for the fit parameters are summarized on the right.

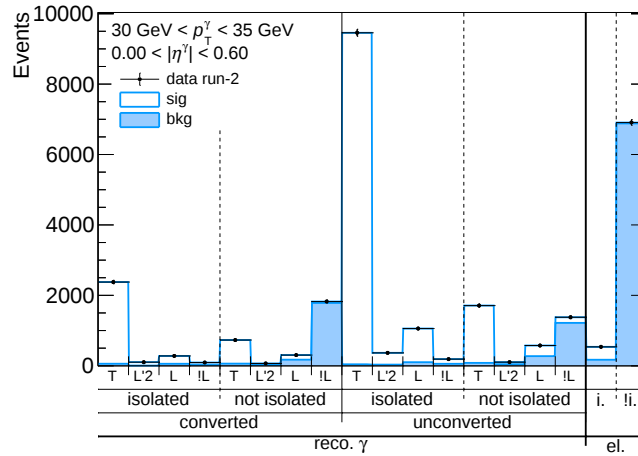


Figure 6.4.: Fit result in terms of number of signal and background events per photon category.

6.4. Systematic uncertainties

The main caveats of the fit are related to the choice of the parametric function for the distribution of the invariant mass of signal and background events and two systematic variations are considered to get a rough estimate of the related uncertainties.

The signal function does not describe the shape of the mass distribution in the high mass tail well. This is depicted in Fig. 6.5 for the MC samples where the photon candidates match to true photons and for the corresponding data category. The bias of the insufficient signal shape in the high mass tails is addressed by assigning the following systematic uncertainty. The difference between the fit result to the signal only model in truth matched signal MC (cf. Fig. 6.5 top right) and a signal+background fit in the signal MC (cf. Fig. 6.5 top left) is assigned as uncertainty. This takes into account that part of the high mass signal could be absorbed by the background shape. A template based method using the MC prediction as signal shape could improve upon this bias, but would come at the cost of other MC related uncertainties on the modelling of the mass shape e.g. related to the energy scale and resolution. In the parametric fits used here the mass shape parameters are free and can be different in data and MC. In general the tails contribute only at the sub-percent level to the signal distributions (cf. Fig. 6.3) and therefore the uncertainty related to the signal-shape mismatch is also low.

The influence of the choice of the background shape is studied by switching to a different parametric function describing a generic peak, which is called *BukinPdf* [134] and implemented in ROOT. The fit to data is redone and the difference to the nominal values is taken as systematic uncertainty. The difference of the shapes is illustrated in the background enriched region with non isolated electrons in Fig. 6.6.

The model assumes that the mass shapes for signal and background are the same in each control region. This assumption is not fully valid, e.g. the energy resolution of converted and unconverted photons is different, but describes the data sufficiently within the limited statistics. In future studies an alternative model with different parameters for the mass shape in the different categories could be used to study the impact of this assumption quantitatively.

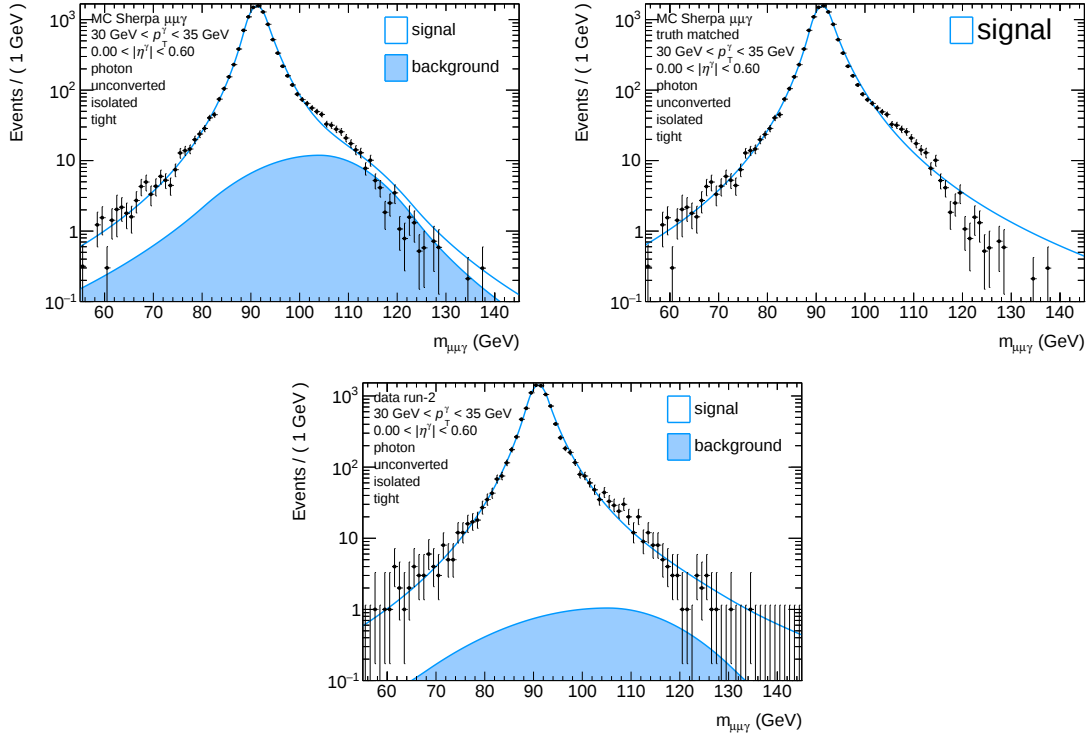


Figure 6.5.: Comparison of the fit result using the signal+background model for fitting the signal MC (top left) and the signal only model (top right) in the category of unconverted, tight and isolated photons. The power law tail does not describe the right hand tails of the signal distribution properly and is partially absorbed by the background model. The difference between the MC signal+background and MC signal only fit results is taken as systematic uncertainty. The bottom plot shows the result of the nominal fit in data in the same region for comparison.

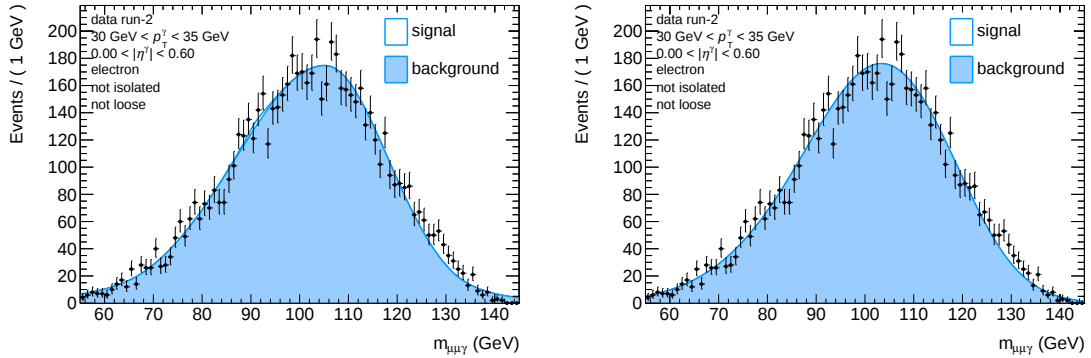


Figure 6.6.: Comparison of the fit result in the category with non isolated electron candidates using different shapes for the background mass distribution. The left plot uses the nominal asymmetric double sided crystal ball function and the right side the alternative BukinPdf used as a systematic variation.

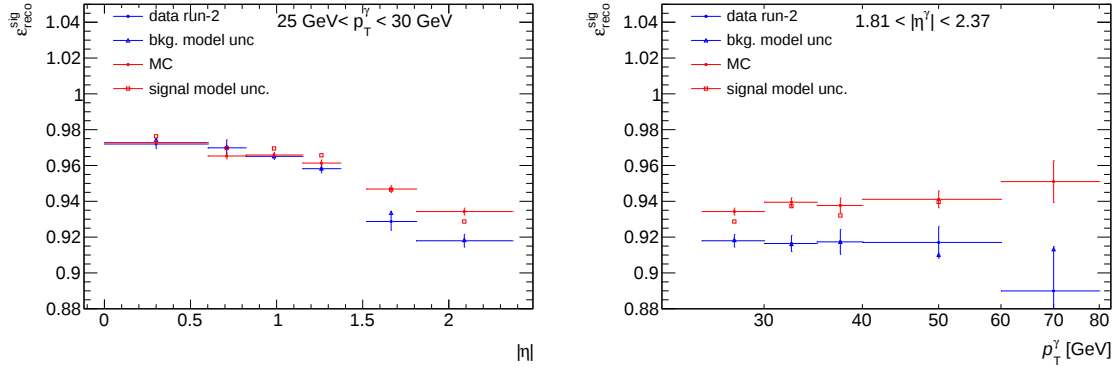


Figure 6.7.: Photon reconstruction efficiency in data (blue) and MC (red) $Z \rightarrow \mu\mu\gamma$ events as a function of $|\eta|$ (left) and p_T (right) of the photon.

6.5. Results

6.5.1. Reconstruction efficiency

The data and MC values for the photon reconstruction efficiency are depicted in Fig. 6.7 as a function of $|\eta|$ and p_T of the photon. The reconstruction efficiencies are decreasing as a function of $|\eta|$ from 98% in the centre to around 92% in the most forward bin. The efficiency values are relatively constant in the p_T range of the study, which is limited due to the decreasing statistics to transverse momenta lower than $p_T < 80$ GeV. This is also visible by the high statistical uncertainty of the values in the last p_T -bin between $60 \text{ GeV} < p_T < 80 \text{ GeV}$, which are excluded in the following considerations. The changes to the data and MC values due to the systematic variations are also depicted. Their impact is usually below 0.5%, increasing to around 1% in a few bins.

In the two $|\eta|$ -bins between $1.52 < |\eta| < 2.37$ the data reconstruction efficiency is significantly lower than the one in MC in all p_T -bins. The data-to-MC ratio is around 98% and is further studied by fitting a constant function to the values in different p_T bins. This is depicted in Fig. 6.8 on the left. The fit is redone for the two systematic variations and the difference to the nominal constant value are added in quadrature to the statistical uncertainty. This procedure of estimating p_T inclusive values is repeated in the different $|\eta|$ -bins and for different data-taking periods. The results are depicted in the right hand plot of Fig. 6.8. The data-to-MC ratios are compatible with one in the bins with $|\eta| < 1.37$ for the full Run-2 data set. Significant deviations from one are observed for $1.52 < |\eta| < 2.37$ for all subsets and the full data. The 2015+2016 values are consistently lower than the values of 2017+2018 in all three bins with $|\eta| > 1.15$. The most significant deviation can be seen in the region with $1.52 < |\eta| < 1.81$, where the data 2015+2016 value is $\epsilon_{\text{reco}}^{\text{data}}/\epsilon_{\text{reco}}^{\text{MC}} = (97.1 \pm 0.5)\%$ compared to $\epsilon_{\text{reco}}^{\text{data}}/\epsilon_{\text{reco}}^{\text{MC}} = (98.7 \pm 0.3)\%$ for 2017+2018.

The results show that the reconstruction efficiency is not well modelled in the simulation of photons with $|\eta| > 1.52$ and that there is a discrepancy in this mis-modelling between 2015+2016 and 2017+2018. The detector material itself has not changed between the different years, therefore any difference in the modelling between the years should be related to different data-taking conditions not properly reflected in MC. Pileup, as one of the main differences between the years, is probably not

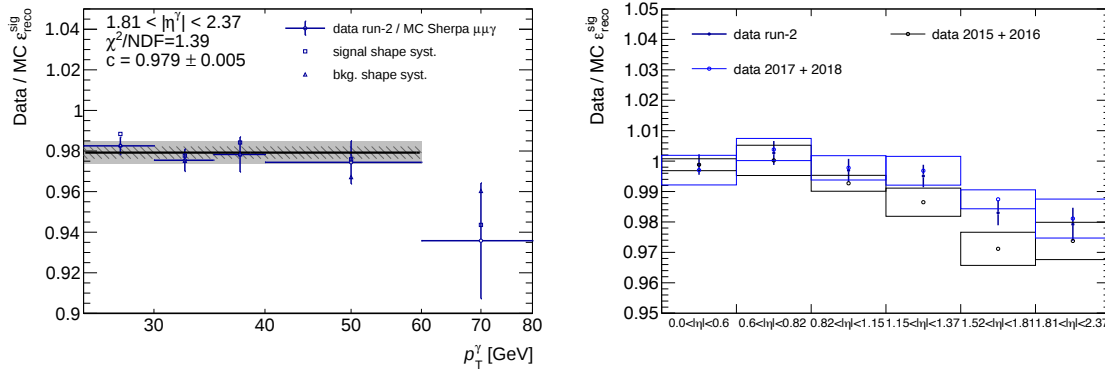


Figure 6.8.: The left plot shows the constant fit to the data-to-MC ratio of the photon reconstruction efficiency ϵ_{reco} as a function of p_T of the photons. The values in the last p_T bin are excluded, because of the limited statistics. The dashed area corresponds to the statistical and the grey area to the full uncertainty on the constant value. The right shows the result of the constant fit in different $|\eta|$ -bins for different data-taking periods: 2015+2016, 2017+2018 and full Run-2.

causing these difference, because the data efficiencies are lower in 2015+2016, although the pileup noise is lower and pileup is expected to deteriorate the tracking efficiencies. The composition of the gas mixture in the TRT is subject to changes due to small gas leaks, which could in turn change e.g. the transition radiation based selection efficiency of electron tracks.

The overall mismatch between the data and MC efficiencies is relatively small, therefore the pragmatic approach pursued by the photon-pair measurement is to correct the MC efficiencies to match the ones measured in $Z \rightarrow \mu\mu\gamma$ data by assigning weights $\epsilon_{\text{reco}}^{\text{data}}/\epsilon_{\text{reco}}^{\text{MC}}$ for both photon candidates in the event depending on the $|\eta|$ region of the respective photon and depending on the data-taking year the MC event should correspond to. The application of these photon reconstruction scale factor weights increases the measured photon-pair cross section value by 1.8% and a similar impact would be expected for other measurements with a photon-pair final state like $H \rightarrow \gamma\gamma$.

6.5.2. Interplay between conversion fractions and identification efficiencies

The central efficiency measurements and corrections are provided and applied independently for photons reconstructed as converted and unconverted. This assumes that the conversion fractions are well modelled in MC and or that selection efficiencies are the same for converted and unconverted photons. The validity of this assumption can be checked with the results of the efficiency fits. As explained before the detector material did not change significantly between the years, that means the true conversion fraction is the same, but the efficiency to reconstruct a true conversion as such and the rate of unconverted photons mis-reconstructed as converted photons can change due to changes in the data-taking conditions impacting the performance of the track reconstruction and selection.

In Fig. 6.9 the fraction of photons reconstructed as converted in 2015+2016 and 2017+2018 data and the corresponding MC is depicted as a function of $|\eta|$. The overall trends agree between data and MC. The MC conversion fractions only change slightly between the years, but the data values vary

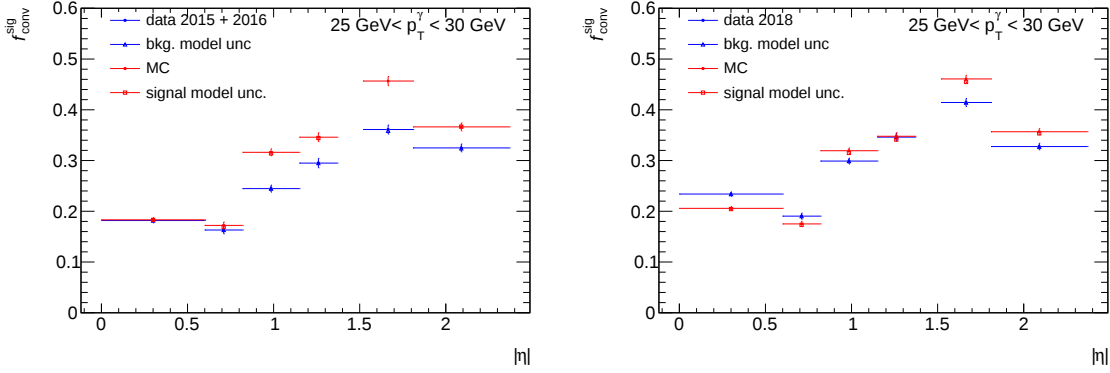


Figure 6.9.: Fraction of photons reconstructed as converted in data (blue) and MC (red) in 2015+2016 data (left) and 2017+2018 data (right).

significantly e.g. going for $|\eta| < 0.6$ from 18% in 2015+2016 to 24% in 2018. In general the values in 2018 are higher than the corresponding values in 2015+2016, which is compatible with a higher fraction of unconverted photons reconstructed as converted due to higher pileup conditions. The conversion fractions are overestimated in MC for $|\eta| > 0.82$.

The conversion fraction itself is not important for most measurements, which are indifferent about the photon conversion type and are taking into account all photon candidates. Problems could arise, if the different conversion fractions would change the overall identification efficiencies.

To check this the full conversion type averaged identification efficiency ε_{id} is calculated from the parameters of the fit in data and MC:

$$\varepsilon_{\text{id}} = f_{\text{conv}} \varepsilon_{\text{L}}^{\text{C}} \varepsilon_{\text{L}/2}^{\text{C}} \varepsilon_{\text{L}/2}^{\text{C}} + (1 - f_{\text{conv}}) \varepsilon_{\text{L}}^{\text{UC}} \varepsilon_{\text{L}/2}^{\text{UC}} \varepsilon_{\text{L}/2}^{\text{UC}} \quad (6.12)$$

The data-to-MC ratios are again fitted with a constant function of p_{T} and the result is shown for the different subsets of the data in different $|\eta|$ regions in Fig. 6.10. The values fluctuate around one and are mostly compatible with one. This means the discrepancies introduced by the different conversion fractions in data and MC are insignificant and well covered by the 1 to 2% uncertainty of the central identification efficiency measurements.

6.5.3. Identification-isolation correlation $R_{\gamma}^{\text{iso-id}}$

At last also the correlation correction factor $R_{\gamma}^{\text{iso-id}}$ for signal can be studied, which is an input to the background estimation of the photon-pair measurement, because it changes the signal migration into background control regions, where both the isolation and identification cuts are failed by the genuine photon. The parameter is defined as the ratio of the isolation efficiency for a photon candidate passing the identification divided by the isolation efficiency for a photon failing the identification. It describes how much the isolation efficiency is lowered for a candidate not passing the identification selections. This parameter is not measured in the standard photon efficiency measurements, because there either isolation or identification are always applied as baseline selections.

For the photon-pair measurement the control regions apply a *Loose'2* baseline selection, therefore

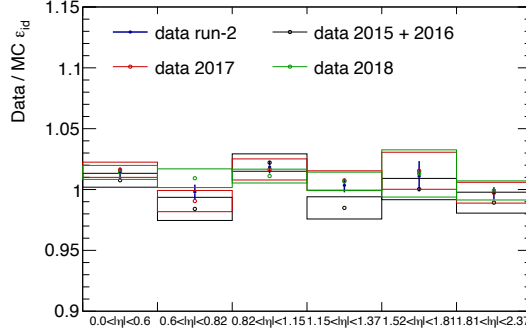


Figure 6.10.: Data-to-MC ratio of conversion type averaged identification efficiency ε_{id} as a function of $|\eta|$ for different data-taking periods.

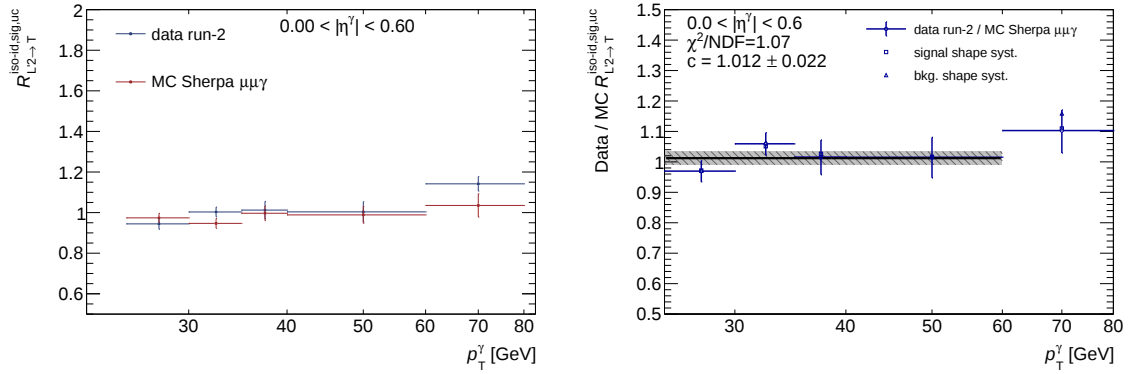


Figure 6.11.: The left plot shows a comparison of the signal correlation correction factor $R_{L'2 \rightarrow T}^{\text{iso-id}}$ between data and MC for unconverted photons in $|\eta| < 0.6$ as a function of p_T . The right hand plot shows a the ratio of the data and MC values and the result of a constant fit.

the correlation correction factor $R_{L'2 \rightarrow T}^{\text{iso-id}}$ of the isolation efficiency for the *Tight* selection with respect to objects passing the *Loose'2* selection is of special interest.

A comparison of a selection of $R_{L'2 \rightarrow T}^{\text{iso-id}}$ values in data and MC for unconverted photons is given in the left hand plot of Fig. 6.11. The R values are close to one indicating the orthogonality of the isolation and identification selection, after the *Loose'2* criterion is passed. The restriction of the statement to *Loose'2* photons is important, because e.g. the cuts on the fraction of the energy deposits in the hadronic calorimeter R_{had} contained in the *Loose'5* identification are not fully orthogonal to the isolation selection, because of the large granularity $\Delta\eta \times \Delta\phi = 0.1 \times 0.1$ of the hadronic calorimeter. This is also reflected by $R_{L \rightarrow L}^{\text{iso-id}}$ values around 0.5 resulting from the fit. In general the R factors of very loose identification criteria have a higher statistical uncertainty because of the lower signal fractions in the relevant categories.

Good agreement of the $R_{L'2 \rightarrow T}^{\text{iso-id}}$ values between data and MC within the uncertainties is observed,

which is checked similarly as before by fitting constant values as a function of p_T in different $|\eta|$ region as illustrated by the right hand plot in Fig. 6.11.

Unfortunately the $R_{L/2 \rightarrow T}^{\text{iso-id}}$ factors for background events can not be estimated by the fit with good precision, because the background fractions in the relevant categories which pass at least *Loose'2* are too low. Extracting $R_{L \rightarrow L/2}^{\text{iso-id}}$ for background from data with good precision would be beneficial, because it could reduce one of the leading uncertainties of the photon-pair measurement.

6.6. Conclusion

A detailed study of photon selection efficiencies was presented. In general the modelling of the efficiencies in simulation is very good and only small differences between the years could be found, which are only partially able to explain the discrepancies seen in the photon-pair measurement (cf. Section 7.7.5). The photon reconstruction efficiency is an important step in the photon selection being responsible for the loss of around 5% of genuine photons especially at high $|\eta|$. The data-to-MC agreement of the conversion fractions and the photon reconstruction efficiencies changes between the years hinting to changes in the data-taking conditions not fully taken into account by the MC. The results presented in this section provide an important tool for all prompt-photon measurements.

Using radiative $Z \rightarrow \mu\mu\gamma$ events limits the range of transverse momenta sufficiently populated for statistically precise statements to $p_T^\gamma < 80$ GeV. Extending the study to higher p_T^γ at the same level of complexity with e.g. single photon events is not straight forward, because there the background can not be estimated based on the distribution of the invariant mass, but identification or isolation criteria need to be utilized.

Chapter 7.

Diphoton Production Measurement

The diphoton production cross section measurement presented in this chapter is the main scientific output of this thesis. The results are published in Ref. [38] and this chapter is based on the descriptions in the paper giving further details especially on parts with major contributions by the author of the thesis. The auxiliary measurements presented in the previous Chapters 5 and 6 provide important information for the diphoton measurement in terms of photon reconstruction and isolation efficiencies.

The presented measurement is the first of its kind at $\sqrt{s} = 13$ TeV. Pair production of prompt¹ photons represents an ideal testing ground for perturbative QCD predictions, because of the large influence of higher-order contributions in fragmentation-like $\gamma\gamma$ +jets configurations (cf. Section 2.3). These $\gamma\gamma$ +jets events are implicitly included by this inclusive diphoton measurement which is based on the properties of the photons in the events with no explicit requirements on the jets. An example of a selected data event with a pair of photon candidates and an additional jet is depicted in Fig. 7.1.

In addition to the sensitivity of the diphoton system to highly energetic QCD jets in the event, the combination of two photons also allows precise measurement sensitive to even very low energetic additional QCD radiation balanced with the transverse momentum of the photon-pair, e.g. with almost back-to-back events with an azimuthal angle between the photons $\Delta\phi_{\gamma\gamma}$ only slightly different from $\Delta\phi_{\gamma\gamma} \approx \pi$.

Furthermore, diphoton production is an important channel for Higgs measurement and BSM searches for which the continuum photon-pair production studied in this measurement is an important background.

The goal of the analysis is to measure particle-level (PL) differential cross sections as a function of several kinematic observables of the diphoton system. PL refers to the properties of the particles as would be measured by a perfect detector with 100% selection efficiency and perfect resolution. In contrast, detector level (DL) refers to the properties of the reconstructed particle candidates, which are affected by the limited resolution and efficiency of the detector. The measurement is performed in a fiducial phase space, which is described by PL requirements on the kinematic properties of photon pairs produced in the collision events. The fiducial phase space is chosen such that the photons can be reconstructed by the detector with high efficiency to minimize the extrapolation from the measured DL quantities to the inferred PL quantities. The resulting PL cross sections can be easily reinterpreted by theoreticians requiring minimal knowledge of the experimental details.

The data and MC samples used for the analysis are described in Sections 7.1 and 7.2. Candidates

¹Prompt refers to photons not produced by a hadron decay

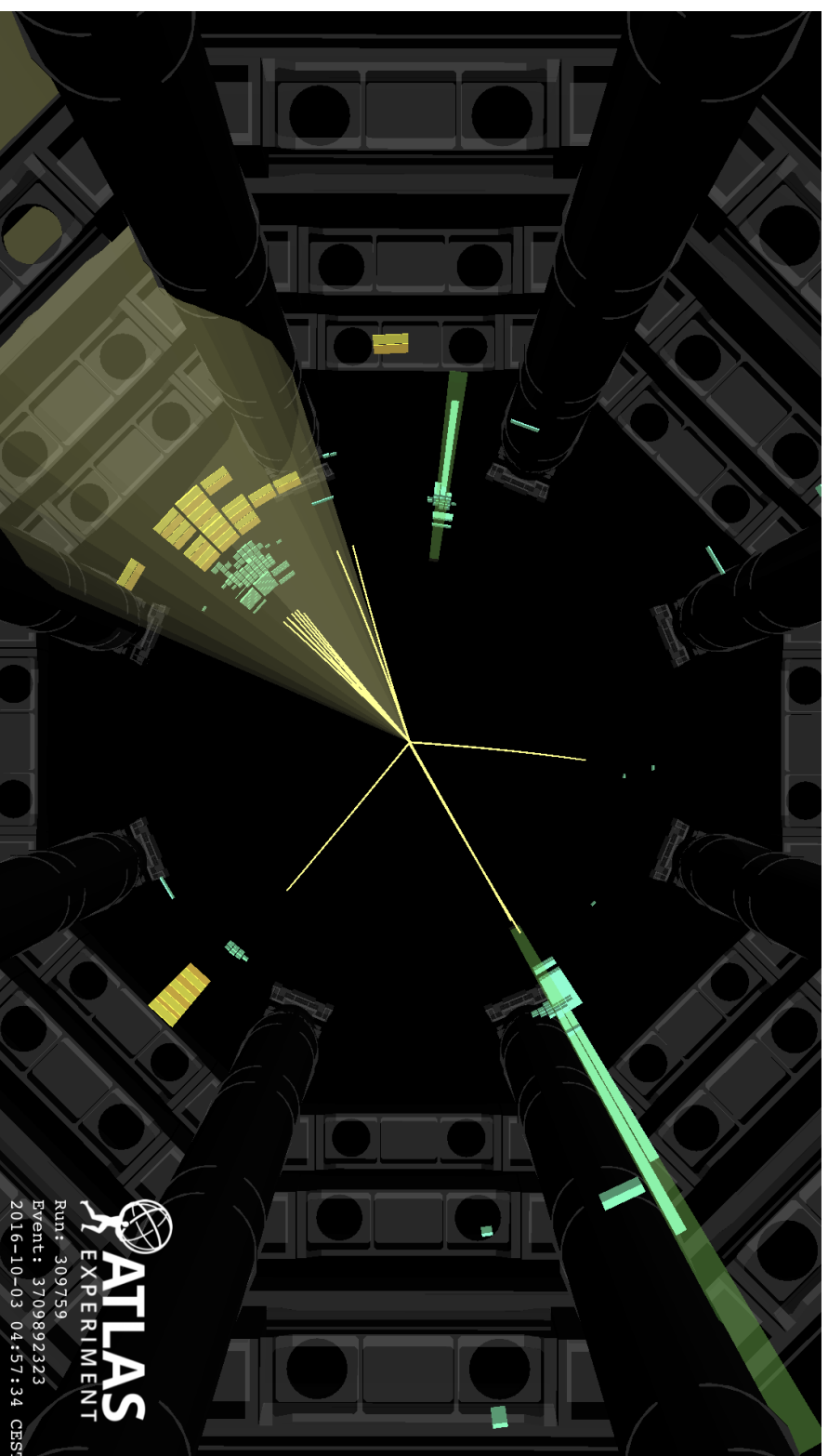


Figure 7.1.: Diphoton event candidate recorded by ATLAS in 13 TeV collisions. The two transparent green bands indicate to the two photons, while the yellow cone corresponds to a jet reconstructed with the anti- k_t algorithm and $R = 0.4$. In this energetically asymmetric photon pair candidate, the leading photon has a transverse momentum of $p_{T,\gamma_1} = 641$ GeV, while the sub-leading photon has $p_{T,\gamma_2} = 231$ GeV [38].

of diphoton events are selected based on the detector level requirements described in Section 7.3. The different observables in which the differential measurement is performed are summarized in Section 7.4. The fraction of genuine photon-pair events and background events is estimated in Section 7.5. In Section 7.6 the fiducial space definition and unfolding is described, which is correcting the DL signal yields for detector inefficiencies and resolution effects to calculate the PL signal yields. In Section 7.7 different sources of uncertainties on the result are discussed. Section 7.8 introduces different theory predictions which are compared to the measured values in Section 7.9.

7.1. Data samples

The 139 fb^{-1} of pp -collision data of the $\sqrt{s} = 13\text{ TeV}$ LHC Run-2 recorded by ATLAS are used. Compared to previous measurements (cf. Section 2.4) this dataset enables a measurement with an unprecedented kinematic range extending to $m_{\gamma\gamma} > 1\text{ TeV}$ and excellent statistics. Only data with stable beam and detector conditions [114] is considered. The primary diphoton triggers described in Section 3.2.5 are used to select event candidates.

7.2. Simulated samples

Different MC samples are used in the following for the background estimation, for the unfolding of detector effects, and as theoretical predictions in the final comparison to the measured data. These samples are centrally produced and validated in ATLAS and processed with the detector simulation and reconstruction as described in Section 3.2.6.

7.2.1. Diphoton signal samples

Simulated samples of prompt diphoton production from the MC generators SHERPA and PYTHIA are used.

SHERPA

The nominal samples used to estimate quantities of the signal process are simulated with the SHERPA 2.2 [36] generator. For these samples fixed-order calculations for $pp \rightarrow \gamma\gamma + 0, 1\text{jet}$ at NLO and $pp \rightarrow \gamma\gamma + 2, 3\text{jet}$ at LO are matched and merged with the SHERPA parton shower based on Catani-Seymour dipoles [126, 127] using the MEPS@NLO prescription [51, 52]. The virtual QCD correction for matrix elements at NLO accuracy are provided by the OPENLOOPS library [135, 136]. Samples are generated using the NNPDF3.0NNLO set [137], along with the dedicated set of tuned parton-shower parameters developed by the SHERPA authors. Both, the direct and fragmentation component of isolated photon production are included by setting the merging scale dynamically in the scheme of [40]. In addition, the loop-induced $gg \rightarrow \gamma\gamma$ box process is included in these samples at LO accuracy.

The fixed-order calculations used for these samples require the leading (subleading)² photon to be above $p_{T,\gamma} > 20(18)\text{ GeV}$, their separation to be $\Delta R_{\gamma\gamma} > 0.2$, and a very loose smooth-cone photon

²Leading and subleading refer to the photon with the largest and second-largest transverse momentum.

isolation [45] with $\epsilon = 0.1$, $n = 2$, $\delta_0 = 0.1$ (cf. Section 2.3).

PYTHIA

The alternative PYTHIA samples are simulated based on LO matrix elements and the PYTHIA 8.186 [44] parton shower using the NNPDF2.3LO [120] PDF set with the A14 shower tune [138]. Different modes with different numbers of photons produced in the parton shower are produced separately: The direct $pp \rightarrow \gamma\gamma$ component with two photons from the matrix element; the single-fragmentation component with one photon in the $pp \rightarrow \gamma + \text{jet}$ matrix element and one additional photon produced in the parton shower; and the double-fragmentation component with $pp \rightarrow \text{jet} + \text{jet}$ matrix elements and two photons produced in the parton shower. The production of photons in the parton shower has the advantage of not requiring any isolation cut on the photons.

The PYTHIA samples are affected by a duplication issue caused in the central MC production. This results in a loss of effective statistics by a factor of 10, which limits the usability of the sample for the analysis. Fixed samples are in preparation, but were not ready in time for this analysis. An alternative sample besides the SHERPA sample is necessary to estimate uncertainties on the analysis from the modelling of the specific diphoton production samples used for the analysis. The main impact of these differences between SHERPA and PYTHIA is expected in the PL photon isolation, because PYTHIA generates photons inclusively, e.g. without isolation cut through the parton shower. The impact of these differences is estimated by reweighting the PL isolation distribution in the SHERPA samples to match the ones in PYTHIA (cf. Appendix A). The differences of the analysis with the nominal and reweighted SHERPA sample are assigned as a systematic uncertainty related to the physics modelling.

7.2.2. Electron background samples

The background from electrons mis-identified as photons is estimated based on MC samples of prompt electron production from Drell-Yan processes like $Z/\gamma^*(\rightarrow ee)$ and $W(\rightarrow e\nu)$. Their impact will be described in Section 7.5.6.

The samples have been generated using POWHEG BOX v2 [115, 117] interfaced to the PYTHIA 8.186 [44] parton shower model. Photos++ 3.52 [139] is used for QED emissions from electroweak vertices and charged leptons. The W/Z samples are normalised to the NNLO cross sections calculated as described in Ref. [140]. The $p_T(Z)$ spectrum in the $Z \rightarrow ee$ sample is corrected based on the results of the measurement in Ref. [141].

7.2.3. $\gamma + \text{jet}$ background

Samples with $\gamma + \text{jet}$ events are used for cross checks with the data-driven background estimation. The same configuration as for the SHERPA signal samples described above is used to match and merge matrix elements of $pp \rightarrow \gamma + 1, 2$ jets at NLO and $pp \rightarrow \gamma + 3, 4$ jets at LO with the SHERPA parton shower.

7.3. Event selection

Events passing the primary diphoton triggers are considered. Photon candidates in these events are preselected if they pass the *Loose'5* identification (cf. Section 4.4), are in the well instrumented regions $|\eta| < 1.37$ or $1.52 < |\eta| < 2.37$, and match to the direction of a photon of the diphoton trigger. Events with less than two preselected photons are rejected. The leading and subleading photons in terms of p_T are selected and the criteria in the following paragraphs are applied to this pair of photons. The photon preselection is important to avoid selecting the wrong photon candidates in diphoton + jet events, where also the jet could create a high- p_T photon candidate.

The (sub)leading photon is required to have a transverse momentum of $p_{T,\gamma_{1(2)}} > 40(30)$ GeV. This requirement is chosen sufficiently higher than the p_T requirement of $p_T > 35(25)$ GeV of the photon-pair trigger to be at the plateau of the trigger efficiency.

In the signal regions both photons are required to pass the *Tight* identification. The photons are also required to be isolated with an isolation cut on $E_T^{\text{cone}20}$ as defined in Section 4.5. This means the definition does not include the new developments of Chapter 5, because not all centrally provided calibrations are ready for the new isolation variables. The insights of Section 5.7 are an important input to the estimation of the pileup related uncertainties of the isolation efficiency in Section 7.7.4. The isolation requirement for the signal region is $E_T^{\text{cone}20} < 0.05 \cdot p_{T,\gamma_{1(2)}}$, which was chosen to minimize the overall uncertainties of the analysis as described in Appendix B.

The angular separation of the photons is required to be $\Delta R > 0.4$. This has the advantage of non-overlapping isolation cones reducing the correlations between the isolation efficiencies of both objects.

7.4. Observables

In principle six degrees of freedom are needed to describe the momenta $p_{\gamma_{1(2)}}$ of the two photons, e.g. the transverse momenta $p_{T,\gamma_{1(2)}}$, the azimuthal angles $\phi_{\gamma_{1(2)}}$ and the rapidities $\eta_{\gamma_{1(2)}}$.

Because of the axial symmetry around the z -axis of the experiment the azimuthal orientation of the diphoton system is ideally uniformly distributed and does not carry interesting information about the collision event. This means the individual azimuthal angles can be replaced by the azimuthal angular separation $\Delta\phi_{\gamma\gamma}$ between the momenta of the photons. Furthermore any good observable of the diphoton system should be invariant under boosts along the z -axis, because the momentum fractions of the two initial state partons are probabilistic. This means the observables should only depend on the rapidity difference $\Delta\eta = |\eta_{\gamma_1} - \eta_{\gamma_2}|$ and not on the individual rapidities of the photons, which leaves four degrees of freedom e.g. p_{T,γ_1} , p_{T,γ_2} , $\Delta\phi_{\gamma\gamma}$ and $\Delta\eta_{\gamma\gamma}$.

The measurement is performed independently in bins of eight observables described in the following:

- The transverse momenta of the leading photon p_{T,γ_1} and subleading p_{T,γ_2} photon. These observables are the main addition with respect to the set of observables included in the previous measurement by ATLAS at $\sqrt{s} = 8$ TeV [69].
- The acoplanarity $\pi - \Delta\phi_{\gamma\gamma}$ is used. This observable is e.g. sensitive to soft wide-angle QCD radiation close to the back-to-back configurations $\Delta\phi_{\gamma\gamma} = \pi$. For a proper display of this region

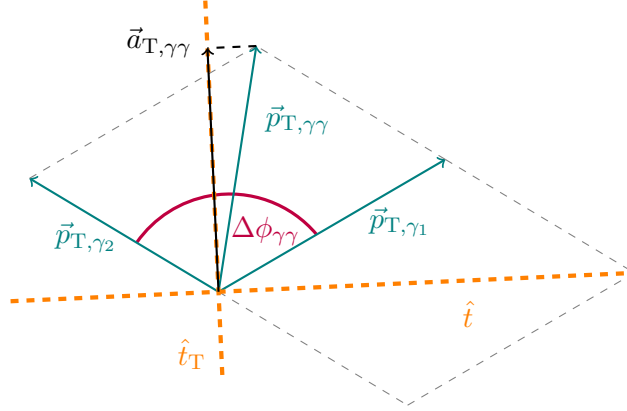


Figure 7.2.: Illustration of different observables in the transverse plane.

an axis logarithmic in $\pi - \Delta\phi_{\gamma\gamma}$ is preferable over simply using $\Delta\phi_{\gamma\gamma}$. The regions with low $\Delta\phi_{\gamma\gamma}$ indicate additional highly energetic QCD jets in the events.

- The invariant mass $m_{\gamma\gamma}$ of the photon pair,

$$m_{\gamma\gamma} = \sqrt{2p_{T,\gamma 1}p_{T,\gamma 2}(\cosh \Delta\eta_{\gamma\gamma} - \cos \Delta\phi_{\gamma\gamma})}, \quad (7.1)$$

which is especially relevant because the measured continuous spectrum constitutes the main background for Higgs measurements and BSM searches.

- The transverse momentum of the photon pair,

$$p_{T,\gamma\gamma} = |\vec{p}_{T,\gamma 1} + \vec{p}_{T,\gamma 2}| = \sqrt{p_{T,\gamma 1}^2 + 2p_{T,\gamma 1}p_{T,\gamma 2} \cos \Delta\phi_{\gamma\gamma} + p_{T,\gamma 2}^2}, \quad (7.2)$$

which is indirectly measuring the transverse momentum of additional QCD activity in the event due to transverse momentum conservation. This means the low $p_{T,\gamma\gamma}$ regime is sensitive to soft radiation, which can not be described perturbatively, while the high $p_{T,\gamma\gamma}$ regime corresponds to events with additional hard jets which are contained in (N)NLO QCD calculations. For events with low $\Delta p_T = p_{T,\gamma 1} - p_{T,\gamma 2}$ in the back-to-back limit $p_{T,\gamma\gamma}$ can be approximated as

$$p_{T,\gamma\gamma} \stackrel{\Delta\phi_{\gamma\gamma} \rightarrow \pi}{\approx} \sqrt{(\Delta p_T)^2 + \frac{(\pi - \Delta\phi_{\gamma\gamma})^2}{2} p_{T,\gamma 1} p_{T,\gamma 2}} \\ \stackrel{\Delta p_T^2 \ll p_{T,\gamma 1} p_{T,\gamma 2}}{\approx} |\pi - \Delta\phi_{\gamma\gamma}| \sqrt{\frac{p_{T,\gamma 1} p_{T,\gamma 2}}{2}} + \mathcal{O}\left(\frac{(\Delta p_T)^2}{\sqrt{p_{T,\gamma 1} p_{T,\gamma 2}}}\right),$$

which shows that it can be measured with approximately the same relative uncertainty as the

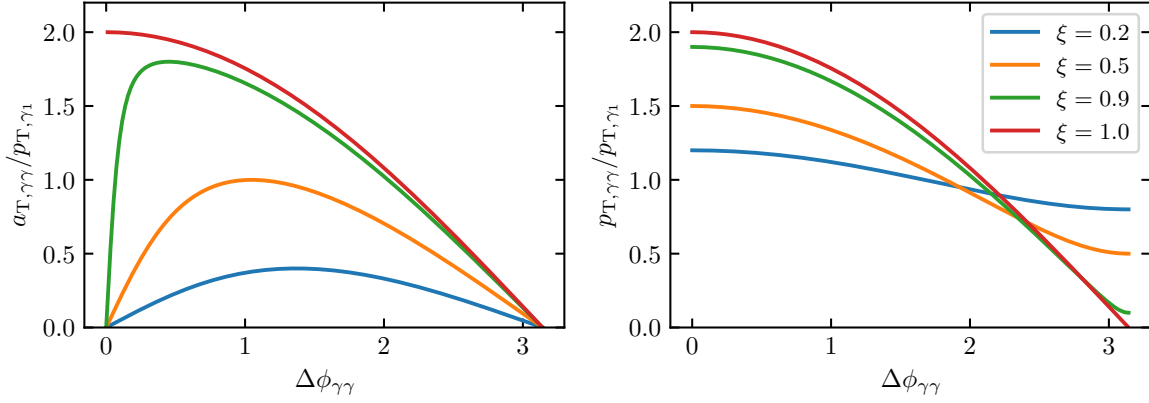


Figure 7.3.: Values of $a_{T,\gamma\gamma}/p_{T,\gamma 1}$ (left) and $p_{T,\gamma\gamma}/p_{T,\gamma 1}$ (right) as a function of $\Delta\phi_{\gamma\gamma}$ for different momentum fractions $\xi = p_{T,\gamma 2}/p_{T,\gamma 1}$.

individual photon momenta, although the absolute value of $p_{T,\gamma\gamma}$ might be low.

- The observable $\mathbf{a}_{T,\gamma\gamma}$ was first introduced in Ref. [142] as an observable similar to $p_{T,\gamma\gamma}$ for back-to-back configurations, but with a better resolution because of a lower sensitivity to variations collinear to the photons (e.g. to Δp_T). This is discussed in more detail in Ref. [143]. The geometric relations of the different observables defined in the transverse plane are depicted in Fig. 7.2. The observable $a_{T,\gamma\gamma}$ is the component of $\vec{p}_{T,\gamma\gamma}$ perpendicular to the thrust axis $\hat{t}$. The thrust axis is defined as:

$$\hat{t} = \frac{(\vec{p}_{T,\gamma 1} - \vec{p}_{T,\gamma 2})}{|\vec{p}_{T,\gamma 1} - \vec{p}_{T,\gamma 2}|} \quad (7.3)$$

The direction perpendicular to the thrust axis $\hat{t}_T$ is:

$$\hat{t}_T = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \hat{t} \quad (7.4)$$

The projection of $p_{T,\gamma\gamma}$ along $\hat{t}_T$ defines $a_{T,\gamma\gamma}$:

$$a_{T,\gamma\gamma} = p_{T,\gamma\gamma} \cdot \hat{t}_T = (\vec{p}_{T,\gamma 1} + \vec{p}_{T,\gamma 2}) \cdot \hat{t}_T = \frac{2p_{T,\gamma 1}p_{T,\gamma 2} \sin \Delta\phi_{\gamma\gamma}}{\sqrt{p_{T,\gamma 1}^2 - 2p_{T,\gamma 1}p_{T,\gamma 2} \cos \Delta\phi_{\gamma\gamma} + p_{T,\gamma 2}^2}} \quad (7.5)$$

Defining the ratio $\xi = p_{T,\gamma 2}/p_{T,\gamma 1}$ the observables $a_{T,\gamma\gamma}$ and $p_{T,\gamma\gamma}$ can be expressed as:

$$a_{T,\gamma\gamma} = p_{T,\gamma 1} \frac{2\xi \sin \Delta\phi_{\gamma\gamma}}{\sqrt{1 - 2\xi \cos \Delta\phi_{\gamma\gamma} + \xi^2}} \quad p_{T,\gamma\gamma} = p_{T,\gamma 1} \sqrt{1 + 2\xi \cos \Delta\phi_{\gamma\gamma} + \xi^2} \quad (7.6)$$

The variation of $a_{T,\gamma\gamma}/p_{T,\gamma 1}$ and $p_{T,\gamma\gamma}/p_{T,\gamma 1}$ with $\Delta\phi_{\gamma\gamma}$ and ξ is compared in Fig. 7.3. For approximately symmetric configurations ($\xi > 0.9$) $a_{T,\gamma\gamma}$ and $p_{T,\gamma\gamma}$ show very similar behaviour if $\Delta\phi_{\gamma\gamma} > 0.5$. Around $\Delta\phi_{\gamma\gamma} \approx \pi$ it is visible that $a_{T,\gamma\gamma}$ does not depend on ξ , while $p_{T,\gamma\gamma}$ strongly

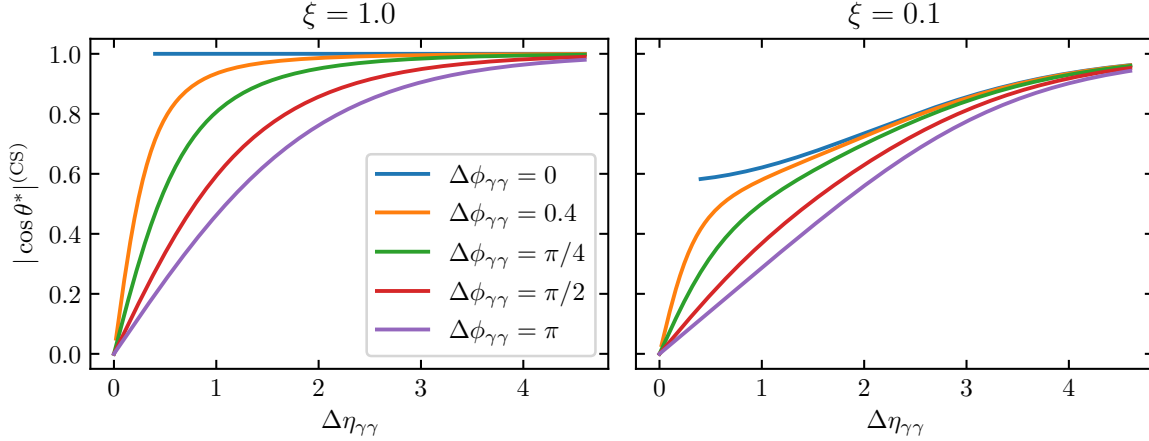


Figure 7.4.: Values of $|\cos \theta^*|^{(\text{CS})}$ as a function of $\Delta\eta_{\gamma\gamma}$ for different $\Delta\phi_{\gamma\gamma}$ for a symmetric $\xi = 1$ (left) and an asymmetric $\xi = 0.1$ (right) configuration.

changes even from $\xi = 1$ to $\xi = 0.9$. This makes $a_{\text{T},\gamma\gamma}$ a superior probe for the momentum of soft radiation at $\Delta\phi_{\gamma\gamma} \rightarrow \pi$. Although low $a_{\text{T},\gamma\gamma}$ values can be also a sign of $\Delta\phi_{\gamma\gamma} \rightarrow 0$ the impact of these events is suppressed, because of the requirement of $\Delta R_{\gamma\gamma} > 0.4$ of the analysis.

- The absolute value of the cosine of the scattering angle with respect to the z -axis in the Collins-Soper frame [144]:

$$|\cos \theta^*|^{(\text{CS})} = \left| \frac{\sinh \Delta\eta_{\gamma\gamma}}{\sqrt{1 + (p_{\text{T},\gamma\gamma}/m_{\gamma\gamma})^2}} \cdot \frac{2p_{\text{T},\gamma 1} p_{\text{T},\gamma 2}}{m_{\gamma\gamma}^2} \right|, \quad (7.7)$$

which is used to study the spin and parity of the Higgs boson [145, 146]. Using again $\xi = p_{\text{T},\gamma 2}/p_{\text{T},\gamma 1}$ the ratio $(p_{\text{T},\gamma\gamma}/m_{\gamma\gamma})^2$ occurring in the calculation can be expressed as:

$$(p_{\text{T},\gamma\gamma}/m_{\gamma\gamma})^2 = \frac{1 + 2\xi \cos \Delta\phi_{\gamma\gamma} + \xi^2}{2\xi(\cosh \Delta\eta_{\gamma\gamma} - \cos \Delta\phi_{\gamma\gamma})}.$$

Similarly the $p_{\text{T},\gamma 1}$ in the second factor of Eq. (7.7) cancels and $|\cos \theta^*|^{(\text{CS})}$ can be expressed in terms of $\Delta\phi_{\gamma\gamma}$, $\Delta\eta_{\gamma\gamma}$ and ξ . The dependency of $|\cos \theta^*|^{(\text{CS})}$ on these variables is illustrated in Fig. 7.4. In general $|\cos \theta^*|^{(\text{CS})}$ is monotonically increasing with $\Delta\eta_{\gamma\gamma}$. High values of $|\cos \theta^*|^{(\text{CS})}$ at low $\Delta\eta_{\gamma\gamma}$ are only possible for symmetric $\xi \approx 1$ events with low $\Delta\phi_{\gamma\gamma}$.

- An angular variable defined as

$$\phi_\eta^* = \tan \frac{\pi - \Delta\phi_{\gamma\gamma}}{2} \quad \sin \theta_\eta^* = \tan \frac{\pi - \Delta\phi_{\gamma\gamma}}{2} \sqrt{1 - \left(\tanh \frac{\Delta\eta_{\gamma\gamma}}{2} \right)^2} \quad (7.8)$$

is used, which was introduced in Ref. [143]. As depicted in Fig. 7.5 it varies strongly with $\Delta\phi_{\gamma\gamma}$, giving an emphasis on the regions near $\Delta\phi_{\gamma\gamma} = 0$ and $\Delta\phi_{\gamma\gamma} = \pi$. The variation with $\Delta\eta_{\gamma\gamma}$

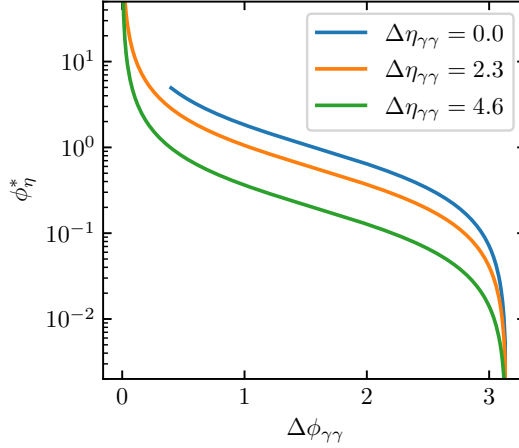


Figure 7.5.: Values of ϕ_η^* as a function of $\Delta\phi_{\gamma\gamma}$ for different $\Delta\eta_{\gamma\gamma}$.

is relatively mild in comparison reducing ϕ_η^* by at most 80% for the maximum of $\Delta\eta_{\gamma\gamma} \approx 4.8$ which can be measured by the ATLAS detector.

The bins in which the cross-sections are measured are optimized for each observable. The bins are required to be larger than four times the detector resolution, which is estimated from the distribution of the difference between particle-level and detector-level observables $x_{\text{detector}} - x_{\text{particle}}$ in the SHERPA MC signal samples. The resolution is determined by the standard deviation of the Gaussian cores of the distributions. The binning restriction based on the detector resolution reduces the corrections needed in the unfolding. In addition to the resolution restriction the bins are required to have enough statistics to get a statistical uncertainty of $< 10\%$ based on the signal expectation. For the observables $|\cos\theta^*|^{(\text{CS})}$, ϕ_η^* and $\pi - \Delta\phi_{\gamma\gamma}$ which are measured with a very high resolution and high statistics the bin size is enlarged in some regions to achieve a bin width which is visible in the plots. This optimized binning is used for all plots in the following.

7.5. Background estimation

The number of events passing the signal region event selection described in Section 7.3 are counted for each bin of the eight observables. Besides the signal of prompt photon pairs ($\gamma\gamma$) there are several background processes contributing to the event yields, which are estimated as described in this section.

The data-driven estimation for the main backgrounds where the leading photon candidate ($j\gamma$), the subleading photon candidate (γj) or both (jj) are mis-identified jets is described in Section 7.5.1. Additional contributions from electrons (ee) and from single photon production in different interaction vertices (PU) due to pileup are also included (cf. Sections 7.5.6 and 7.5.7).

7.5.1. Jet background

The jet backgrounds in the signal region mostly consists of jets including a high energetic neutral meson decaying to a collimated photon pair. Because of the very specific configuration of these jets

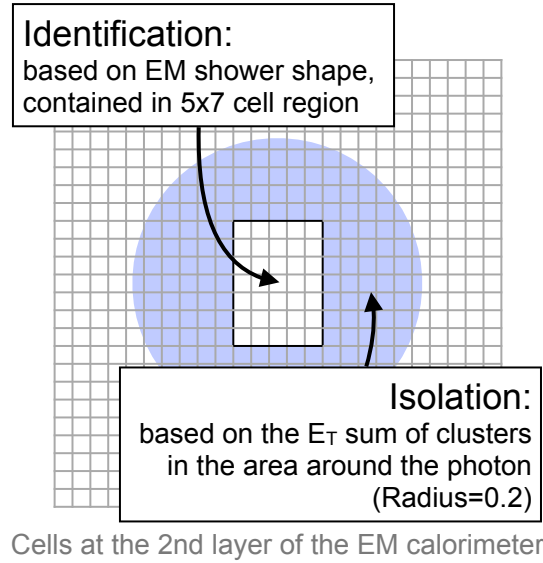


Figure 7.6.: Illustration of the calorimeter cells in the middle layer around a photon candidate. The cells in the rectangular window in the centre are used to calculate the photon identification variables and the energy deposited in this central window is subtracted from the isolation energy.

consisting of a fairly isolated hadron and because there are no dedicated measurements to study the detector response for such jets, the simulated samples of the jet backgrounds can not be used directly for the estimation. Furthermore background samples with high statistics come at high computational costs, because of the high background rejection of the signal region selection.

A data-driven estimation technique for the jet background is used instead which relies on isolation and identification information of the photon candidates. The approach is an extension of the estimation method used for ATLAS single photon measurements [147–156] and similar to the one of previous photon pair measurements by ATLAS [67, 68].

The method relies on data control regions with either or both of the photon candidates failing the signal-region isolation criterion, the signal-region identification criterion or both criteria. The candidates in the background control regions are still required to satisfy loose baseline criteria to reduce the correlation between the identification and isolation efficiencies. As described in Section 6.5.3 this is not the case for very loose identification criteria, for which the isolation efficiency is significantly higher for candidates passing it compared to similar candidates failing it.

The requirement for the candidates failing the signal region *Tight* identification is to still pass the *Loose2* identification (cf. Section 4.4). This means the photon identification cuts requiring a narrow shower in the middle layer of the calorimeter and a small relative amount of energy in the hadronic calorimeter are passed. In addition most of the strip-layer cuts are passed. Therefore the shower of the photon candidate in the control regions is still required to be narrowly collimated in a small window. For the calculation of the isolation variables, the window of cells used for the photon identification cuts is removed as depicted in Fig. 7.6 and described earlier in Section 4.5 to reduce the

Table 7.1.: Numbering scheme for the signal region and the background control regions. P indicates a passed criterion and F a failed one.

γ_1 id.	P								F							
γ_2 id.	P				F				P				F			
γ_1 iso.	P		F		P		F		P		F		P		F	
γ_2 iso.	P	F	P	F	P	F	P	F	P	F	P	F	P	F	P	F
index	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16

correlation between the identification and isolation criteria.

The requirement for the candidates failing the signal region isolation cut is to still pass $E_{T,\gamma_{1(2)}}^{\text{cone20}} < 0.15 \cdot p_{T,\gamma_{1(2)}}$ which removes candidates with large energy deposits in the isolation region which could possibly distort the identification variables.

The passed or failed isolation and identification criteria of both candidates create 15 control regions in addition to the signal region, which are numbered as described in Table 7.1.

The background estimation is based on describing the fraction $f_{p,i}(\vartheta_p)$ of events entering into the $i = 1 \dots 16$ -th region for the each process $p \in \{\gamma\gamma, \gamma j, j\gamma, jj, ee, \text{PU}\}$ with a set of parameters ϑ_p . This means the number of expected events n_i^{exp} in each region can be expressed as:

$$n_i^{\text{exp}} = \sum_p f_{p,i}(\vartheta_p) N_p, \quad (7.9)$$

with N_p being the total number of events in all 16 regions for a process. The parameter of interest: the number of photon-pair events in the signal region $n_{\gamma\gamma,1} = f_{\gamma\gamma,1} N_{\gamma\gamma}$, is estimated base on a Poisson likelihood fit to the observed number of events n_i^{obs} in each region, maximizing:

$$\mathcal{L}(n_{\gamma\gamma,1}, \theta | n_1^{\text{obs}}, \dots, n_{16}^{\text{obs}}) = \prod_{i=1}^{16} \frac{[n_i^{\text{exp}}(n_{\gamma\gamma,1}, \theta)]^{n_i^{\text{obs}}}}{n_i^{\text{obs}}!} e^{-n_i^{\text{exp}}} \quad (7.10)$$

depending on $n_{\gamma\gamma,1}$ and a set of nuisance parameters θ including the background normalisations N_p ($p \in \{\gamma j, j\gamma, jj\}$). The chosen parametrisation of $f_{p,i}(\vartheta_p)$ and, the assumptions and additional nuisance parameter connected to it are explained in the following.

The $f_{p,i}(\vartheta_p)$ are expressed as:

$$\begin{aligned}
 f_{p,i}(\vartheta_p) &= f_{p,i}(\varepsilon_{p,1}^{\text{iso}}, \varepsilon_{p,2}^{\text{iso}}, R_p^{\text{iso}}, \varepsilon_{p,1}^{\text{id}}, \varepsilon_{p,2}^{\text{id}}, R_p^{\text{id}}, R_{p,1}^{\text{iso-id}}, R_{p,2}^{\text{iso-id}}) \\
 &= \begin{cases} \varepsilon_{p,1}^{\text{iso}} & \varepsilon_{p,2}^{\text{iso}} & \varepsilon_{p,1}^{\text{id}} & \varepsilon_{p,2}^{\text{id}} & \text{for } i = 1 \\ \varepsilon_{p,1}^{\text{iso}} & (1 - \varepsilon_{p,2}^{\text{iso}}) & \varepsilon_{p,1}^{\text{id}} & \varepsilon_{p,2}^{\text{id}} & \text{for } i = 2 \\ (1 - \varepsilon_{p,1}^{\text{iso}}) & \varepsilon_{p,2}^{\text{iso}} R_p^{\text{iso}} & \varepsilon_{p,1}^{\text{id}} & \varepsilon_{p,2}^{\text{id}} & \text{for } i = 3 \\ (1 - \varepsilon_{p,1}^{\text{iso}}) & (1 - \varepsilon_{p,2}^{\text{iso}} R_p^{\text{iso}}) & \varepsilon_{p,1}^{\text{id}} & \varepsilon_{p,2}^{\text{id}} & \text{for } i = 4 \\ \varepsilon_{p,1}^{\text{iso}} & \varepsilon_{p,2}^{\text{iso}} R_{p,2}^{\text{iso-id}} & \varepsilon_{p,1}^{\text{id}} & (1 - \varepsilon_{p,2}^{\text{id}}) & \text{for } i = 5 \\ \varepsilon_{p,1}^{\text{iso}} & (1 - \varepsilon_{p,2}^{\text{iso}} R_{p,2}^{\text{iso-id}}) & \varepsilon_{p,1}^{\text{id}} & (1 - \varepsilon_{p,2}^{\text{id}}) & \text{for } i = 6 \\ (1 - \varepsilon_{p,1}^{\text{iso}}) & \varepsilon_{p,2}^{\text{iso}} R_p^{\text{iso}} R_{p,2}^{\text{iso-id}} & \varepsilon_{p,1}^{\text{id}} & (1 - \varepsilon_{p,2}^{\text{id}}) & \text{for } i = 7 \\ (1 - \varepsilon_{p,1}^{\text{iso}}) & (1 - \varepsilon_{p,2}^{\text{iso}} R_p^{\text{iso}} R_{p,2}^{\text{iso-id}}) & \varepsilon_{p,1}^{\text{id}} & (1 - \varepsilon_{p,2}^{\text{id}}) & \text{for } i = 8 \\ \varepsilon_{p,1}^{\text{iso}} R_{p,1}^{\text{iso-id}} & \varepsilon_{p,2}^{\text{iso}} & (1 - \varepsilon_{p,1}^{\text{id}}) & \varepsilon_{p,2}^{\text{id}} R_p^{\text{id}} & \text{for } i = 9 \\ \varepsilon_{p,1}^{\text{iso}} R_{p,1}^{\text{iso-id}} & (1 - \varepsilon_{p,2}^{\text{iso}}) & (1 - \varepsilon_{p,1}^{\text{id}}) & \varepsilon_{p,2}^{\text{id}} R_p^{\text{id}} & \text{for } i = 10 \\ (1 - \varepsilon_{p,1}^{\text{iso}} R_{p,1}^{\text{iso-id}}) & \varepsilon_{p,2}^{\text{iso}} R_p^{\text{iso}} & (1 - \varepsilon_{p,1}^{\text{id}}) & \varepsilon_{p,2}^{\text{id}} R_p^{\text{id}} & \text{for } i = 11 \\ (1 - \varepsilon_{p,1}^{\text{iso}} R_{p,1}^{\text{iso-id}}) & (1 - \varepsilon_{p,2}^{\text{iso}} R_p^{\text{iso}}) & (1 - \varepsilon_{p,1}^{\text{id}}) & \varepsilon_{p,2}^{\text{id}} R_p^{\text{id}} & \text{for } i = 12 \\ \varepsilon_{p,1}^{\text{iso}} R_{p,1}^{\text{iso-id}} & \varepsilon_{p,2}^{\text{iso}} R_{p,2}^{\text{iso-id}} & (1 - \varepsilon_{p,1}^{\text{id}}) & (1 - \varepsilon_{p,2}^{\text{id}} R_p^{\text{id}}) & \text{for } i = 13 \\ \varepsilon_{p,1}^{\text{iso}} R_{p,1}^{\text{iso-id}} & (1 - \varepsilon_{p,2}^{\text{iso}} R_{p,2}^{\text{iso-id}}) & (1 - \varepsilon_{p,1}^{\text{id}}) & (1 - \varepsilon_{p,2}^{\text{id}} R_p^{\text{id}}) & \text{for } i = 14 \\ (1 - \varepsilon_{p,1}^{\text{iso}} R_{p,1}^{\text{iso-id}}) & \varepsilon_{p,2}^{\text{iso}} R_p^{\text{iso}} R_{p,2}^{\text{iso-id}} & (1 - \varepsilon_{p,1}^{\text{id}}) & (1 - \varepsilon_{p,2}^{\text{id}} R_p^{\text{id}}) & \text{for } i = 15 \\ (1 - \varepsilon_{p,1}^{\text{iso}} R_{p,1}^{\text{iso-id}}) & (1 - \varepsilon_{p,2}^{\text{iso}} R_p^{\text{iso}} R_{p,2}^{\text{iso-id}}) & (1 - \varepsilon_{p,1}^{\text{id}}) & (1 - \varepsilon_{p,2}^{\text{id}} R_p^{\text{id}}) & \text{for } i = 16, \end{cases}
 \end{aligned}$$

in terms of eight parameters per process:

- The isolation $\varepsilon_{p,1,(2)}^{\text{iso}}$ and identification $\varepsilon_{p,1,(2)}^{\text{id}}$ efficiencies of the (sub-)leading photon candidate with respect to the baseline selections of the control regions,
- The correlation-correction factor for the isolation (identification) requirement R_p^{iso} (R_p^{id}) describing the change of the sub-leading photon candidate efficiency, if the leading photon fails the respective requirement,
- The correlation-correction factor $R_{p,1(2)}^{\text{iso-id}}$ for the (sub-)leading photon quantifying the change of the isolation efficiency for candidates failing the identification requirement compared to candidates passing it.

Describing the event fractions in the 16 regions with only 8 parameters implies that a few assumptions are made, e.g. that the identification of the leading photon and the isolation of the subleading photon are uncorrelated within each process. Given that the correlation corrections taken into account are relatively close to one, it can be assumed that the impact of the even more intricate correlations is small.

The full set of nuisance parameters included in the fit are:

$$\theta = \{N_{\gamma j}, \varepsilon_{\gamma j,2}^{\text{id}}, \varepsilon_{\gamma j,2}^{\text{iso}}, N_{j\gamma}, \varepsilon_{j\gamma,1}^{\text{id}}, \varepsilon_{j\gamma,1}^{\text{iso}}, N_{jj}, \varepsilon_{jj,1}^{\text{id}}, \varepsilon_{jj,1}^{\text{iso}}, \varepsilon_{jj,2}^{\text{id}}, \varepsilon_{jj,2}^{\text{iso}}, R_{jj}^{\text{id}}, R_{jj}^{\text{iso}}\}. \quad (7.11)$$

This means e.g. all jet related isolation and identification efficiencies are estimated directly from the data. The total number of nuisance parameters is 13. The addition of the target parameter $n_{\gamma\gamma,1}$ leaves two degrees of freedom for the fit to the 16 regions.

The main challenge of the background estimation is to estimate the values and uncertainties of the remaining parameters not included in θ which are fixed before the fit. This is described in the following sections including also the event fractions $f_{\text{PU},i}$ and $f_{ee,i}$ and corresponding event counts N_{PU} and N_{ee} . The fit is performed for the central values of the fixed parameters and redone for each systematic uncertainty.

7.5.2. Signal parameters

The eight values describing the $\gamma\gamma$ signal distribution over the 16 regions:

$$\vartheta_{\gamma\gamma} = \{\varepsilon_{\gamma\gamma,1}^{\text{id}}, \varepsilon_{\gamma\gamma,2}^{\text{id}}, R_{\gamma\gamma}^{\text{id}}, \varepsilon_{\gamma\gamma,1}^{\text{iso}}, \varepsilon_{\gamma\gamma,2}^{\text{iso}}, R_{\gamma\gamma}^{\text{iso}}, R_{\gamma\gamma,1}^{\text{iso-id}}, R_{\gamma\gamma,2}^{\text{iso-id}}\} \quad (7.12)$$

are estimated from the SHERPA MC signal sample for each bin of each observable. The photon identification and isolation variables are corrected in the MC based on the measurements in [103] with shifts to the variables as described in Sections 4.4 and 4.5. In addition the nominal isolation efficiencies are calculated with a pileup reweighting of $1/f_{\mu\text{-scale}} = 1/1.2$, which improves the data-MC agreement of the isolation distribution as shown in Section 5.7. The identification efficiencies are corrected based on the data-MC identification efficiency ratios measured in [103]. From these ratios event weights based on the photon identification status are calculated as described in Appendix C, which corrects not only the signal-region, but also the control-region yields.

The systematic uncertainties affecting the photon isolation and identification are discussed in detail in Sections 7.7.4 and 7.7.6.

In Fig. 7.7 the estimated isolation and identification efficiencies for the subleading photon in the different bins of p_{T,γ_2} are depicted. The identification efficiencies for the *Tight* requirement with respect to *Loose'2* are very high $\varepsilon > 97\%$, which means only a small fraction of signal is present in the control regions where e.g. the subleading photon does not pass the identification. The isolation efficiencies are lower in comparison and especially at low p_T , because of the p_T dependent isolation requirement, indicating more signal in the respective control regions. The systematic uncertainties on the individual efficiencies are typically below 1%.

Values for $R_{\gamma\gamma,2}^{\text{iso-id}}$ are depicted in Fig. 7.8 as a function of p_{T,γ_2} . For the signal this parameter does not have a large impact on the background estimation, because it is only relevant for regions which are suppressed by $(1-\varepsilon_{\gamma\gamma,2}^{\text{id}})$. It is still taken into account and the values are interesting, because of the implications for the $R_j^{\text{iso-id}}$ parameters for photon candidates from jets. For signal at low p_T the values in Fig. 7.8 are significantly below one, indicating a reduced isolation efficiency for photons failing the identification. This implies that the correlation corrections $R_j^{\text{iso-id}}$ for background candidates from jets, which usually have a wider shower shape than the signal, also can not be assumed to be one which motivates the estimation discussed in Section 7.5.4. For high p_{T,γ_2} the $R_{\gamma\gamma,2}^{\text{iso-id}}$ are increasing to

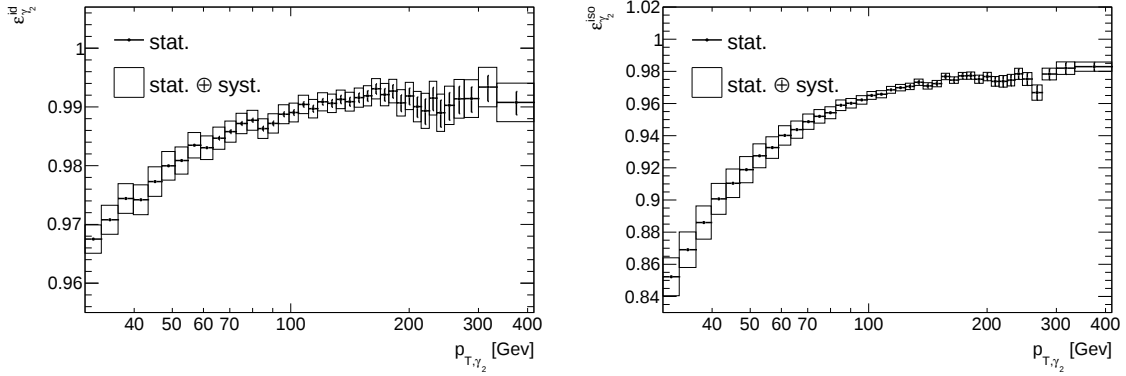


Figure 7.7.: Identification efficiency $\varepsilon_{\gamma\gamma,2}^{\text{id}}$ (left) and isolation efficiency $\varepsilon_{\gamma\gamma,2}^{\text{iso}}$ (right) as a function of p_{T,γ_2} for the subleading photon in $\gamma\gamma$ signal events in the SHERPA MC samples.

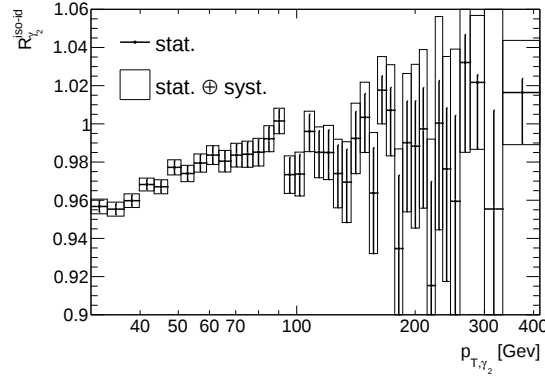


Figure 7.8.: Isolation-identification correlation correction factor $R_{\gamma\gamma,2}^{\text{iso-id}}$ as a function of p_{T,γ_2} for the subleading photon in $\gamma\gamma$ signal events in the SHERPA MC samples.

values compatible with one.

The values of $R_{\gamma\gamma}^{\text{iso}}$ and $R_{\gamma\gamma}^{\text{id}}$ are depicted as function $m_{\gamma\gamma}$ in Fig. 7.9. The values are shown as a function of $m_{\gamma\gamma}$, because low values of $m_{\gamma\gamma} < 70$ GeV correspond to low angular separations for the photons with $p_{T,\gamma_{1(2)}} > 40(30)$ GeV selected for this analysis. The correlation correction for the identification $R_{\gamma\gamma}^{\text{id}}$ is very close to one regardless of $m_{\gamma\gamma}$, which shows that the identification requirements of the two photons are independent. In contrast the correction for the isolation $R_{\gamma\gamma}^{\text{iso}}$ is around $R_{\gamma\gamma}^{\text{iso}} = 0.98$, which can be explained with pileup noise being approximately uniformly distributed over the whole event and affecting both photons similarly. In addition $R_{\gamma\gamma}^{\text{iso}}$ is decreasing to $R_{\gamma\gamma}^{\text{iso}} = 0.96$ for low $m_{\gamma\gamma}$. Despite the requirement of $\Delta R > 0.4$ between both photons ensuring non-overlapping isolation regions, this could be caused by an additional jet in the region between the photon candidates, which partially enters into both regions. This is a common topology in $\gamma\gamma + 2$ jet events, where one of the jets is accompanied by two fragmentation photons.

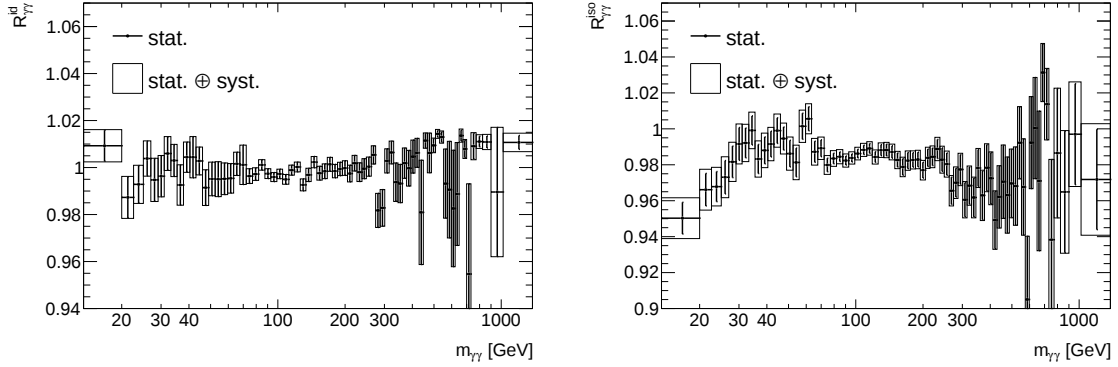


Figure 7.9.: Correlation correction factor between the leading and subleading photon for the identification $R_{\gamma\gamma}^{\text{iso}}$ (left) and the isolation $R_{\gamma\gamma}^{\text{id}}$ (right) as a function of $m_{\gamma\gamma}$ in signal SHERPA MC samples.

7.5.3. Prompt-photon isolation and identification efficiencies in γj and $j\gamma$ events

The isolation and identification efficiencies $\varepsilon_{\gamma j,1}^{\text{iso}}$, $\varepsilon_{j\gamma,2}^{\text{iso}}$, $\varepsilon_{\gamma j,1}^{\text{id}}$, $\varepsilon_{j\gamma,2}^{\text{id}}$ for the prompt photons in the γj and $j\gamma$ backgrounds are fixed to the respective values for the $\gamma\gamma$ signal. Although there are γj samples (cf. Section 7.2.3), their statistics is relatively poor, because of the background suppression of the identification and isolation selections. To avoid large statistical fluctuations in the parameters, it is beneficial to use the $\gamma\gamma$ values instead. The efficiency values derived from the γj samples are compared to the respective $\gamma\gamma$ values and the ratio as a function of all observables is compatible with one within statistical uncertainties. The impact of changing the prompt photon identification (isolation) efficiencies of the γj and $j\gamma$ processes by a conservative variation of 2(4)% around the nominal $\gamma\gamma$ values is checked. It changes the resulting target parameter $n_{\gamma\gamma,1}$ by less than 1% and is therefore negligible.

7.5.4. Isolation–identification correlation for misidentified jets

The values of the isolation–identification correlation correction parameters:

$$R_{\gamma j,2}^{\text{iso-id}}, R_{j\gamma,1}^{\text{iso-id}}, R_{jj,1}^{\text{iso-id}}, R_{jj,2}^{\text{iso-id}}, \quad (7.13)$$

for photon candidates from jets are determined based on a validation region in data and the statistically limited information of the γj MC sample. The parameter for the subleading candidate in γj events $R_{\gamma j,2}$ is studied as a function of p_{T,γ_2} . The values for bins of other observables and processes, e.g. the leading candidate in $j\gamma$ or either candidate in jj , are calculated evaluating $R_{\gamma j,2}(p_{T,\gamma_2})$ at the average p_T of the respective candidate in the bin of the observable.

The values of $R_{\gamma j,2}^{\text{iso-id}}$ in the MC sample are depicted in Fig. 7.10 (left) as a function of p_{T,γ_2} . No significant trends are observed and a constant function is fit to the values to extract an average of $R_{\gamma j,2}^{\text{iso-id,MC}} = 0.990 \pm 0.025$.

The data validation region is defined based on the tracking isolation $p_{T,\gamma_2}^{\text{cone20}}$ (cf. Section 4.5) of the

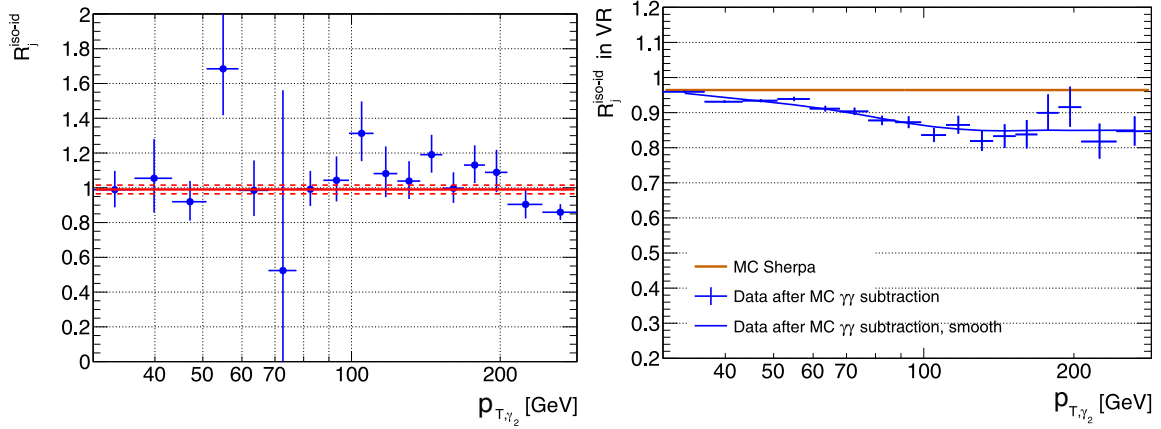


Figure 7.10.: Value of $R_{\gamma j,2}^{\text{iso-id}}$ in simulated MC samples for γj events as a function of p_{T,γ_2} (left). On the right the validation region values of $R_{\gamma j,2}^{\text{iso-id}}$ for data after the signal subtraction (blue) are compared to the result of a constant fit (orange) to the validation region MC values.

subleading photon candidate. A requirement of:

$$p_{T,\gamma_2}^{\text{cone20}} > 0.02 \cdot p_{T,\gamma_2} + 1.5 \text{ GeV} \quad (7.14)$$

is used to create a region with a large fraction of γj events. The validation-region values of $R_{\gamma j,2}^{\text{iso-id}}$ in the background MC sample are used to check if the tracking isolation cut is biasing them. Similarly as before a constant function as a function of p_{T,γ_2} is fitted and yields $R_{\gamma j,2}^{\text{iso-id,MC-VR}} = 0.96 \pm 0.04$, which is roughly compatible³ with $R_{\gamma j,2}^{\text{iso-id,MC}}$.

The data events in the validation region are corrected for $\gamma\gamma$ signal contamination based on the expectation from the SHERPA signal samples. The values of $R_{\gamma j,2}^{\text{iso-id,data-VR}}$ are compared to $R_{\gamma j,2}^{\text{iso-id,MC-VR}}$ in Fig. 7.10 (right). The data values are compatible to the MC value at low p_{T,γ_2} , but show a downward trend, which reaches a plateau of $R_{\gamma j,2}^{\text{iso-id,data-VR}} \approx 0.85$ around $p_{T,\gamma_2} \approx 100 \text{ GeV}$.

The data values depend on the signal subtraction and the MC value can not be estimated reliably as a function of p_{T,γ_2} , because of poor statistics. The mean between the p_T dependent data values and the fixed MC value is used to describe the nominal $R_{\gamma j,2}^{\text{VR}}(p_{T,\gamma_2})$ values and a p_{T,γ_2} dependent uncertainty is assigned, such that the fixed MC value as well as the data validation region values are covered. At last, the $R_{\gamma j,2}^{\text{VR}}(p_{T,\gamma_2})$ values are extrapolated from the validation region based on the ratio of the MC values $R_{\gamma j,2}^{\text{iso-id,MC}}/R_{\gamma j,2}^{\text{iso-id,MC-VR}} = 0.99/0.96 = 1.03 \pm 0.03$ and the statistical uncertainty on the ratio is assigned as an additional flat uncertainty on $R_{\gamma j,2}(p_{T,\gamma_2})$.

The values of $R_{\gamma j,2}(p_{T,\gamma_2})$ and their MC statistical and total uncertainty are depicted in Fig. 7.11. These uncertainties constitute one of the main systematic uncertainties on the final results, particularly important in regions with low signal purity, and will be shown in Section 7.7.3.

³The comparison is not straight forward, because the validation region is a subset of the full sample, which means that the statistical uncertainties are correlated.

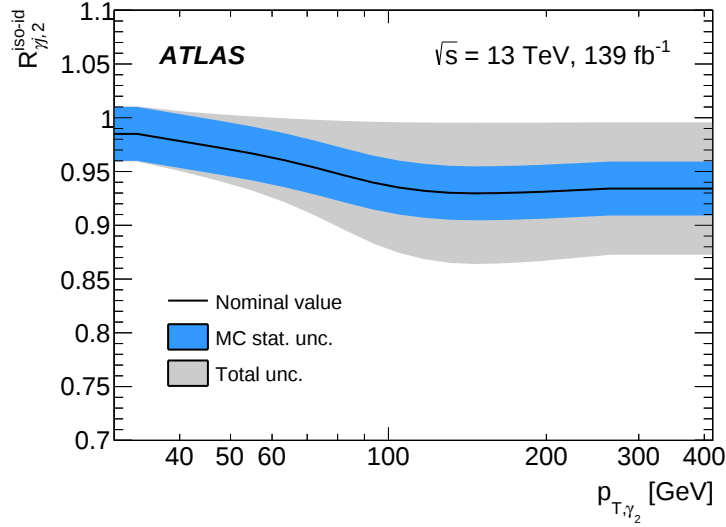


Figure 7.11.: Correction factor $R_{\gamma j, 2}^{\text{iso-id}}$ for the isolation–identification correlation, for jets misidentified as photons [38]. The nominal value (black) as well as the MC statistical (blue) and total uncertainty (grey) are depicted.

7.5.5. Correlation parameters in γj and $j\gamma$ events

The isolation-correlation correction and identification-correlation correction factors for γj and $j\gamma$ events:

$$R_{\gamma j}^{\text{iso}}, R_{j\gamma}^{\text{iso}}, R_{yy}^{\text{id}}, R_{jj}^{\text{id}} \quad (7.15)$$

are set based on the comparison to the corresponding jj and $\gamma\gamma$ values. Conservative uncertainties are assigned, which show only a small impact on the fit result compared to other systematic variations.

As shown for the signal in Section 7.5.2 the $R_{\gamma\gamma}^{\text{iso}}$ parameter describing the correlation between the isolation efficiencies of both candidates is slightly below one $R_{\gamma\gamma}^{\text{iso}} \approx 0.98$. The parameters for R_{jj}^{iso} parameter for the jj background is a free parameter determined in the fit and the results are in the range $0.9 < R_{jj}^{\text{iso}} < 1$. The values of $R_{\gamma j(j\gamma)}^{\text{iso}}$ for the γj ($j\gamma$) background should be somewhere in the region between the jj and $\gamma\gamma$ values. A value of $R_{\gamma j}^{\text{iso}} = R_{j\gamma}^{\text{iso}} = 0.95 \pm 0.05$ is chosen with a systematic uncertainty covering values between 0.9 and 1. The impact of this systematic uncertainty will be shown in Section 7.7.3 and is subleading compared to other systematic uncertainties.

The parametrisation of $f_{j\gamma, i}$ is slightly altered from what is shown in section Section 7.5.1 such that $R_{j\gamma}^{\text{iso}}$ applies to the isolation efficiency of the leading candidate. This means for both, $j\gamma$ and γj , the R^{iso} parameter is changing the isolation efficiency of the mis-identified jet for the case that the photon fails the isolation cut.

Similar arguments as for R^{iso} are used for fixing $R_{\gamma j}^{\text{id}}$ and $R_{j\gamma}^{\text{id}}$. The values of R_{yy}^{id} and R_{jj}^{id} fluctuate around 1 with values usually in the region of 1 ± 0.02 . Varying $R_{\gamma j}^{\text{id}}$ and $R_{j\gamma}^{\text{id}}$ to 0.98 or 1.02 changes the result for $n_{\gamma\gamma, 1}$ by less than 0.4% which is negligible compared to other uncertainties. The value of $R_{\gamma j}^{\text{id}}$ and $R_{j\gamma}^{\text{id}}$ are therefore fixed to one in the fit.

7.5.6. Electron background

As explained in Chapter 4 the signatures of photons and electrons in the EM calorimeter are very similar and the main disambiguation is based on tracks in the inner detector. This means that e.g. inefficiencies in the tracking can cause electrons to be mis-identified as photons.

The number of events where the photon candidate is a mis-identified electron are estimated based on MC samples (cf. Section 7.2.2). The samples include the Drell-Yang $Z/\gamma^* \rightarrow ee$ process and also the small contributions from $W \rightarrow e\nu$ are contained.

The expected number of electron events in the signal region is around 2.6% of the number of all data events in the signal region. This fraction rises up to around 15% in the $m_{\gamma\gamma}$ bin containing m_Z . Several corrections and systematic uncertainties are considered to validate the MC based approach:

- A 5% normalisation uncertainty is assigned,
- A reweighting based on the measurement in Ref. [141] is applied to correct the $p_{T,Z}$ spectrum and a systematic variation switching off the reweighting is introduced,
- A data-driven correction factor to the $e \rightarrow \gamma$ mis-identification rate is applied, which was provided to the analysis. It is measured in $Z \rightarrow ee$ events comparing the size of the mass peak in reconstructed ee and $e\gamma$ events. A conservative uncertainty is assigned by comparing the result derived with the correction factor to the result derived without it.

The impact of these uncertainties is only relevant for $m_{\gamma\gamma} \sim m_Z$ and will be shown in Section 7.7.3.

7.5.7. Pileup background

The last process which needs to be considered before estimating the $\gamma\gamma$ signal yields with the fit is the pileup background, which consists of two γj events originating from different proton–proton interactions of the same bunch crossing. A candidate for such an event is displayed in Fig. 7.12. The number of pileup background events is estimated in a data-driven approach and the distribution as a function of the different observables is determined based on randomly matching two MC γj events.

It is challenging to extrapolate the trajectory of unconverted photons without a track in the inner detector to the beam axis, although a rough estimate can be calculated from the tilt and position of the calorimeter cluster. The estimation of the amount of pileup background relies on events with two converted photons with two tracks with hits in the silicon detector instead. For these photons a precise extrapolation to the beam axis is possible using the position of the calorimeter cluster and of the conversion vertex in the inner detector. In addition the photon are required to be in the central $|\eta| < 1.37$ region of the detector, because the extrapolated z_γ position is determined less precisely for trajectories with a small angle θ to the beam axis. The estimated distance between the z -positions of the vertices associated to the photons $|\Delta z| = |z_{\gamma_1} - z_{\gamma_2}|$ is used to discriminate between photon pairs from the same and different interactions. The variable $\Delta\phi_{\gamma\gamma}$ is another property of the photon pair which can be used to create regions with lower and higher fractions of pileup background. For photons from different vertices $\Delta\phi_{\gamma\gamma}$ should be distributed uniformly except for a suppression at low $\Delta\phi_{\gamma\gamma}$ caused by the requirement of $\Delta R_{\gamma\gamma} > 0.4$. For photons from the same interaction configurations with both photons being approximately back-to-back are dominant.

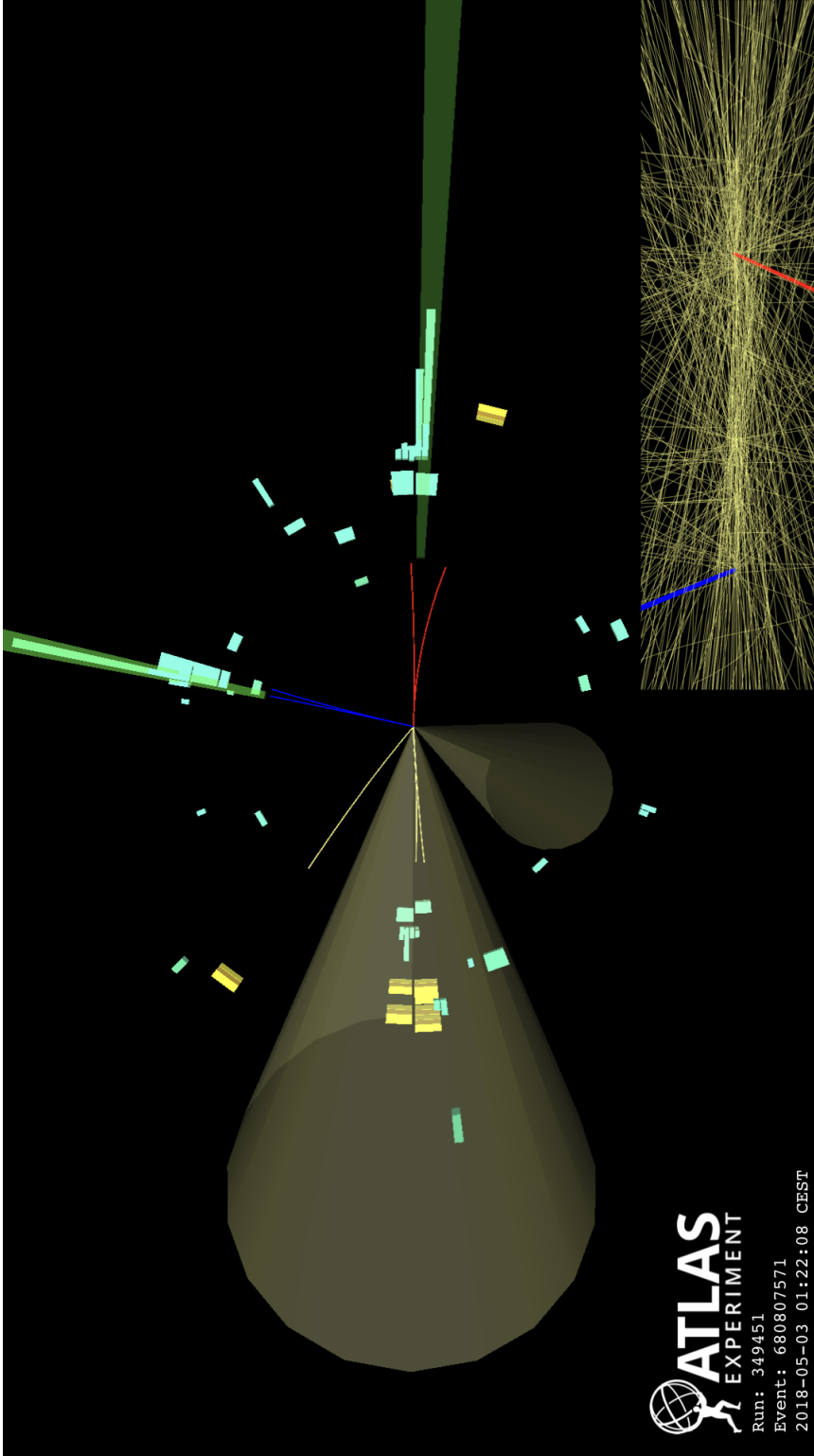


Figure 7.12.: Event display of a pileup-background candidate. The event is passing the signal region selection of the analysis. The green cuboids represent the photon candidates of the event and the yellow cones correspond to jets reconstructed with the anti- k_t algorithm with $R = 0.4$. Both photons are matched to pairs of tracks with hits in the silicon tracker (blue and red lines) which are compatible with a photon conversion occurring in the inner detector material. Both photons are located in the barrel of the EM calorimeter with $\eta_1 = 0.21$ and $\eta_2 = -0.44$. A projection into a plane containing the beam axis is shown in the small inset on the bottom right. The extrapolation of the conversion tracks to the beam axis yields a distance of $\Delta z = 92$ mm between the primary vertices [38].

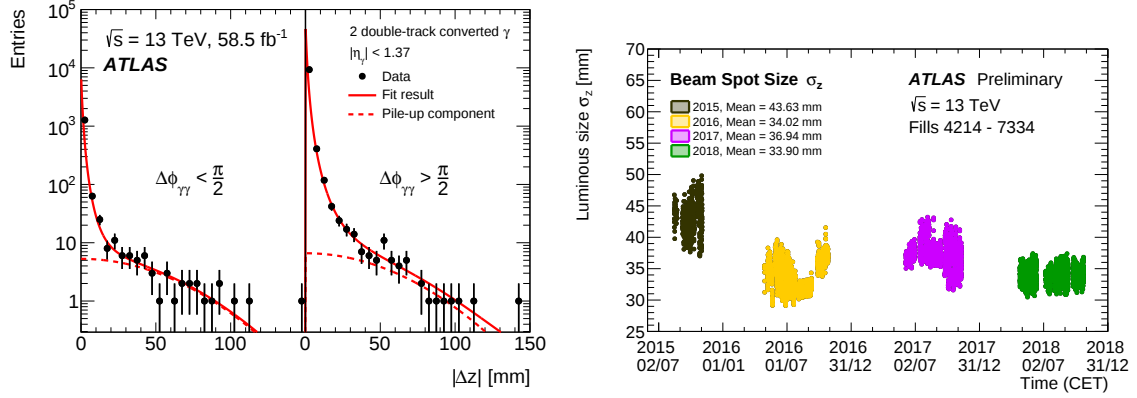


Figure 7.13.: The distribution of the distance between the extrapolated photon trajectories on the beam axis $|\Delta z|$ (left) for events with two converted photons with silicon tracks and in the central $|\eta_\gamma| < 1.37$ region for two $\Delta\phi_{\gamma\gamma}$ categories [38]. Standard deviation of the distribution of primary interaction vertices along the beam axis (right) during Run-2 of the LHC [157].

The $|\Delta z|$ distribution in two regions of $\Delta\phi_{\gamma\gamma}$ is depicted in Fig. 7.13 (left). A two-component fit is used to determine the number of pileup background events. The $|\Delta z|$ distribution for photons from the same interaction is strongly peaked at zero and can be described by a power-law function. The pileup background distribution is given by a Gaussian with a width of $\sigma_{|\Delta z|} = \sqrt{2} \times \sigma_z$ with σ_z being approximately the beam-spot size in the z -direction, which is the standard deviation of the z -position of interaction vertices. The value of σ_z is determined here directly from the z_γ distribution, but is very similar to the values reported in [157] and depicted in Fig. 7.13 (right). For the pileup background estimation only the 2018 dataset is used, because it has a high number of interactions per bunch crossing (and therefore more pileup background) and a stable value of σ_z . The number of pileup events estimated by the simultaneous fit to both $\Delta\phi_{\gamma\gamma}$ regions is then extrapolated from the events in 2018 to the full dataset based on the luminosity and pileup conditions of the other years. Furthermore the efficiencies of the η - and conversion-type selections are corrected based on the expectations from MC simulations.

The photon-pair events of the pileup background described by the Gaussian distribution in $|\Delta z|$ can also contain background events where one of the photon is a mis-identified jet. These background events are contained in the γj , $j\gamma$ and jj component of the fit model already. To estimate the amount of genuine $\gamma\gamma$ events from pileup the background estimation fit is performed for the events with $|\Delta z| > 48$ mm in the tails of the distribution depicted in Fig. 7.13 (left).

The resulting fraction of $\gamma\gamma$ pileup events in the signal region is $(0.6 \pm 0.4)\%$. The uncertainty is dominated by the limited statistics for the background estimation fit. Due to the small size of the background the influence on the result and its uncertainty are mostly negligible except for high $|\cos\theta^*|^{(\text{CS})}$ where a contribution of up to 6% of all data events in the signal region is estimated.

The photon-pair measurement is the second analysis by ATLAS after the $Z\gamma$ measurement [131] to estimate this background, where a photon is coming from a different proton–proton interaction. This background is of special relevance for photons, because of the limited vertex association capabilities

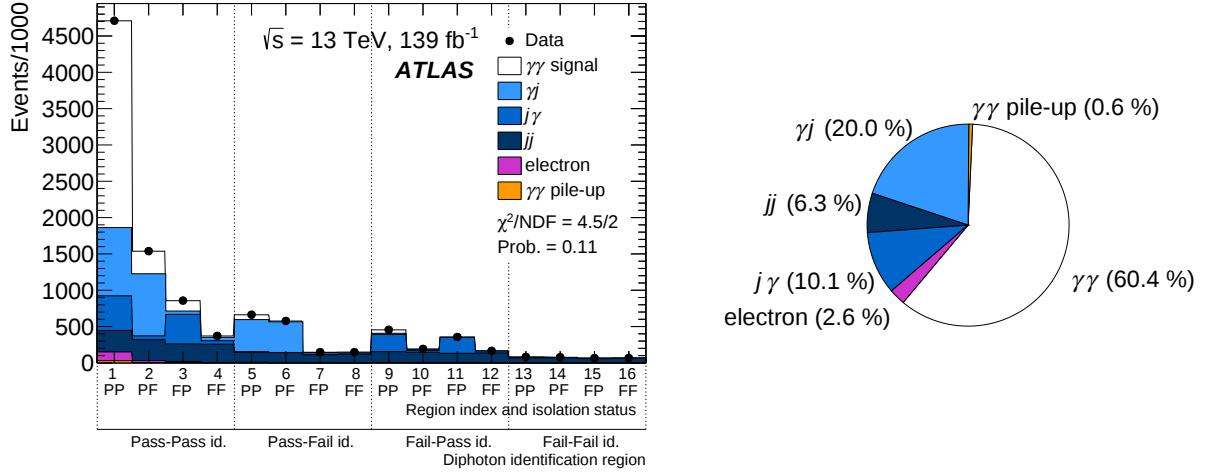


Figure 7.14.: On the left the event yields of the full data sample in the 16 regions, numbered as described in Table 7.1, are compared to the signal and background yields resulting from the fit [38]. On the right the signal region ($i = 1$) fractions of the signal and the backgrounds are visualized.

for unconverted photons and will gain further importance for future LHC runs with higher pileup conditions.

7.5.8. Results

With all the inputs in place the fit can be performed to estimate the signal $\gamma\gamma$ contribution in the signal region $n_{\gamma\gamma,1}$ alongside with the γj , $j\gamma$ and jj contributions as discussed in Section 7.5.1.

The fit result for the inclusive⁴ dataset is compared in Fig. 7.14 to the data yields in the signal region and the different control regions. The signal purity in the signal region is $(60.4 \pm 3.0)\%$. Most of the signal is concentrated in the signal region. The regions 5-6 where the leading photon passes the identification and isolation cuts, but the subleading photon fails the identification are dominated by γj background. Similarly regions 9 and 11 have a large contribution of $j\gamma$ background. The region with failed isolation or identification cuts for both photons are enriched in jj background. The contributions of ee and PU are only visible in the signal region, because they have similar isolation and identification efficiencies as the $\gamma\gamma$ signal.

The χ^2 -value of the fit of $\chi^2 = 4.5$ is calculated taking into account the statistical and systematic uncertainties⁵ and corresponds to a p -value of $p = 0.11$ for the two degrees of freedom of the fit. This indicates that the model is able to describe the data properly.

The background estimation is performed independently for each bin of each observable. The resulting differential signal and background fractions in the signal region as a function of the different

⁴Inclusive refers here to the full dataset not binned in any observable.

⁵The χ^2 value is calculated based on the inverse of the covariance matrix Σ^{-1} of the total uncertainty: $\chi^2 = \sum_{ij} (n_i^{\text{obs}} - n_i^{\text{exp}})(\Sigma^{-1})_{ij}(n_j^{\text{obs}} - n_j^{\text{exp}})$

Table 7.2.: Overview of the event selection at the detector level and at the particle level, i.e. definition of the fiducial phase space.

Selection	Detector level	Particle level
Photon kinematics	$p_{T,\gamma_{1(2)}} > 40 \text{ (30) GeV}, \quad \eta_\gamma < 2.37$ excluding $1.37 < \eta_\gamma < 1.52$	
Photon identification	tight	stable, not from hadron decay
Photon isolation	$E_T^{\text{cone20}} < 0.05 \cdot p_{T,\gamma}$	$E_{T,\text{PL}}^{\text{cone20}} < 0.09 \cdot p_{T,\gamma}$
Diphoton topology	$N_\gamma \geq 2, \quad \Delta R_{\gamma\gamma} > 0.4$	

observables are depicted in Fig. 7.15. The signal purity ranges from 30% at low $m_{\gamma\gamma}$ to 80% at high p_{T,γ_2} . The purities are lower in regions with low p_T candidates. Furthermore regions with low $\Delta\phi_{\gamma\gamma}$ of the photon candidates like high ϕ_η^* or low $m_{\gamma\gamma}$ show a large fraction of $j\gamma$ events, which correspond to events with a low p_T photon radiated in the vicinity of a high p_T jet. In these regions the usually subleading $j\gamma$ contribution rises up to the level of the γj contribution. The ee contribution is mainly important around $m_{\gamma\gamma} \sim m_Z$, where it is around 15%. The PU contribution is mostly negligible except for high $|\cos\theta^*|^{(\text{CS})}$, where it increases to more than 5%. These events are usually characterized by a high $\Delta\eta_{\gamma\gamma}$ as discussed in Section 7.4.

7.6. Unfolding

The number of signal region $\gamma\gamma$ events $n_{\gamma\gamma,1}$ in each bin of the observables resulting from the background estimation is used to calculate particle-level (PL) differential cross sections. This procedure is referred to as unfolding and involves the correction of detector effects e.g. caused by the limited detector resolution and efficiencies.

To avoid theory based extrapolations the cross section is measured in a PL fiducial phase space, which is closely matching the detector level (DL) requirements described in Section 7.3. If e.g. the measurement would be unfolded to a phase space involving photons with a lower p_T as included in the DL selection, the unfolding would depend on predictions for the p_T spectrum of the photons.

The DL and corresponding PL selections for the analysis are summarized in Table 7.2. The PL requirements on the photon kinematics and diphoton topology are exactly matching the DL ones.

The photons are required to be prompt, which means not from a hadron decay on PL. This requirement is fulfilled for the DL yields in the signal region after the background estimation. There are however events passing this PL selection which are rejected by the corresponding DL photon identification requirements which have a limited signal efficiency.

The photon isolation requirement needs to be included also on PL. On the one hand higher-order calculations of photon production require an isolation cut meaning that calculations are more easily compared to a measurement in a fiducial phase space also involving an isolation cut. On the other hand the events passing the DL selections are not sensitive to highly non-isolated photons, because of the photon isolation and identification requirements. The definition of the PL isolation variable $E_{T,\text{PL}}^{\text{cone20}}$ and the choice of the PL cut will be discussed in detail in Section 7.6.5.

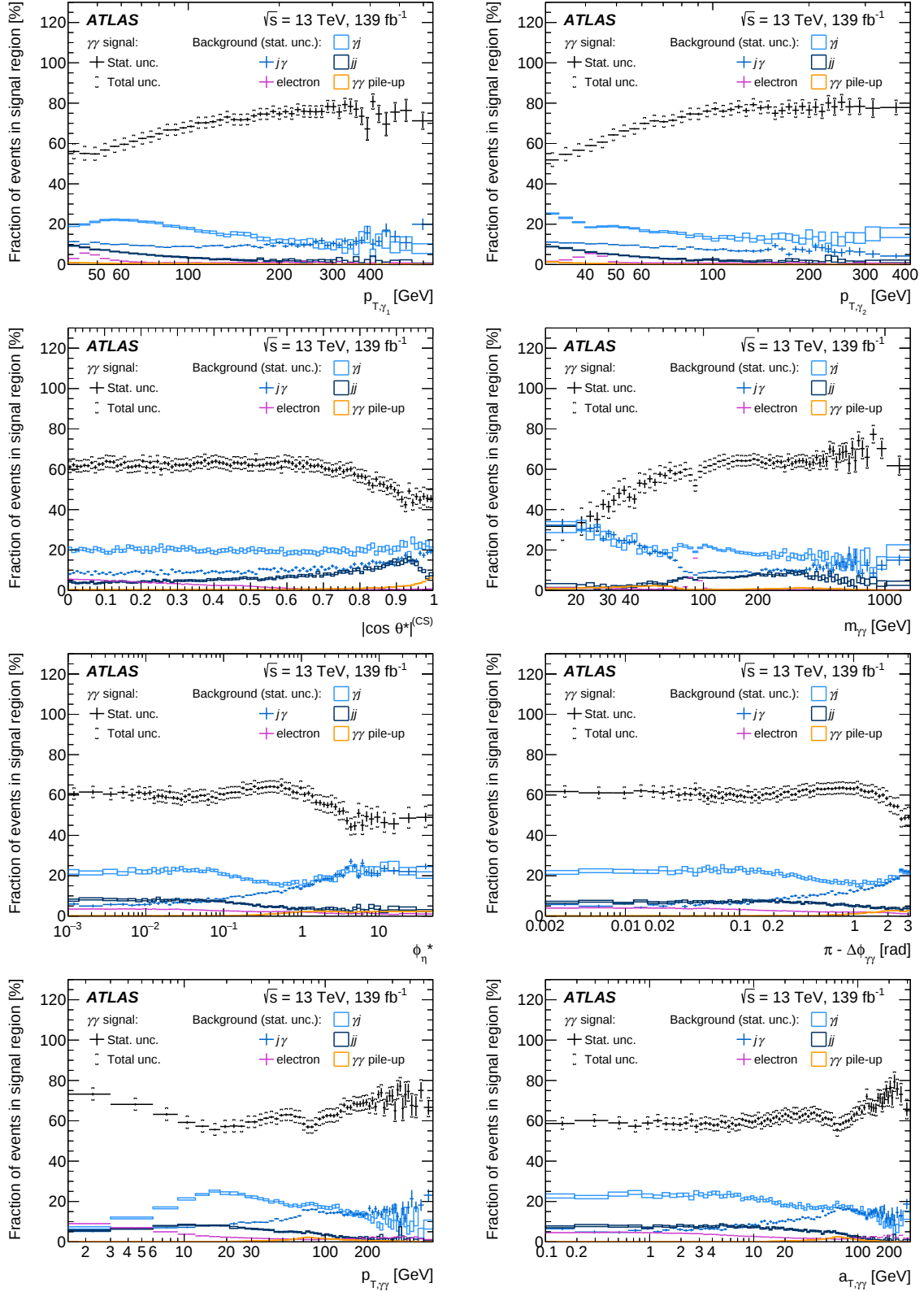


Figure 7.15.: Sample decomposition as a function of p_{T,γ_1} , p_{T,γ_2} , $|\cos \theta^*|^{(CS)}$, $m_{\gamma\gamma}$, ϕ_η^* , $\pi - \Delta\phi_{\gamma\gamma}$, $p_{T,\gamma\gamma}$ and $a_{T,\gamma\gamma}$. For the $\gamma\gamma$ signal fraction, the total uncertainty is shown, while for the background fractions only the data and Monte Carlo statistical uncertainty component is shown [38].

The PL cross section $\left(\frac{d\sigma_{\gamma\gamma}}{dx}\right)_{j_{\text{PL}}}$ in the j_{PL} -th PL bin of an observable x given the number of signal events $n_{i_{\text{DL}}}$ in the $i_{\text{DL}} \in \{1, \dots, n_{\text{det.}}\}$ DL bins of the observable are calculated as follows:

$$\left(\frac{d\sigma_{\gamma\gamma}}{dx}\right)_{j_{\text{PL}}} = \frac{1}{(\Delta x)_{j_{\text{PL}}}} \epsilon_{j_{\text{PL}}}^{-1} \sum_{i_{\text{DL}}=1}^{n_{\text{det.}}} p(j_{\text{PL}}|i_{\text{DL}}) n_{i_{\text{DL}}} f_{i_{\text{DL}}}, \quad (7.16)$$

with the fiducial correction $f_{i_{\text{DL}}}$, the unfolding matrix $p(j_{\text{PL}}|i_{\text{DL}})$, the efficiency correction $\epsilon_{j_{\text{PL}}}^{-1}$, the PL bin width $(\Delta x)_{j_{\text{PL}}}$ and the integrated luminosity $\mathcal{L}$ of the dataset. For this measurement the PL binning is the same as the DL one.

Inputs to the unfolding are determined based on the SHERPA signal MC sample and systematic uncertainties addressing imperfections in the detector simulation and possible biases from the theory modelling of the signal are taken into account.

The unfolding can be factorised into three steps:

1. Fiducial correction,
2. Resolution correction,
3. Efficiency correction,

which are discussed in the following sections.

7.6.1. Fiducial correction

At first the number of events $n_{i_{\text{DL}}}$ is corrected for *unmatched* events, which are also referred to as *non-fiducial* events. Unmatched events are passing the DL requirements, but are not in the PL phase space. This can e.g. happen if the DL p_{T} is shifted above the threshold value due to detector resolution effects, although the PL p_{T} value is below. The corresponding fiducial correction $f_{i_{\text{DL}}}$ is calculated as follows:

$$f_{i_{\text{DL}}} = \frac{N_{i_{\text{DL}}}^{\text{DL} \cap \text{PL}}}{N_{i_{\text{DL}}}^{\text{DL}}} \quad (7.17)$$

with $N_{i_{\text{DL}}}^{\text{DL} \cap \text{PL}}$ being the number of events passing the PL and DL requirements with respect to all events passing the DL requirements $N_{i_{\text{DL}}}^{\text{DL}}$ in the MC signal sample in the i_{DL} bin.

The fiducial correction as a function of the two observables p_{T,γ_2} and $m_{\gamma\gamma}$ is depicted in Fig. 7.16 for different steps of the PL selection with respect to all events passing the DL selection. Usually the correction factors are above $f > 0.9$ and the main corrections are caused by the PL p_{T} and isolation cuts.

The influence of the p_{T} cuts is large in regions enriched in photons close to the p_{T} thresholds of the fiducial phase space, e.g. $p_{\text{T},\gamma_2} \sim 30$ GeV or $m_{\gamma\gamma} \sim 70$ GeV. The region around $m_{\gamma\gamma} \sim 70$ GeV, which is the sum of the p_{T} thresholds, marks the transition of a region dominated by approximately back-to-back configurations for $m_{\gamma\gamma} > 70$ GeV to a boosted region with small angular separations for $m_{\gamma\gamma} < 70$ GeV.

The contributions of the PL isolation cuts to the fraction of unmatched events are also the largest at low p_{T} . The isolation cuts are chosen relative to the candidate p_{T} and are therefore at only a

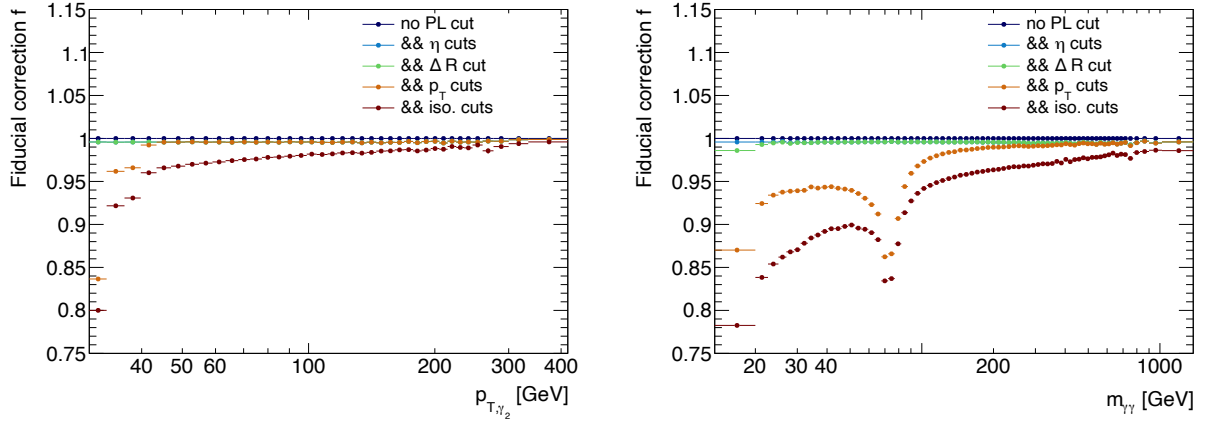


Figure 7.16.: The fiducial correction is shown as a function of p_{T,γ_2} and $m_{\gamma\gamma}$. The different colours indicate different steps in the PL selection. The lowest points correspond to the fiducial correction for the full PL selection. The denominator for all points is the number of all MC photon-pair events which pass the DL selection. Plots for all observables are shown in Fig. D.1.

few GeV in this region. Especially due to the high pileup noise the detector resolution for such low energy deposits in the calorimeter is limited and it occurs that the DL isolation requirements are passed, although the PL ones are failed. The fiducial correction depends on the fraction of events in the MC samples, which are slightly non-isolated on PL, such that they occasionally still pass the DL requirement. The sensitivity to the modelling of the PL isolation distribution is estimated based on a comparison between SHERPA and PYTHIA8 as described in Appendix A. The corresponding uncertainties are at the percent level (cf. Section 7.7.4).

7.6.2. Resolution correction

The resolution correction is applied after the fiducial correction, e.g. to yields which pass both, the PL and DL requirements. Due to detector resolution effects an event in a PL observable bin j_{PL} can migrate to e.g. a different bin $i_{\text{DL}} \neq j_{\text{PL}}$ on DL. The conditional probability for the migrations are summarized in the response matrix $r(i_{\text{DL}}|j_{\text{PL}})$:

$$\sum_{j_{\text{PL}}=1}^{n_{\text{bins}}} r(i_{\text{DL}}|j_{\text{PL}}) n_{j_{\text{PL}}} = n_{i_{\text{DL}}}. \quad (7.18)$$

They are estimated from the MC signal samples and relatively symmetric as depicted in Fig. 7.17. The response matrices have large fractions in the diagonal with $r(i_{\text{DL}} = j_{\text{PL}}|j_{\text{PL}}) > 0.75$ for most bins (cf. Fig. 7.18), which is a consequence of choosing the bin sizes to be a larger than four times the detector resolution. This choice limits the influence of the resolution corrections.

The main systematic uncertainties visibly changing the response matrices are related to the photon-energy scale (cf. Section 7.7.7).

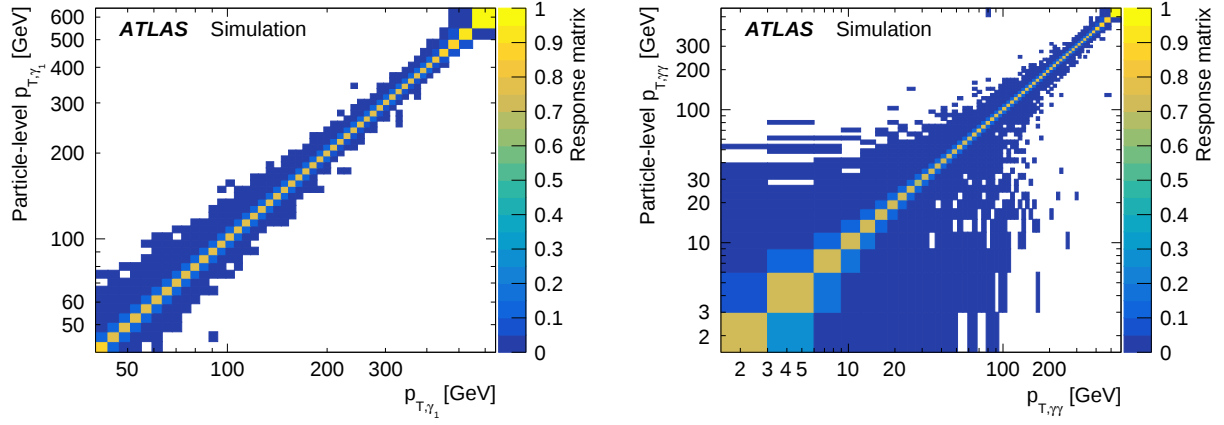


Figure 7.17.: Response matrices for p_{T,γ_1} and $p_{T,\gamma\gamma}$ containing the conditional probability for a event in a certain particle-level bin to migrate to the different detector-level bins. Plots for all observables are shown in Fig. D.2.

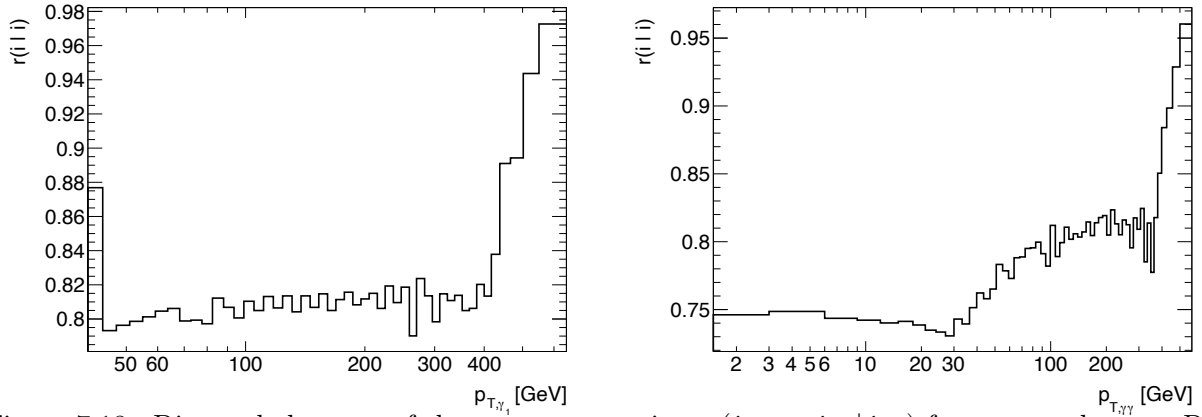


Figure 7.18.: Diagonal elements of the response matrices $r(i_{DL} = j_{PL} | j_{PL})$ for p_{T,γ_1} and $p_{T,\gamma\gamma}$. Plots for all observables are shown in Fig. D.3.

The goal of the unfolding is to calculate the unfolding matrix $p(j_{\text{PL}}|i_{\text{DL}})$ which inverts the response matrix $r(i_{\text{DL}}|j_{\text{PL}})$. The elements give the probabilities for an event in the i_{DL} bin to be originating from a certain PL bin j_{PL} and can be calculated using Bayes theorem:

$$p(j_{\text{PL}}|i_{\text{DL}}) = \frac{r(i_{\text{DL}}|j_{\text{PL}})p(j_{\text{PL}})}{p(i_{\text{DL}})} = \frac{r(i_{\text{DL}}|j_{\text{PL}})p(j_{\text{PL}})}{\sum_{k_{\text{PL}}} r(i_{\text{DL}}|k_{\text{PL}})p(k_{\text{PL}})}, \quad (7.19)$$

with the PL and DL distributions $p(j_{\text{PL}})$ and $p(i_{\text{DL}})$. This shows that the migrations depend on the PL spectra. The Bayesian unfolding [158, 159] used for this measurement is based on an iterative approach to reduce the sensitivity to the PL MC spectra and to regularize the unfolding matrix.

The first iteration of the unfolding matrix $p_0(j_{\text{PL}}|i_{\text{DL}})$ is given by Eq. (7.19) and purely based on the quantities from signal MC also for $p(j_{\text{PL}})$. For the further iterations the measured data is unfolded with the unfolding matrix of the previous iteration:

$$p_n(j_{\text{PL}}) = \sum_{i_{\text{DL}}}^{n_{\text{bins}}} p_{n-1}(j_{\text{PL}}|i_{\text{DL}}) \frac{n_{i_{\text{DL}}}^{\text{data}}}{\sum_{k_{\text{DL}}}^{n_{\text{bins}}} n_{k_{\text{DL}}}^{\text{data}}}$$

and used instead of the signal MC $p(j_{\text{PL}})$ in Eq. (7.19). A number of $n = 3$ iterations is used for this analysis which sufficiently reduces the uncertainties related to the bias from the MC prior $p_0(j_{\text{PL}}|i_{\text{DL}})$ which are estimated in Section 7.7.8 and are below 0.2% in all observable bins except for low $p_{\text{T},\gamma\gamma}$ where they reach 1%.

7.6.3. Efficiency correction

At last the efficiency correction is applied correcting for events which are in the PL phase space, but do not pass the DL selections. The efficiency corrections for the j_{PL} PL bin is calculated as follows:

$$\varepsilon_{j_{\text{PL}}}^{-1} = \frac{N_{j_{\text{PL}}}^{\text{PL}}}{N_{j_{\text{PL}}}^{\text{PL} \cap \text{DL}}},$$

with the number of events in MC in the j_{PL} PL bin passing the PL selection $N_{j_{\text{PL}}}^{\text{PL}}$ and the events passing both the PL and DL selection $N_{j_{\text{PL}}}^{\text{PL} \cap \text{DL}}$.

The efficiencies ε for subsequent requirements of the DL selection are depicted in Fig. 7.19 for the observables p_{T,γ_2} and $m_{\gamma\gamma}$.

The photon identification cuts remove around 70 to 80% of the PL photon-pair events, which aligns approximately with the expectations from squaring the efficiencies in Fig. 4.4 showing results from the central measurements for identification efficiencies of single photons. The related uncertainties will be discussed in Section 7.7.6.

The DL p_{T} cuts are important for events enriched in photons close to the p_{T} thresholds, similar as was the case for the fiducial correction in Fig. 7.16. The efficiency correction of the DL p_{T} cuts partially cancels with the fiducial correction of the PL p_{T} cuts, because of the symmetric detector response.

The photon DL isolation cuts further reduce the efficiencies, especially at low p_{T} where the requirement is most stringent. This relatively large reduction of the efficiency is expected even

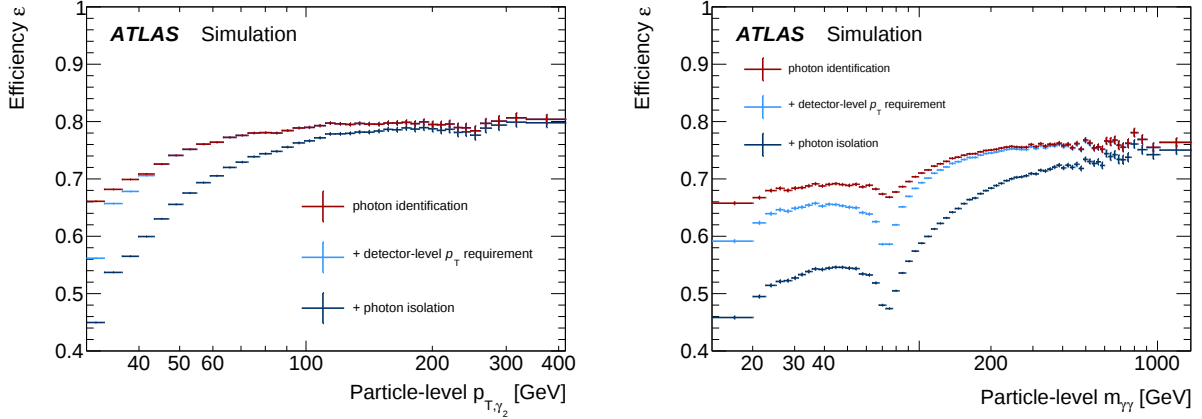


Figure 7.19.: Detector efficiency for different steps of the detector-level selection for events passing all particle-level cuts for p_{T,γ_2} and $m_{\gamma\gamma}$ [38]. Plots for all observables are shown in Fig. D.4.

though the photons are required to pass the PL isolation cuts, because of the limited resolution of the calorimetric isolation driven by pileup noise. The uncertainties related to the photon isolation efficiency are one of the most dominant sources of uncertainty and will be discussed in Section 7.7.4.

7.6.4. Overall corrections

The corrections associated to the different steps of the unfolding with their respective systematic uncertainties are depicted in Fig. 7.20 for p_{T,γ_2} and $m_{\gamma\gamma}$. The unfolding is mainly driven by the detector-efficiency correction and the dominant systematic uncertainties are entering through them. The fiducial correction is relatively small in comparison, but has significant impact e.g. at low p_{T,γ_1} , where it partially cancels with the detector-efficiency correction. The impact of the resolution correction is usually less than 4% in most bins. The only exception is the region with low $p_{T,\gamma\gamma}$, where it can reach 10%.

7.6.5. Particle-level isolation requirement

The PL isolation cut is optimized to reflect the DL isolation cut as close as possible. The first step to achieve this is defining a PL isolation variable $E_{T,PL}^{cone20}$ closely matching the DL one. It is defined as the transverse component of the summed momenta of all stable non-pileup particles excluding muons and neutrinos in a $\Delta R < 0.2$ cone around the photon.

Similar to the DL definition in Section 4.5 the PL isolation is corrected for the ambient energy density. Pileup particles are excluded from the PL isolation definition, which means the PL ambient energy subtraction is only targeting the contribution of the soft homogeneous emission of additional particles from the so-called underlying event of the primary interaction. On DL this contribution is included as a small part of the pileup subtraction. The PL subtraction method is equivalent to the DL one, but uses the momenta of stable non-pileup particles excluding muons and neutrinos for the calculation of the central- and forward energy densities instead of the momenta of topological clusters as inputs.

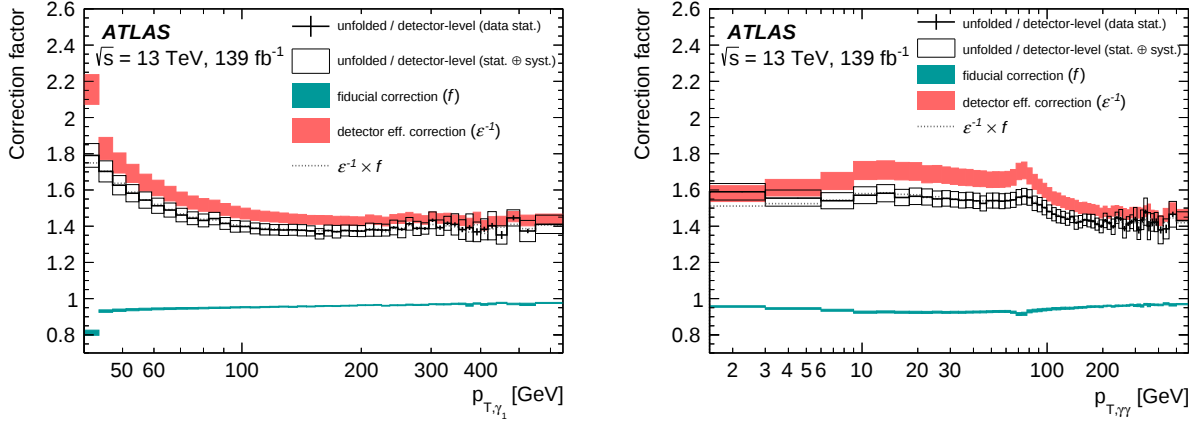


Figure 7.20.: Different components of the unfolding procedure are depicted for p_{T,γ_1} and $p_{T,\gamma\gamma}$. The green area shows the fiducial correction f and the red area the detector-efficiency correction ε^{-1} . The filled areas correspond to the systematic uncertainties of the respective correction. The black line is the ratio of the unfolded result and the detector-level signal yields (the overall unfolding correction). The product $\varepsilon^{-1} \times f$, which corresponds to ignoring any migrations in the unfolding procedure, is depicted with a dashed line. Comparing the dashed line and the black line shows the impact of the resolution corrections [38]. Plots for all observables are shown in Fig. D.5.

Similar to the DL isolation cut the PL isolation cut is performed relative to the photon transverse momentum. The PL isolation threshold:

$$E_{T,PL,\gamma_{1(2)}}^{\text{cone20}} < E_{T,PL,\min}^{\text{cone20}} + \xi \cdot p_{T,\gamma_{1(2)}}, \quad (7.20)$$

is optimized with respect to the two parameters: The relative isolation fraction ξ and the isolation threshold $E_{T,PL,\min}^{\text{cone20}}$.

The mean of the relative DL isolation $E_T^{\text{cone20}}/p_{T,\gamma}$ is calculated in bins of the relative PL isolation $E_{T,PL}^{\text{cone20}}/p_{T,\gamma}$ in the SHERPA signal sample applying all PL and DL selections (cf. Table 7.2) except for the isolation cuts. The results for the subleading photon in events with low $30 \text{ GeV} < p_{T,\gamma_2} < 50 \text{ GeV}$ are depicted in Fig. 7.21. A linear function is approximated to find the PL relative isolation threshold ξ most closely matching the DL requirement of $E_T^{\text{cone20}}/p_{T,\gamma} = 0.05$. The procedure is repeated for different p_T -bins separately for the leading and subleading photon.

The PL ξ values are approximately twice the DL fraction of 0.05. This is caused by using the EM calibrated energy of the topological clusters for the calculation of the DL isolation energy, which does not take into account the smaller calorimeter signal for hadrons compared to the one for electrons or photons with the same energy. The e.g. different energy losses, dead-material and out-of-cluster deposits for hadrons are taken into account applying the local hadronic calibration (LCW) instead [104]. The mean ratio of the LCW and EM calibrated energies of clusters in the isolation cone of $Z \rightarrow ee$ events⁶ is around 2 matching the ratio of the PL to DL relative isolation threshold

⁶The isolation of the probe electrons from the $Z \rightarrow ee$ events in Chapter 5 is used, because the LCW calibrated energy

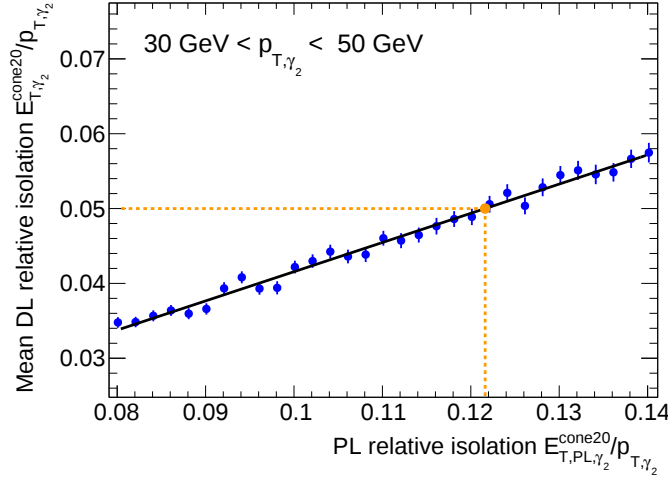


Figure 7.21.: Mean relative DL isolation energy as a function of the relative PL isolation energy. A linear fit is performed to the points and the green point indicates the PL cut, which matches best to the DL isolation working point.

estimated here. Using LCW calibrated clusters for the DL isolation could lead to more similar selection criteria on the PL and DL isolation, but preliminary studies show that the signal-efficiency versus background-rejection performance is slightly deteriorated.

The ξ -values estimated from the linear fit are cross checked by evaluating the magnitude of the unfolding corrections as a function of ξ . Again all PL and DL selections except for the isolation criteria are applied to the MC events. In this set of event the fraction of *missed* and *unmatched* events is calculated as a function of ξ . Missed events refer to events not passing the DL isolation cut, but passing the PL isolation cut and unmatched events refer to events passing the DL isolation cut, but not passing the PL isolation cut. The results for the isolation cut on the subleading photon candidate in a low and high p_{T,γ_2} bin are depicted in Fig. 7.22. For very tight PL isolation requirements (low ξ) the fraction of unmatched events is rising, because the PL requirement gets tighter than the fixed DL one. For high ξ the fraction of missed events is rising, because non-isolated photons are getting included into the PL selection. The fraction of events which need correction are much higher at low p_{T,γ_2} than at high p_{T,γ_2} , because of the stricter isolation requirements in terms of absolute energies at low p_T and the limited detector resolution. This limited resolution is also the reason for the wide plateau, which the summed values are reaching at low p_T compared to the sharp minimum at high p_T . For both cases the ξ -value resulting from the linear fit yield values where the fraction of events needing correction is approximately minimal, which means the cross-check succeeded.

The ξ -values are different for high and low p_T . The PL isolation threshold $E_{T,PL,min}^{cone20}$ (cf. Eq. (7.20)) could be used to stabilize the ξ values as a function of p_T . The linear fit shown in Fig. 7.21 is repeated for different relative PL isolation definitions:

$$\xi = (E_{T,PL,\gamma_{1(2)}}^{cone20} - E_{T,PL,min}^{cone20})/p_{T,\gamma}, \quad (7.21)$$

of the topological clusters is not available by default, but calculated for this specific sample.

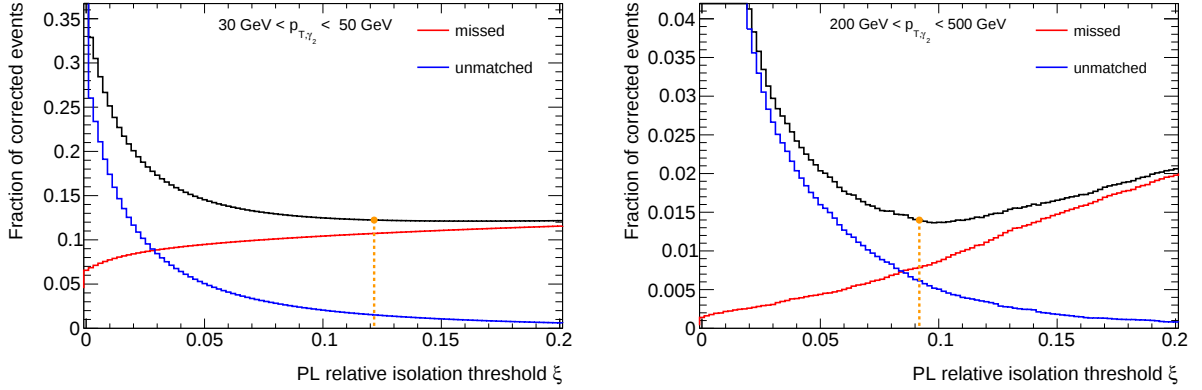


Figure 7.22.: Fraction of missed (red) and unmatched (blue) events and their sum (black) due to the subleading photon isolation requirements normalised to the number of events passing all PL and DL requirements up to the isolation ones. The left plot is for a low $30 \text{ GeV} < p_{T,\gamma_2} < 50 \text{ GeV}$ and the right plot for a high $200 \text{ GeV} < p_{T,\gamma_2} < 500 \text{ GeV}$ bin. The orange dot represents the optimal ξ value estimated from the linear fit to the mean DL relative isolation as a function of the relative PL isolation in this bin.

with different values of $E_{T,PL,min}^{\text{cone20}}$. The resulting ξ thresholds are depicted in Fig. 7.23 on the left. The thresholds are most stable for $E_{T,PL,min}^{\text{cone20}} = 1 \text{ GeV}$ and converge all to a similar value of around $\xi = 0.09$. In the end the PL cut with $\xi = 0.09$ and $E_{T,PL,min}^{\text{cone20}} = 0 \text{ GeV}$ is chosen to simplify the interpretation of the results for theorists and because the influence of $E_{T,PL,min}^{\text{cone20}}$ on the fraction of corrected events is small, which is shown on the right hand side of Fig. 7.23.

The same studies as shown here for the subleading photon are performed for the leading photon. The results are very similar indicating that the same PL isolation cuts can be used for the leading and subleading candidate.

Using an appropriate cut as discussed in this section does reduce the uncertainties. The main uncertainty altered by the choice of the PL isolation cut is related to the modelling of the PL isolation distribution (cf. Section 7.7.4). Using e.g. a very strict PL isolation cut, would lead to a large fiducial correction depending on a good modelling of the PL isolation and correspondingly higher uncertainties.

7.7. Uncertainties

The different uncertainties on the unfolded results are discussed in this section. At first an overview of the different sources of uncertainties and their impact on the result is given in Section 7.7.1 and the technical aspects of the estimation of the systematic uncertainties are discussed (cf. Section 7.7.2). Afterwards the different sources of uncertainty are discussed in more detail in Sections 7.7.3 to 7.7.9.

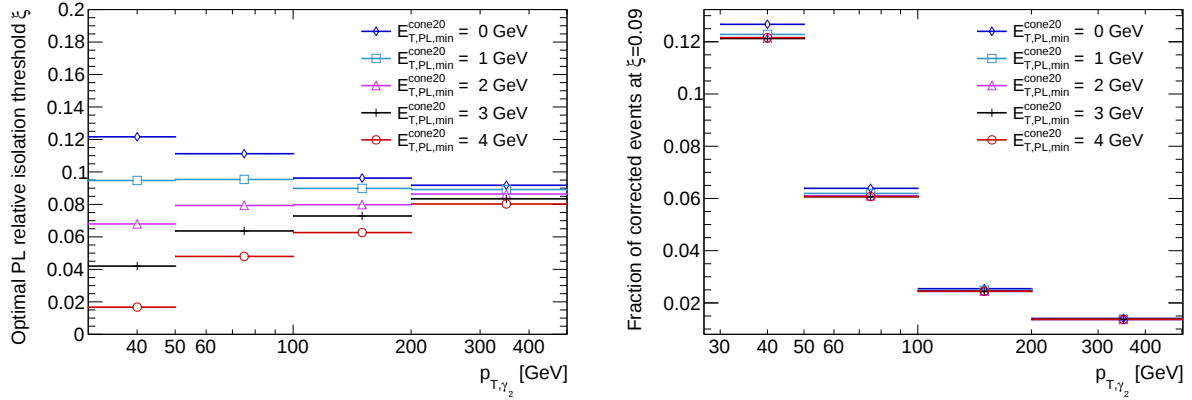


Figure 7.23.: On the left the optimal relative PL cut from the method shown in Fig. 7.21 for different values of $E_{T,PL,min}^{cone20}$ is depicted as a function of p_{T,γ_2} for the subleading photon. The right plot shows the fraction of events needing correction for $\xi = 0.09$ for the same $E_{T,PL,min}^{cone20}$ values.

7.7.1. Overview

The relative systematic and statistical uncertainties on the integrated fiducial cross-section grouped into different categories are summarized in Table 7.3. The calculation and result of the integrated fiducial cross-section will be discussed in Section 7.9.1. The total relative uncertainty is 7.5%. The leading category of uncertainties is related to the background estimation (cf. Section 7.7.3), followed by uncertainties related to the photon isolation (cf. Section 7.7.4), the stability of the measured result across the different data-taking years (cf. Section 7.7.5), and the photon identification and reconstruction (cf. Section 7.7.6). Other uncertainties related to the unfolding method (cf. Section 7.7.8) are relatively small. The uncertainty on the integrated luminosity of the full dataset is 1.7% [160] and directly translates to a relative uncertainty on the measured result of the same size. The data and MC statistical uncertainties are estimated based on pseudo-experiments (cf. Section 7.7.9). The uncertainties on the modelling of the photon energy scale (cf. Section 7.7.7) have a negligible impact on the integrated cross-section result.

The relative uncertainties of each category in Table 7.3 and the total uncertainty are depicted in Fig. 7.24 as a function of the different observables. The total uncertainty is in the range from 6 to 12% in all bins except for low $m_{\gamma\gamma} < 50$ GeV. The uncertainties related to the background estimation are especially dominant in regions with low signal purity. Photon energy related uncertainties become important only for high p_{T,γ_1} , p_{T,γ_2} or $m_{\gamma\gamma}$. Some region like high p_{T,γ_1} , p_{T,γ_2} or $m_{\gamma\gamma}$ are limited by data statistics. At low p_{T,γ_1} the photon isolation related uncertainties are dominant.

7.7.2. Systematic uncertainty estimation and combination method

The systematic uncertainties are estimated based on two-point variations, which means the whole analysis is repeated using the up- and down-variation of an uncertain parameter to propagate the effect to the measured result. The variations cover the 1σ region of the parameter, e.g. corresponding

Table 7.3.: Breakdown of the relative uncertainties in the integrated fiducial cross-section measurement. The uncertainties are grouped into different categories and the first row of each category shows the sum in quadrature of its components [38].

Source	Relative uncertainty [%]
Background estimation	4.3
$R_j^{\text{iso-id}}$	4.2
$\gamma\gamma$ pile-up background	0.6
$R_{\gamma j}^{\text{iso}}$	0.5
Electron background	0.2
Photon isolation	4.1
Pile-up reweighting	3.5
Data-driven correction	1.9
Theory modelling of isolation	0.6
Photon reconstruction and identification	3.0
Photon identification	2.9
Photon reconstruction	0.4
Other	3.5
Data-period stability	2.9
Luminosity	1.7
Trigger efficiency	0.7
Theory modelling of p_{T,γ_1}	0.2
MC statistical uncertainty	0.1
Unfolding method	<0.1
Photon energy	0.5
Total systematic uncertainty	7.5
Data statistical uncertainty	0.3

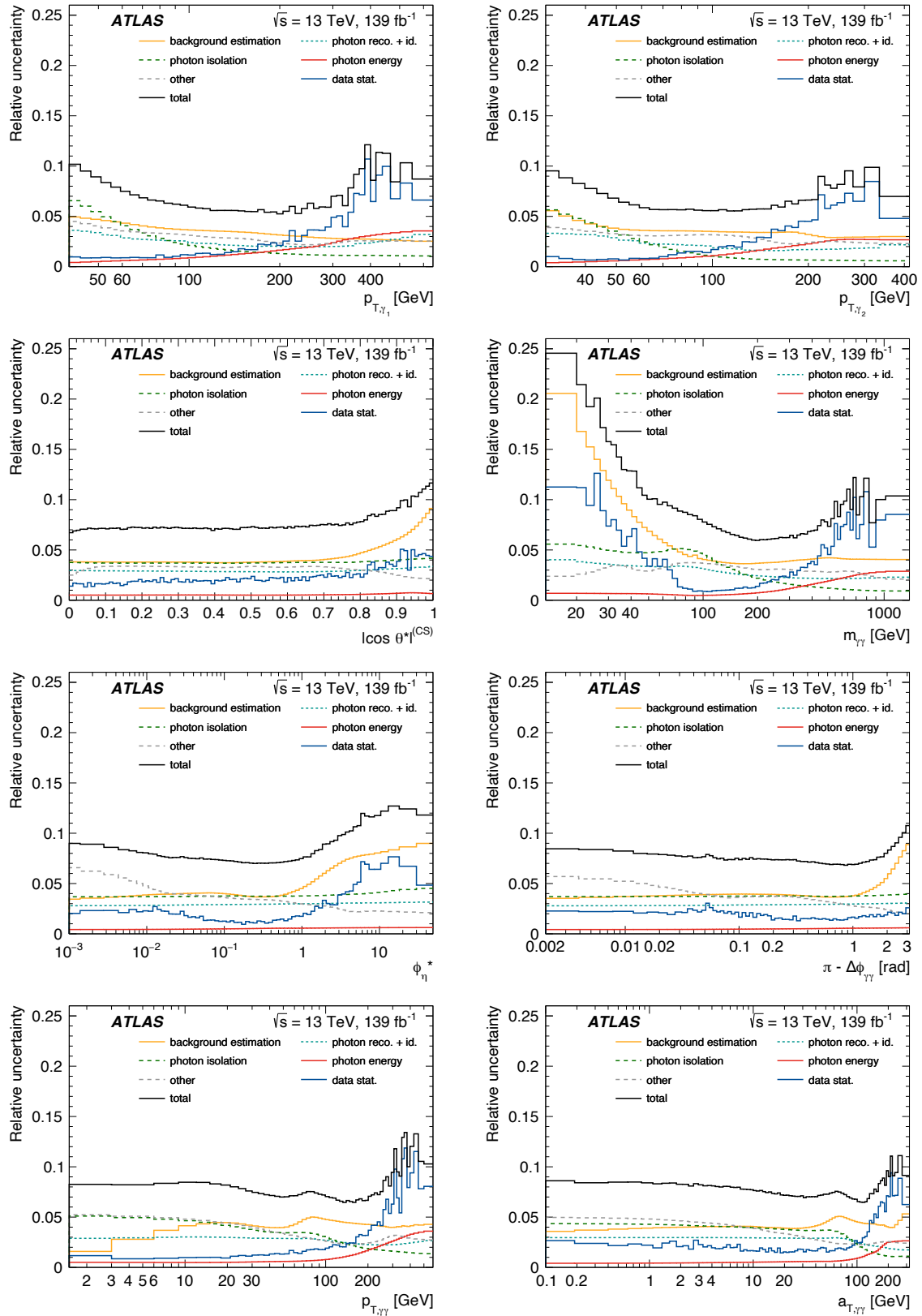


Figure 7.24.: The relative uncertainties in the unfolded result associated with different categories of uncertainties as grouped in Table 7.3 are summarised [38].

to a 68% confidence interval. Propagating the systematic variations takes the correlation of different steps in the analysis into account. This means, if e.g. the up-variation increases the yield in both, the background estimation and the unfolding, the effects are added linearly. Furthermore the correlation ρ_{ij} of an uncertainty between different observable bins i and j are encoded by the relative sign

$$\rho_{ij} = \text{sig}(\Delta_i \times \Delta_j) \quad (7.22)$$

of the deviations Δ_i and Δ_j of a variation to the nominal result in each bin.

The nominal results and the result of each of the more than 180 individual systematic up- and down variations is published on the HEPData portal [161, 162] to provide complete information about the uncertainties. To get a simplified interpretation and comprehensible visualization of the uncertainties different sources are combined. This is done assuming Gaussian distributed uncertainties and necessitates the combination of the up- and down variation in each bin into a symmetric uncertainty

$$\sigma_i = \frac{|\Delta_i^{\text{up}}| + |\Delta_i^{\text{down}}|}{2}. \quad (7.23)$$

The correlation structure of the uncertainty between different bins is retained by defining a multivariate Gaussian based on the covariance matrix

$$\Sigma_{ij} = \sigma_i \sigma_j \text{sig}(\Delta_i^{\text{up}} \times \Delta_j^{\text{up}}). \quad (7.24)$$

Using the up-variation to calculate the correlation gives in almost all cases the same result as using the down variation, because the Δ_i^{up} and Δ_i^{down} have opposite signs except for some rare edge cases.

The covariance matrix Σ_{ij} for a single systematic uncertainty is not invertible, which means the corresponding multivariate Gaussian distribution of the result $\vec{y}$:

$$f(\vec{y}) = \frac{1}{\sqrt{(2\pi)^{n_{\text{bins}}} |\det \Sigma|}} \exp [(\vec{y} - \vec{y}^{\text{nom}}) \Sigma^{-1} (\vec{y} - \vec{y}^{\text{nom}})], \quad (7.25)$$

is not a proper function, but can be described as the product distribution of a $(n_{\text{bins}} - 1)$ dimensional δ -distribution and a 1-dimensional Gaussian in the n_{bins} -dimensional space of the results. The δ -distribution is aligned orthogonal to the direction between the up- and down variation $\vec{y}^{\text{down}} - \vec{y}^{\text{up}}$ and the Gaussian is aligned with the direction of the variation.

The benefit of this description in terms of multivariate Gaussian distributions is that the distribution corresponding to the total uncertainty can be calculated by simply adding the n_{syst} individual covariance matrices Σ^{unc} , because the sum of two (multivariate) Gaussians is again Gaussian. The total covariance is then given by:

$$\Sigma^{\text{tot}} = \sum_i^{n_{\text{unc}}} \Sigma_i^{\text{unc}}. \quad (7.26)$$

7.7.3. Background estimation

In this subsection the uncertainties only affecting the background estimation are discussed. Other uncertainties e.g. changing the identification and isolation efficiencies change both the background

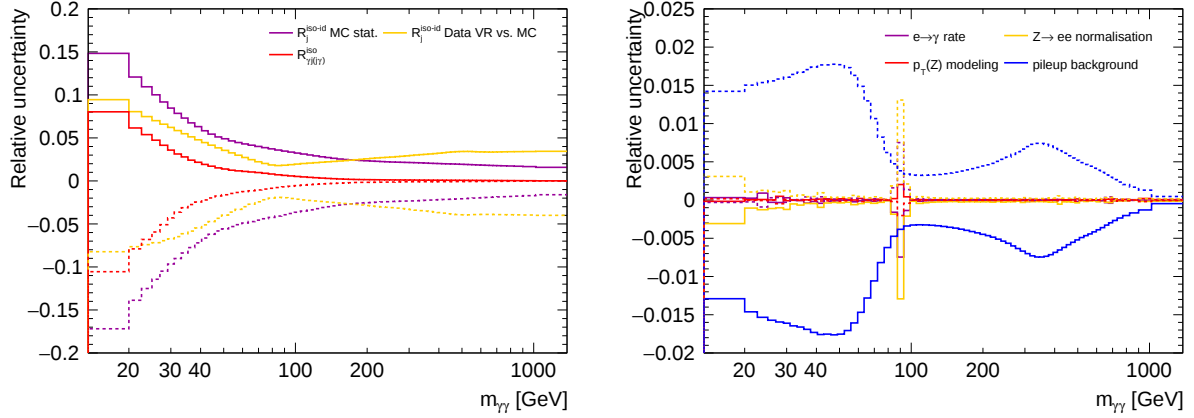


Figure 7.25.: Relative uncertainties as a function of $m_{\gamma\gamma}$ for different sources of systematic uncertainties affecting only the background estimation. The solid line represents the up-variation and the dashed line the down-variation. The left hand plot shows the contributions from the uncertainty on the $R_j^{\text{iso-id}}$ and $R_{j(\gamma j)}^{\text{iso}}$ parameters. The right plot shows the uncertainties related to the subleading electron and pileup backgrounds.

estimation and the unfolding and are discussed in the respective sections together.

The largest components of the background estimation uncertainties and thus also of the whole measurement are related to the correction factor for the identification-isolation correlation of misidentified photon candidates from jets, which were discussed in Section 7.5.4. The relative uncertainty related to the up-and down variation of the two $R_j^{\text{iso-id}}$ uncertainty components are depicted in Fig. 7.25 (left) as a function of $m_{\gamma\gamma}$. The p_T independent uncertainty component related to the limited MC statistics for the extrapolation from the validation region to the signal region is dominant in regions with low p_T photon candidates. At high $m_{\gamma\gamma}$, which corresponds to high p_T photons, the other p_T dependent uncertainty component becomes dominant, which is related to the data-to-MC comparison in the validation region. In general the background estimation uncertainties are most important for low purity regions, like low $m_{\gamma\gamma}$ where the purity is estimated to be around only 30%.

The uncertainties from the correction for the isolation correlation in γj and $j\gamma$ events (cf. Section 7.5.5) is in general negligible except for low $m_{\gamma\gamma}$ where it reaches 8%.

The uncertainties related to the electron background (cf. Section 7.5.6) and the pileup background (cf. Section 7.5.7) are depicted in Fig. 7.25 (right) and are mostly negligible compared to the other uncertainties.

7.7.4. Photon isolation

The photon isolation uncertainties are usually the second largest source of uncertainty as shown in Fig. 7.24. Three different sources of uncertainty are considered and are affecting the $\gamma\gamma$ signal parameters used in the background estimation (cf. Section 7.5.2), and the fiducial and efficiency corrections in the unfolding (cf. Sections 7.6.1 and 7.6.3):

- Modelling of the pileup noise of the signal isolation distribution

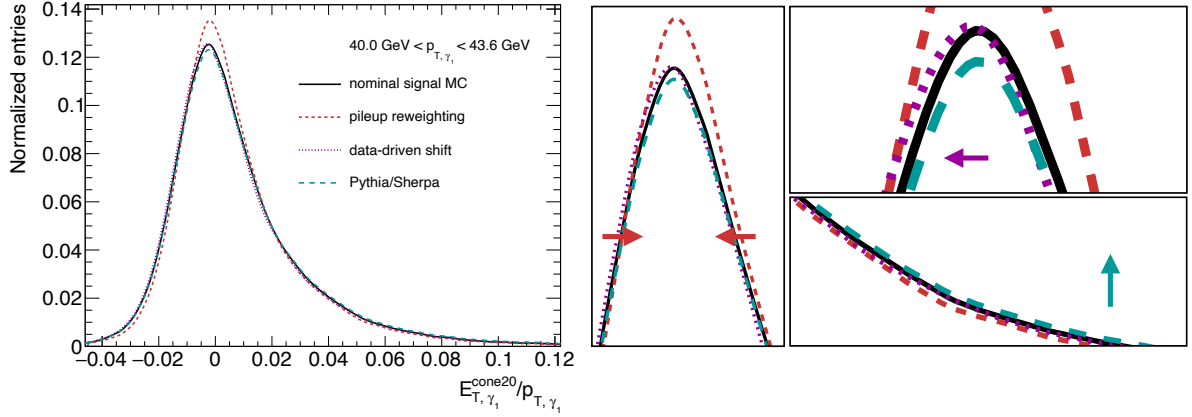


Figure 7.26.: Illustration of the MC signal isolation distribution and the different systematic uncertainties affecting it.

- Simulation of the energy leakage of the photon entering into the isolation region
- Theory modelling of non-isolated photons

The impact of the different systematic variations used to estimate the influence of these uncertainties on the photon isolation distribution are depicted in Fig. 7.26.

The pileup noise is mostly changing the width of the isolation distribution and changes to the pileup reweighting (cf. Section 5.2.2) scaling the amount of pileup in MC up-and down are used to estimate the corresponding uncertainty. The studies of the calorimetric isolation of electrons in $Z \rightarrow ee$ events in Section 5.7 motivates weighting down the pileup in MC $f_{\mu\text{-scale}} = 1/1.2$ for the calculation of the nominal isolation related values. A conservative uncertainty is assigned by using the default $f_{\mu\text{-scale}} = 1/1.03$ as the up-variation and $f_{\mu\text{-scale}} = 1/1.4$ as the down-variation. In the unfolding the pileup is only changed for the efficiency correction related to the photon isolation. Otherwise the default pileup reweighting is used, because the decline of the photon identification efficiencies as a function of number of pileup interactions is well modelled. This is achieved by factorizing the efficiency correction into multiple steps similar as depicted in Fig. 7.19 and determining the factor corresponding to the isolation selection with the different variations of the pileup reweighting. The influence of the pileup reweighting on the fiducial correction has been checked and is below 1% everywhere.

The energy of the photon in the core of the isolation region is subtracted and the residual energy leaking out of the core area is corrected based on the expectations in simulated samples (cf. Section 4.5). If the energy leakage is not correctly modelled this would lead to a shift of the peak position between the data and MC isolation distributions. This shift is centrally measured in bins of p_T and η [103]. The result is applied as a correction to the MC isolation and referred to as data-driven shift. The data-driven shifts are switched off for the down-variation and applied twice for the up-variation of the corresponding systematic uncertainty.

The theory modelling of non-isolated photons can bias the determination of the signal migration into the isolation control regions in the background estimation, and the fiducial and efficiency correction in the unfolding. For the fiducial correction photons passing only the DL but not the PL

isolation cut are relevant and the isolation control regions require slightly non-isolated DL photons $0.05 < E_{T,\gamma}^{\text{cone20}}/p_{T,\gamma} < 0.15$. The uncertainty related to the fraction of such not-fully isolated photons is estimated based on the comparison of the PL isolation distribution in the PYTHIA and SHERPA signal samples (cf. Section 7.2.1). The PYTHIA sample does not have any restriction on the isolation values of the photons, because they are simulated as part of the parton shower. The SHERPA sample is using NLO matrix elements which require a loose parton-level smooth-cone isolation. Both the SHERPA and the PYTHIA sample can contain configurations with very non-isolated photons up to $E_{T,\text{PL}}^{\text{cone20}}/p_{T,\gamma} \sim 1$ they are just more frequent in the PYTHIA sample. To avoid the severely restricted statistics of the PYTHIA sample the SHERPA sample is reweighted to match the relative PL isolation distribution in the PYTHIA sample as a systematic variation as described in Appendix A. This Pythia/Sherpa weight is applied as a variation to the SHERPA sample and the analysis is rerun. The Pythia/Sherpa weighted sample corresponds to the up-variation of the uncertainty and the down-variation is defined by applying the inverse weight allowing for asymmetric effects due to the steeply falling isolation distribution. As depicted in Fig. 7.26 the weight affects the tails of the DL isolation distribution.

The influence of the different systematic variations on the subsequent steps of the analysis and the final result are depicted in Fig. 7.27. The largest variations of the result of up to 6% at low p_{T,γ_1} are caused by the pileup reweighting. Increased pileup (up-variation) increases the resulting signal yield of the background estimation, because the fraction of signal migrating into the background control regions is increased, which reduces the overall background normalisation. Similarly, the isolation efficiency correction in the unfolding is increased, because the efficiencies are deteriorated for higher pileup. Therefore the uncertainties on the background estimation and the efficiency correction add up to the value on the full result. The influence of the pileup noise is reduced in regions with high p_T photons, because of the looser isolation requirements.

For low p_T the variations caused by the data-driven shifts are smaller than the ones from the pileup reweighting, but show similar trends. At high p_T the energy from the photon leaking into the isolation region and the corresponding uncertainties from the shifts become more important having approximately the same size as the pileup reweighting uncertainty.

The Pythia/Sherpa reweighting is the only variation with significant impact on the fiducial correction. Increasing the fraction of PL non-isolated photons (up-variation) increases the number of unmatched events in the MC sample reducing the correction factor f and thus the final result. On the other hand the number of $\gamma\gamma$ signal in the isolation control regions is also increased, which increases the estimated signal fraction in the signal region as just explained for the pileup reweighting. This means the effects from the background estimation and the fiducial correction partially cancel and the uncertainty on the final result is reduced. The effects of the Pythia/Sherpa reweighting are most visible at low $m_{\gamma\gamma}$, which consists of events with additional jets providing the recoil for the boosted photon system and sometimes entering into the isolation region of the photons.

The MC photon isolation distribution and the assigned uncertainties are cross-checked with the data distribution as depicted in Fig. 7.28. The comparison is based on the isolation of the leading photon in events with all signal region cuts applied except for the isolation requirement on the leading photon. The comparison is shown for events in the first p_{T,γ_1} bin. The background distribution is added to the signal MC shape based on the distribution in the data control regions, where the leading candidate fails the tight identification. The signal migrating into these control regions is subtracted from the

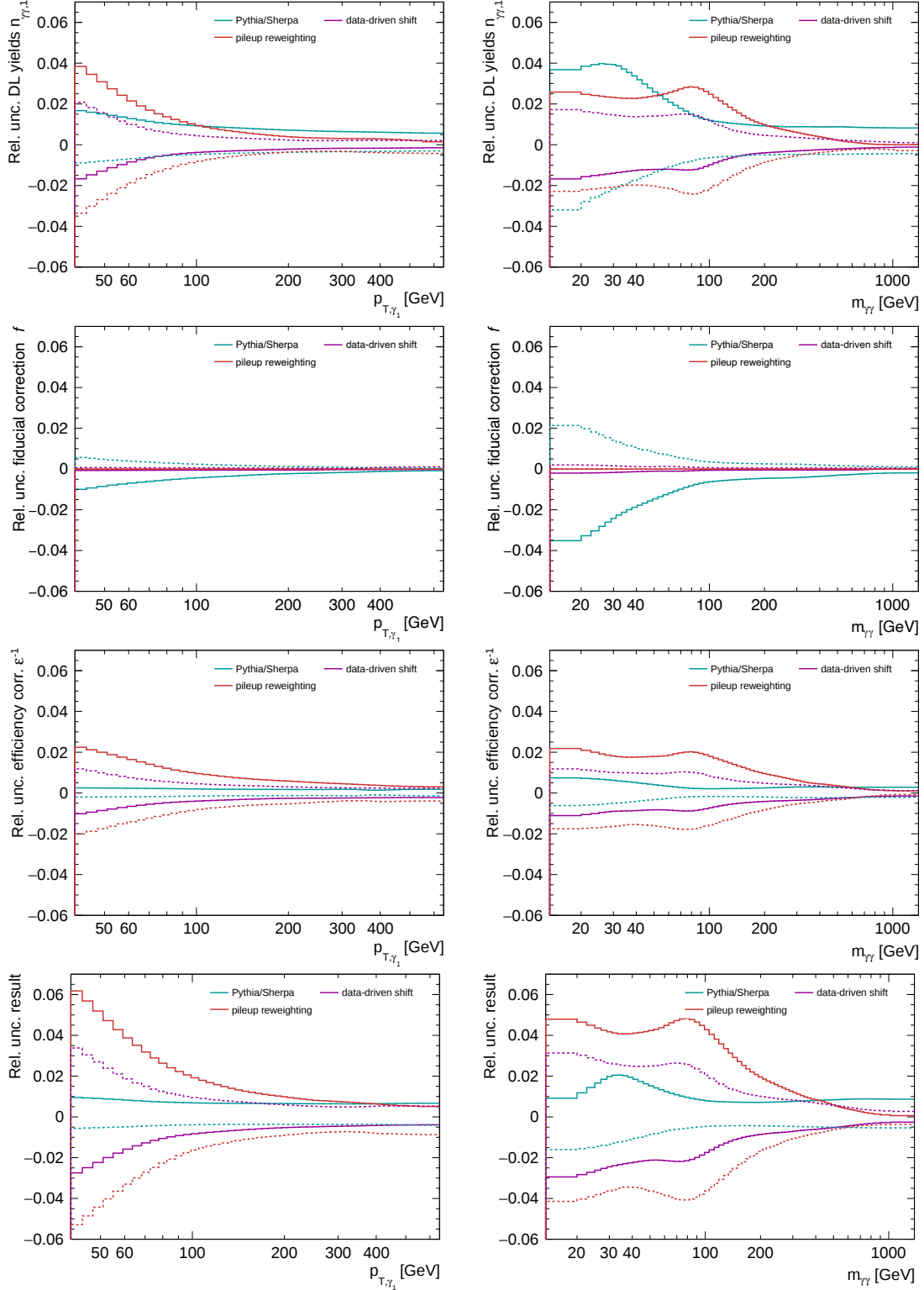


Figure 7.27.: Systematic variations of the different steps of the analysis related to the photon isolation for the observables p_{T,γ_1} (left) and $m_{\gamma\gamma}$ (right). The solid line shows the up-variation and the dashed line the down variation. The first row shows the changes to the DL signal yield after the background estimation. The second row shows the influence on the fiducial correction and the third row on the efficiency correction. The last row shows the full influence on the final result. All curves are smoothed for better visibility. 109

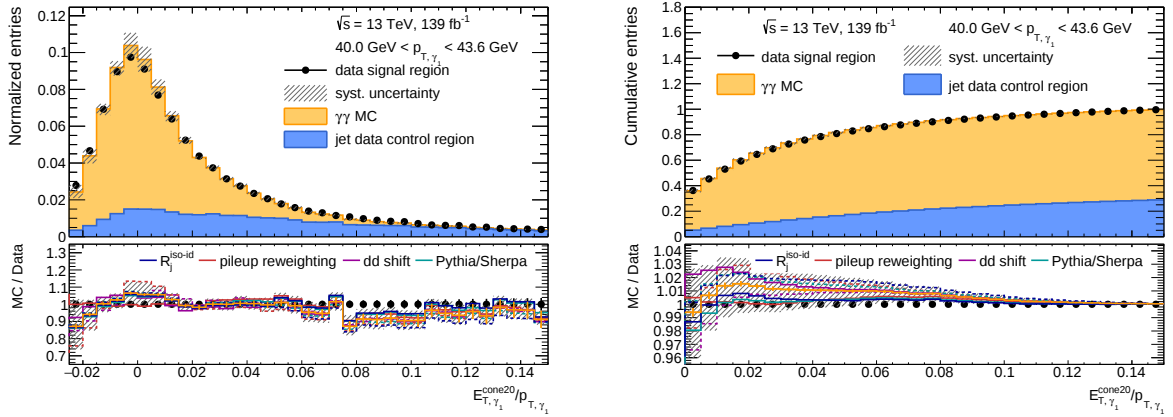


Figure 7.28.: Comparison of the relative photon isolation distribution of the leading photon between data and MC in the signal region without a requirement on the leading photon isolation. On the left the normalized histograms and on the right the cumulative distributions are compared. The shape of the isolation distribution for the jet background is taken from the data control regions, where the leading photon fails the *Tight* identification criterion. The signal-to-background fractions are taken as resulting from the background estimation fit. Different systematic uncertainties on the MC/Data ratio are considered: The three uncertainties changing the MC signal shape and the uncertainty on $R_j^{\text{iso-id}}$ changing the signal-to-background fraction in the fit.

background based on the signal MC shape and the signal fractions in the control regions resulting from the background estimation fit (cf. Section 7.5.8). The signal-to-background fraction in the signal region is also taken from the fit results and the background and signal shape are added accordingly. The data and MC+background distributions are normalized to unity and compared. Different systematic uncertainties on the comparison are considered: The three uncertainties discussed in this subsection which change the isolation distribution of the signal and the influence of $R_j^{\text{iso-id}}$ (cf. Section 7.5.4) on the signal-to-background fraction. Besides the normalized distributions also the integrated cumulative distributions are compared, which are the relevant quantity for the determination of the isolation efficiency. The data and MC distributions show good agreement within the assigned uncertainties.

7.7.5. Data-period stability

The measurement is performed independently with the data from different years and the result is compared. The datasets of 2015 and 2016 are combined to get sufficient statistics. If the influence of the changing experimental conditions on the analysis are represented by the MC samples and their uncertainties, the ratio of the measured cross-sections in the different years should be compatible with unity.

The ratios between the 2015+2016 and 2018 results for p_{T,γ_1} are depicted in Fig. 7.29. To reduce the influence of statistical fluctuations on the ratios the values are smoothed based on the **SmoothSuper** function implemented in ROOT [163]. The statistical uncertainty on the smoothed values is estimated

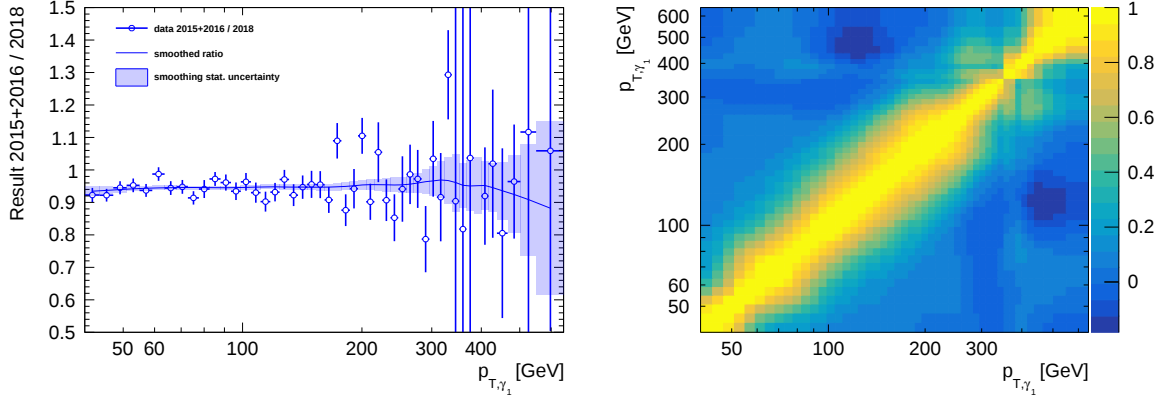


Figure 7.29.: Ratio of the measured cross section 2015+2016 and 2018 data as a function of p_{T,γ_1} (left) including the uncertainty from data statistics. The ratios are smoothed to reduce the impact of statistical fluctuations. The right plot shows the correlation of the statistical uncertainties of the smoothed values.

using toys. The ratio values are varied by adding Gaussian noise according to the statistical uncertainty of the points and these toys are again smoothed. The standard deviation of the values of the smoothed curves of the different toys is used to estimate the statistical uncertainty. The smoothed curve and the statistical uncertainty are also depicted in Fig. 7.29 and a significant offset from one with no clear trends as a function of p_{T,γ_1} is observed. The smoothed value at a certain p_{T,γ_1} corresponds to a weighted average over the values in a region around this p_{T,γ_1} . Therefore the smoothing introduces correlations between the statistical uncertainties of the ratio values in different p_{T,γ_1} bins, which is shown in Fig. 7.29 and also estimated from the toys.

Besides the statistical uncertainties there are also systematic uncertainties affecting the ratios between the year. Most systematic uncertainties are considered as correlated and of similar size in the different years and should therefore not change the ratios.

The leading uncertainty of the analysis related to the isolation-identification correlation of mis-identified photon candidates (cf. Section 7.7.3) is considered fully correlated. The $R_j^{\text{iso-id}}$ values in the data validation regions (cf. Section 7.5.4) of the separate years are compared and the values are compatible.

Although correlated between the years, the isolation uncertainty related to the pileup noise (cf. Section 7.7.4) has a different size for the respective years, because the pileup conditions changed Fig. 3.2. The pileup reweighting has a smaller impact for the lower pileup conditions in 2015+2016 than in e.g. for 2018, which means that e.g. the ratio of the down-variation of 2015+2016 to the down-variation in 2018 is different from the nominal ratio.

The luminosity uncertainty is also only partially correlated between the years [160] and the influence of the uncorrelated parts on the ratio are taken into account.

The remaining uncertainties, which are dominantly related to the photon identification efficiency, are considered fully correlated and neglected in the determination of the data-period stability uncertainty. Testing this assumption was part of the motivation for the measurements in Chapter 6.

The smoothed ratios between the different years including the discussed systematic and statistical

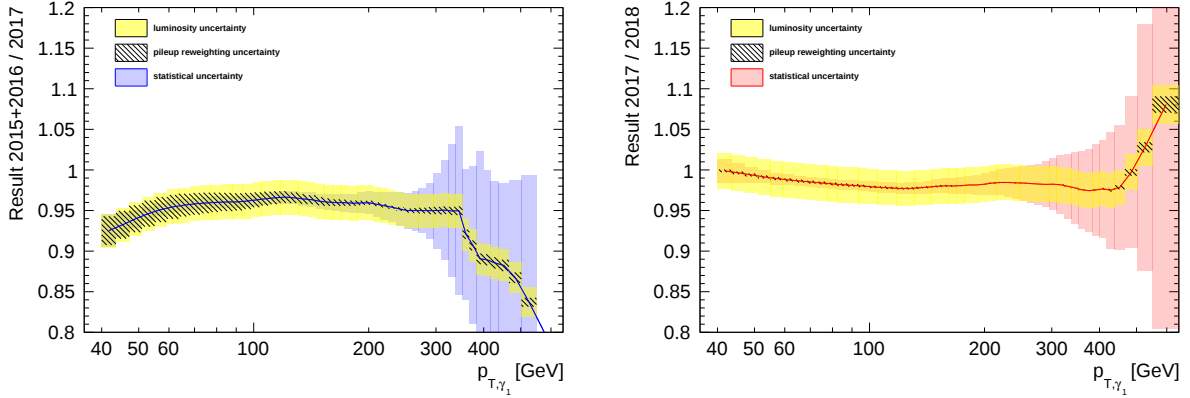


Figure 7.30.: Smoothed ratio between the measured cross-sections in different data-taking periods showing the systematic uncertainty from the pileup reweighting and the luminosity uncertainty. The left hand plot shows the ratio 2015+2016 / 2017 and the right hand plot shows the ratio 2017 / 2018. The plots for all observables are depicted in Figs. D.6 and D.7.

uncertainties is depicted in Fig. 7.30. The ratio of the 2015+2016 to the 2017 result is around 0.95 showing a significant difference to unity. The pileup reweighting uncertainties on the ratio are with around 2% the largest at low p_{T,γ_1} due to the p_T dependency of the isolation cut. The systematic variation scaling down the pileup by 1/1.4 in the MC for the isolation efficiency corrections gives ratios closer to one, which are compatible with a constant value as a function of p_{T,γ_1} . The uncertainty on the ratio of the 2015+2016 to the 2017 luminosity is 2.2%. None of the uncertainties considered are a probable explanation for the 5% difference. In contrast the ratio of the 2017 to the 2018 result shows good agreement. The pileup uncertainty on this ratio is very small, because the average pileup conditions in 2017 and 2018 are similar.

Multiple possible reasons for the discrepancies between the 2015+2017 and 2017+2018 results are investigated, but none of them are able to explain differences of the observed size. They will be summarized at the end of this section. In the absence of a good explanation for the differences an additional uncertainty is assigned to the result, which covers the discrepancies of the result of each separate year to the result of the combined dataset. The relative data-period stability uncertainty is calculated in each bin of the observables based on the smoothed ratio r , the statistical uncertainty Δr_{stat} , the pileup reweighting uncertainty Δr_{PRW} and the luminosity uncertainty Δr_{lumi} of the ratio:

$$\Delta_{\text{data-period}}/N = \sqrt{\max \left[0, (1 - r)^2 - (\Delta r_{\text{stat}})^2 - (\Delta r_{\text{PRW}})^2 - (\Delta r_{\text{lumi}})^2 \right]}. \quad (7.27)$$

This means the uncertainty is only assigned in bins where the other uncertainties are too small to explain the discrepancies. The data-period stability uncertainty of the combined result is calculated as the envelope (the maximum) of the data-period stability uncertainties of the individual years. The relative data-period stability uncertainty is depicted in Fig. 7.31. The discrepancy of 2015+2016 is the dominant contribution in the high statistics regions. The 2017 or 2018 ratio to the combined

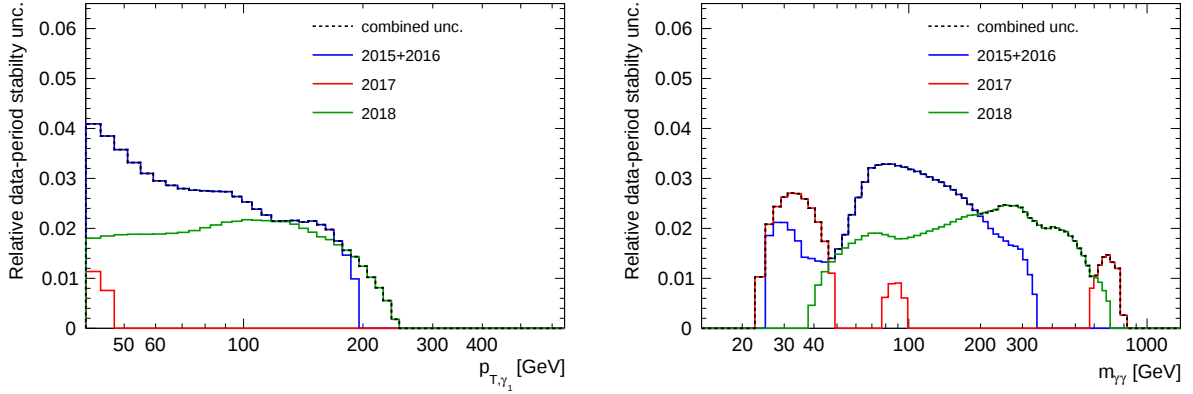


Figure 7.31.: Relative data-period stability uncertainty for the separate years and the combined dataset as a function of p_{T,γ_1} (left) and $m_{\gamma\gamma}$ (right). Plots for all observables are collected in Fig. D.8.

result contribute in regions with relatively low statistics. The uncertainty is typically below 3%. It is the main contribution to the “other” uncertainty category in Fig. 7.24 and usually the third largest uncertainty. Given that there are multiple other systematic uncertainties of similar or larger size removing the data-period stability uncertainty would reduce the total uncertainty by usually only less than 10%.

In the pursuit for the reasons of the offset between the years different hypotheses are checked:

- The most obvious difference between the years are the pileup conditions. The measurement is repeated in a subset of the 2017+2018 data with reduced pileup conditions more similar to the 2015+2016 data. The ratios of the 2015+2016 results to the reduced pileup 2017+2018 results are compatible to the ratios to the full 2017+2018 results. This shows that the different pileup conditions are not the cause of the discrepancies.
- The central photon identification efficiency measurements are performed inclusively for all years and separately for photons reconstructed as converted and unconverted. This measurement is repeated split by year to check for differences in the data-MC ratio of the photon identification efficiencies between the years. The data-MC ratios of the photon identification efficiencies are similar between the years and close to one. The uncertainty from the identification efficiency measurement split by year on the ratio of the measured photon-pair cross sections between the years is around 1%, e.g. too small to explain the 5% differences between 2015+2016 and 2017+2018.
- The number of events passing the signal region selection are checked for each run⁷. The number of selected events is divided by the luminosity of the run and plotted as a function of the average interactions per bunch crossing $\langle\mu\rangle$ for the run, because the selection rates are decreasing linearly as a function of $\langle\mu\rangle$. Similar trends as for the ratio on the measured cross-section are observed,

⁷Run refers here to a single fill of the LHC with two beams of proton bunches and not the complete data-taking campaign.

e.g. a few percent less events per luminosity in 2016 than in 2017 or 2018 at the same $\langle\mu\rangle$. This discrepancy is enhanced for photons reconstructed as converted, which occur less often in 2015+2016 than in 2017 or 2018. Checking the number of selected events per luminosity for each run shows also that there are no missing or pathologic runs in the datasets.

- The influence of the fraction of photons reconstructed as converted on the analysis is checked, by performing the analysis separately for converted and unconverted photons. This means the reconstructed fraction of converted photons passing the event selection is taken from the data in contrast to the nominal method where it is taken from MC. As shown in Section 6.5.2 the conversion fraction is not well modelled in MC and the mismatch is different between the years. Despite this the influence on the photon-pair result is small ($\sim 1\%$), because the difference in the photon isolation and identification efficiencies between converted and unconverted photons is not very large.
- The trigger used for 2015+2016 is different from the trigger for 2017+2018. As described in Section 3.2.5 the identification criterion on the trigger was tighter in 2017+2018 to cope with higher rates. This could explain lower rates in 2017+2018 than in 2015+2016, but not the observed opposite.
- The efficiency measurement in Chapter 6 is largely motivated by the mismatch observed here and studies the identification, isolation and reconstruction efficiency as well as the reconstructed conversion fraction and the interplay of these quantities in different years. The reconstruction efficiency shows small differences in the data-to-MC ratio between the years as shown in Section 6.5.1. This is taken into account as a correction in the photon-pair measurement and reduces the data-period stability uncertainty by approximately one percent point. This is the main improvement of the result published in [38] with respect to the preliminary result presented in [164].
- The compatibility of the observed discrepancy with other ATLAS measurements involving photons is checked. The $H \rightarrow \gamma\gamma$ cross-section measurements with the full Run-2 data [91] have a statistical uncertainties around 5% and are therefore not sensitive enough to resolve the small differences seen in the photon-pair measurement. The $Z\gamma$ measurement [131] observes a ratio of $(98.9 \pm 1.1)\%$ between the 2015+2016 result and the full Run-2 result. This value needs to be squared to compare it to photon-pair results, where all photon selection efficiencies enter twice. The squared value $(97.8 \pm 2.2)\%$ is roughly compatible with the differences observed for the photon-pair measurement.

7.7.6. Photon identification and reconstruction

The photon identification efficiencies in the MC signal samples are corrected to match the measurements in [103] with event weights based on the data-to-MC ratio of the measured efficiencies. Event weights for signal events failing one or either of the identification requirements on the photon are also taken into account in these weights as described in Appendix C, which can have an influence on the inputs to the background estimation.

The uncertainties on the measured data-to-MC ratio of the efficiencies are propagated to the result of this analysis by varying the weights. The data-to-MC ratios are measured in bins of p_T and η , e.g. in independent categories and applied accordingly. Although the efficiency measurements are statistically independent in each p_T and η bin it is recommended to propagate the uncertainty by only one up- and down-variation changing the weights for all p_T and η bins coherently, instead of performing independent variations for the statistical uncertainty in each bin and the different systematic uncertainties. In general this should be a more conservative approach as it overestimates the impact of the statistical uncertainties in the measurement of the photon identification efficiencies.

Similarly, the photon reconstruction efficiency is corrected with the data-to-MC ratios measured in different η bins as presented in Fig. 6.8 and are assumed to be constant as a function of p_T . To a good approximation the correction affects only the efficiency corrections in the unfolding, but not the background estimation where only photons enter which pass the reconstruction. Slight influences on the background estimation can arise if the correction of the photon reconstruction efficiency strongly changes the η distribution and thereby the average of η dependent e.g. isolation efficiencies. The nominal photon reconstruction efficiency correction is applied for the full analysis including the background estimation, but the impact of the variations is only taken into account for the unfolding. In the same way as for the photon identification only one up and down variation is used. The full Run-2 efficiency corrections from Fig. 6.8 and the corresponding uncertainties are used for the nominal analysis with the full Run-2 dataset. For the measurements split by year in Section 7.7.5 the corrections derived for the respective years are used which slightly reduces the difference between 2015+2016 and 2017+2018.

The photon trigger efficiency is corrected based on the measurements in [93], which shows data-to-MC ratios compatible with one. The uncertainties are evaluated only in the unfolding with the same arguments as for the reconstruction efficiency.

The impact of the uncertainties discussed in this section on the steps of the analysis and the full result are depicted in Fig. 7.32. The photon identification uncertainty is the largest of the three and ranges between 2 to 3%. The photon reconstruction and trigger efficiency uncertainties are at the subpercent level. There are multiple reasons for the larger impact of the photon identification. First, the photon identification affects the background estimation changing the migrations of the signal into the control regions. Second, the statistical uncertainties on efficiency ε measurements scales approximately with $\sqrt{\varepsilon(1-\varepsilon)}$ which means they are larger for efficiencies closer to $\varepsilon = 0.5$. Third, the photon identification measurement extends to high $p_T \sim 1$ TeV values with low statistics, where the trigger and reconstruction efficiencies results are only extrapolated. The third point is a caveat of the photon reconstruction and trigger efficiency measurement, which are only measured at low p_T . This can be tolerated given the small impact compared to other uncertainties. As shown in Fig. 7.24 even the impact of the photon identification uncertainty is subdominant compared to e.g. the isolation efficiency.

7.7.7. Photon energy scale

The photon energy-scale and resolution in the MC samples is corrected based on the measurements in [106]. In [106] over 80 independent systematic uncertainties are evaluated which are propagated with separate variations to the result of the photon-pair measurements. The photon-energy scale uncertainties affect mostly the response matrices, slightly distorting the shape of the unfolded PL

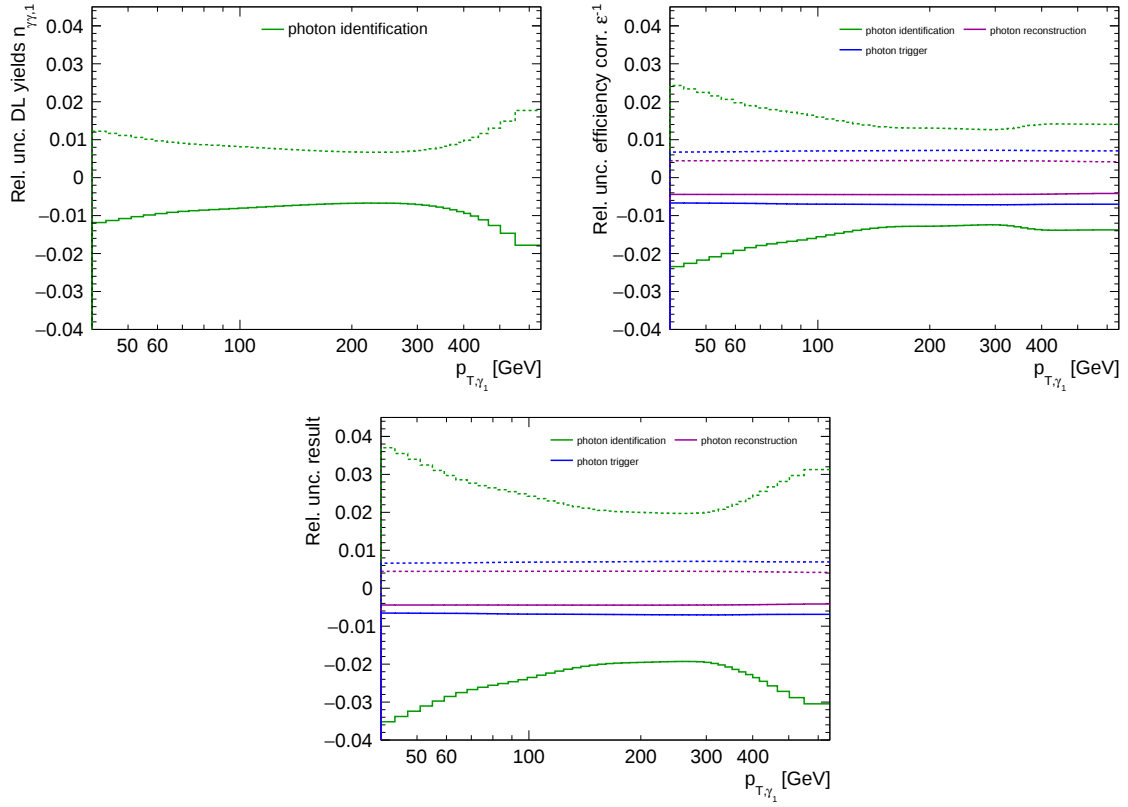


Figure 7.32.: Uncertainties related to photon identification, reconstruction and trigger efficiencies on the background estimation (top left) the efficiency corrections (top right) and the final result (bottom).

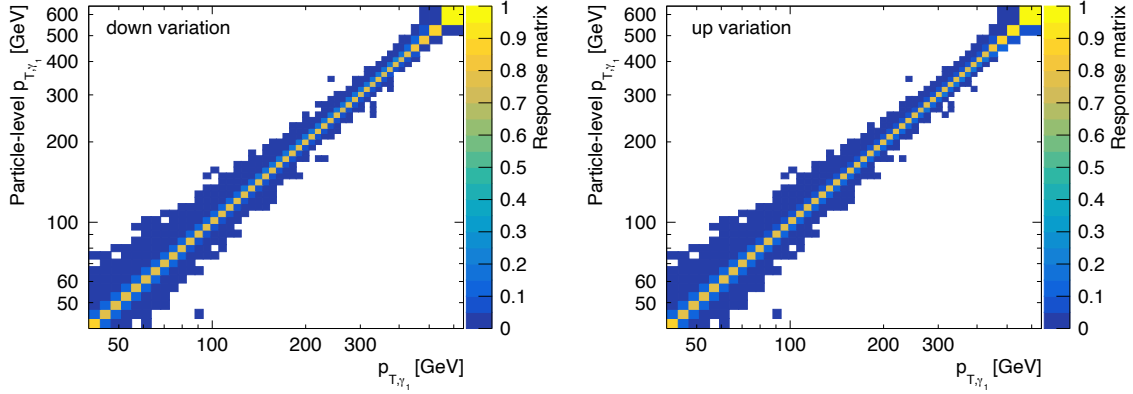


Figure 7.33.: Up (left) and down (right) variations of the response matrix for the systematic uncertainty connected to the linearity of different readout gain configurations.

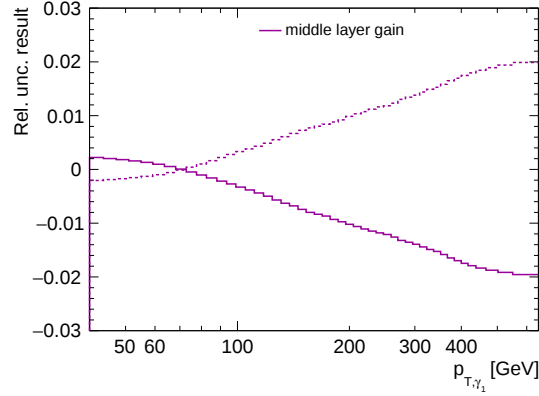


Figure 7.34.: Impact of the up (solid) and down (dashed) variation of the photon energy uncertainty connected to the linearity of different readout gain configurations.

result with respect to the DL yields. The dominant systematic uncertainty is connected to the relative calibration of the different readout gains in the middle layer of the EM calorimeter (cf. Section 8.5 in Ref. [106]).

Although the changes in the response matrices are relatively small even for this most dominant variation as depicted in Fig. 7.33, they have a significant impact of up to a few percent in bins with high p_T photons (cf. Fig. 7.34). The impact of the energy-scale uncertainties on the efficiency and fiducial correction is negligible compared to the influence from the change in the response matrices. The impact of the photon energy resolution uncertainties are negligible everywhere which is a consequence of the wide binning.

The photon energy related uncertainties are in general small compared to other uncertainties (cf. Fig. 7.24). In the regions with high p_T photons where the photon energy related uncertainties rise to up to 4% the uncertainties from the limited data statistics are also rising and the dominant contribution to the total uncertainty.

7.7.8. Unfolding

In this section uncertainties related to the sensitivity of the results to the kinematic distributions in the signal samples are discussed. On the one hand the MC prior distributions enter directly into the first iteration of the unfolding procedure Section 7.6.2. On the other hand they enter indirectly by only unfolding one variable at the time, such that differences in other *hidden* variables could bias e.g. the efficiency corrections.

Uncertainty from MC prior

The bias from the MC prior in the iterative unfolding is estimated based on a data-driven test, which is commonly performed for ATLAS measurements [165]. The details of the procedure are closely following and adopting the developments in [166].

The principal idea is to reweight the MC on PL, such that the DL distributions in data and MC match. The reweighted MC is then used as pseudo-data with a known PL distribution to estimate the bias. The DL distribution in the reweighted MC is unfolded using the prior and response matrix of the nominal MC sample. The unfolded DL distribution of the reweighted MC can then be compared to the known PL distribution of the reweighted MC to estimate the bias, which is assigned as systematic uncertainty.

The weights applied to the PL MC are smoothed to reduce the sensitivity of the estimated bias to statistical fluctuation. The smoothing procedure is taken from [166]. The results are not very sensitive to the smoothing procedure because of the good data statistics. The weights $\mathbf{w}$ are determined by minimizing:

$$\min_{\mathbf{w}} \left(\chi_{\text{MC,data}}^2(\mathbf{w}) + \lambda \sum_{j_{\text{PL}}=2}^{n_{\text{bins}}} (w_{j_{\text{PL}}} - w_{j_{\text{PL}}-1})^2 \right). \quad (7.28)$$

The first term is the χ^2 value calculated between the DL MC and data distributions. The second term adds a penalty for fluctuations in the weight vector $\mathbf{w}$. The penalty is steered by the λ parameter, which is increased starting from zero until the χ^2 gets larger than $\chi^2/\text{ndof} > 1$. This means the smoothest weight configuration which still yields a DL MC distribution which is statistical compatible to the data is used. The χ^2 value is calculated based on the number of DL events in the reweighted MC $n_{\text{rew},i_{\text{DL}}}^{\text{MC}}$, the number of data events $n_{i_{\text{DL}}}^{\text{data}}$ and the statistical uncertainty of the data $\Delta n_{i_{\text{DL}}}^{\text{data}}$:

$$\chi^2(\mathbf{w}) = \sum_{i_{\text{DL}}=1}^{n_{\text{bins}}} \frac{\left(n_{\text{rew},i_{\text{DL}}}^{\text{MC}}(\mathbf{w}) - n_{i_{\text{DL}}}^{\text{data}} \right)^2}{\left(\Delta n_{i_{\text{DL}}}^{\text{data}} \right)^2} \quad (7.29)$$

The reweighting is applied on the PL distribution:

$$n_{\text{rew},i_{\text{DL}}}^{\text{MC}}(\mathbf{w}) = \sum_{j_{\text{PL}}=1}^{n_{\text{bins}}} f_{\text{corr},i_{\text{DL}}}^{-1} r(i_{\text{DL}}|j_{\text{PL}}) \epsilon_{j_{\text{PL}}} n_{j_{\text{PL}}}^{\text{MC}} w_{j_{\text{PL}}}, \quad (7.30)$$

which is calculate based on the fiducial correction $f_{\text{corr},i_{\text{DL}}}$, the response matrix $r(i_{\text{DL}}|j_{\text{PL}})$, the efficiency correction $\epsilon_{j_{\text{PL}}}$ and the PL MC $n_{j_{\text{PL}}}^{\text{MC}}$ distribution.

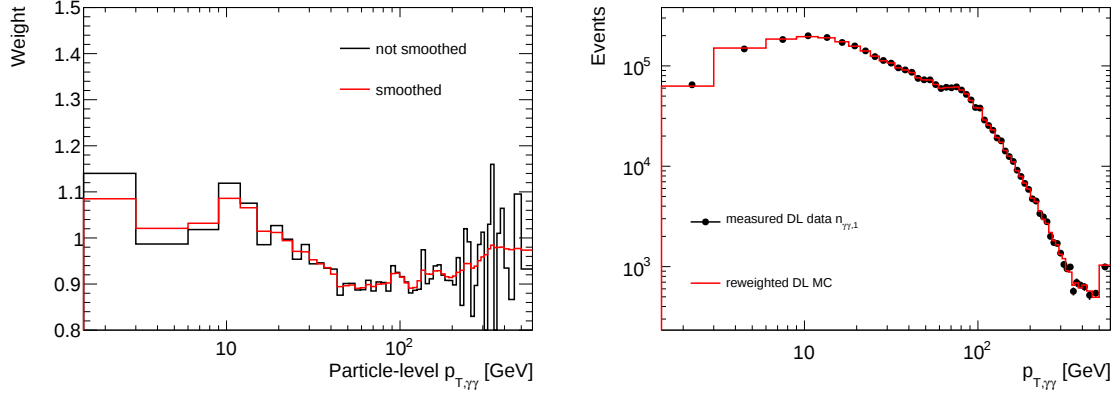


Figure 7.35.: Comparison of PL weights (left) derived for MC to match the DL data with no smoothing ($\lambda = 0$) or choosing λ to get $\chi^2 = 1$. Comparison of the DL distribution of the reweighted MC with the data (right).

The weights for the observable $p_{T,\gamma\gamma}$ are shown in Fig. 7.35 and compared to the not smoothed weights derived with $\lambda = 0$. The DL distribution of the reweighted MC shows good agreement with data. The values for $p_{T,\gamma\gamma}$ are shown because this is the observable for which the largest bias from the prior is observed.

The systematic uncertainty from the bias due to the MC prior is shown in Fig. 7.36 (left) for different numbers of iterations. Even for $p_{T,\gamma\gamma}$ the uncertainties are below 1% when using more than one iteration. The MC priors are stabilizing the results thus increasing the number of iterations does slightly increase the data statistical uncertainty which is shown in Fig. 7.36 (right). For this analysis the number of iterations is chosen to be 3, which reduces the bias down to a negligible level for all observables except $p_{T,\gamma\gamma}$ where it is slightly above 1% in the lowest bin.

Hidden Variable Test

The uncertainty due to hidden variables is also estimated based on a reweighting to the MC sample. The main concern addressed by this systematic uncertainty is that the efficiency correction for a given observable bin depends on the modelling of e.g. the latent p_{T,γ_1} distribution in this bin, because the efficiencies are p_T dependent. The uncertainty is derived by applying the reweighting calculated for p_{T,γ_1} for the uncertainty from the MC prior to the MC sample. The analysis is then redone for the other observables using the reweighted MC observables to estimate the impact of the mis-modelling in the hidden p_{T,γ_1} observable. The signal efficiencies for the background estimation and the unfolding are slightly changed. The impact of using the reweighted MC instead of the nominal MC on the different steps of the analysis are depicted in Fig. 7.37. For this uncertainty there is only one variation and the change of the final result is symmetrized to get the other variation. The uncertainty is below 1% in all bins of all observables.

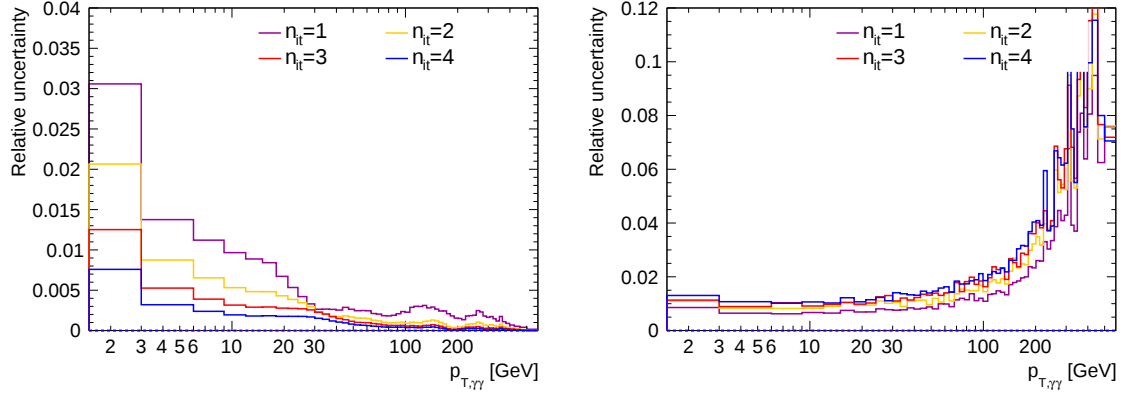


Figure 7.36.: The left plot shows the systematic uncertainty from the bias due to the MC prior for different numbers of iterations in the unfolding procedure. The right hand plot shows the estimated data statistical uncertainty.

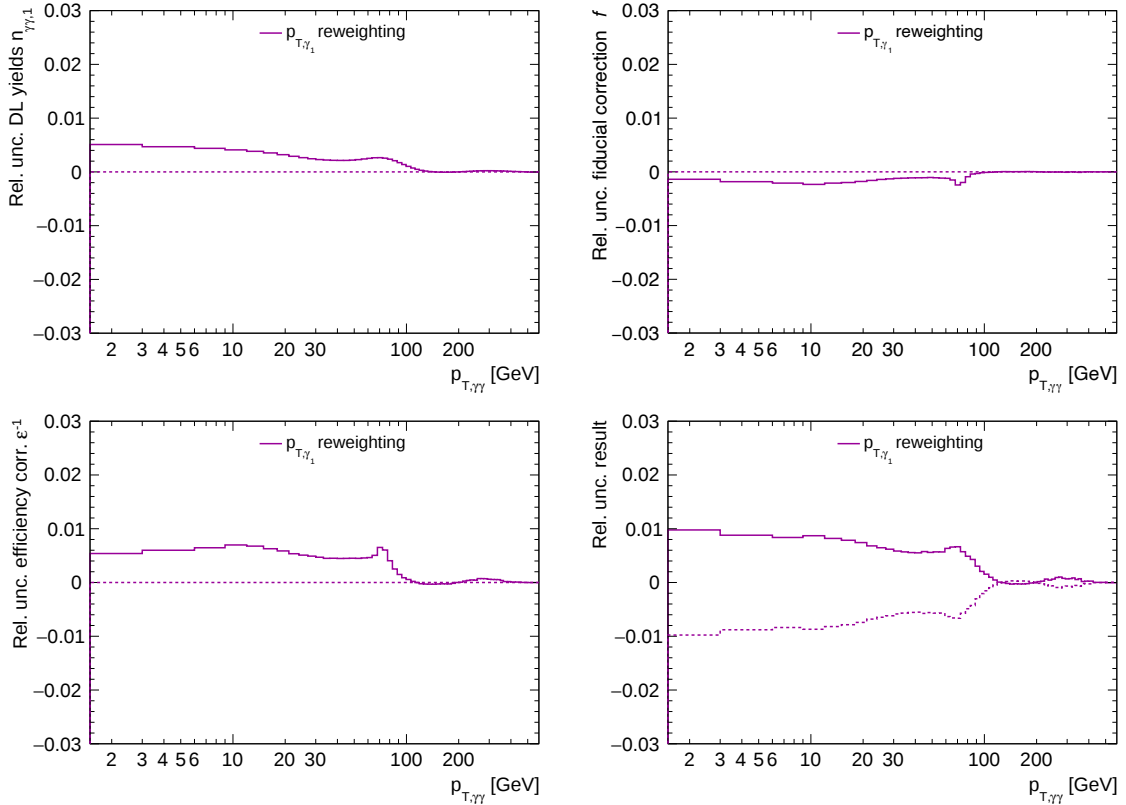


Figure 7.37.: Change of different steps of the analysis using a MC sample reweighted to match the data result for p_{T,γ_1} . The change of the detector level signal after background estimation (top left), the fiducial correction (top right), the efficiency correction (bottom left) and the full result (bottom right) are shown.

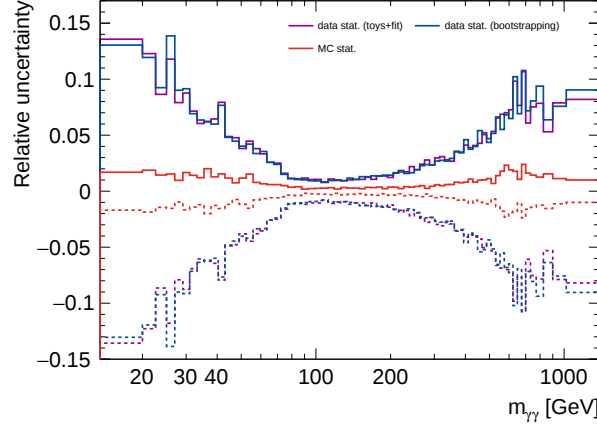


Figure 7.38.: Relative uncertainty due to limited data and MC statistics on the measured cross section as a function of $m_{\gamma\gamma}$.

7.7.9. Data and MC statistical uncertainties

The uncertainty from limited data statistics are estimated by default based on the uncertainty of the likelihood fit of the background estimation. This uncertainty is propagated to the final result using toys, which are generated by adding Gaussian noise according to the uncertainties of the likelihood fit to the detector-level signal yields. Each toy is unfolded and the standard deviation among the results of the toys is used to estimate the statistical uncertainty. Due to the unfolding the yields of multiple DL bins enter into the result of one PL bin, which causes slight correlations between the statistical uncertainty of the result of different bins. These correlations can also be estimated from the toys and are very small between the bins of a single observable, because of the large bin sizes and diagonal response matrices.

To cross check the uncertainty estimation of the likelihood fit, another pseudo-experiment based method referred to as bootstrapping is used [167]. The toys for this method are generated by assigning random Poissonian distributed weights with expectation value one to each event. For each set of randomized data points the background estimation fit and unfolding is performed. The statistical uncertainty based on bootstrapping and based on the likelihood fit are compared in Fig. 7.38 and are compatible. The bootstrapping method also enables the estimation of the correlations of the statistical uncertainty between bins of different observables, which can share large fractions of events.

The correlation matrices for ϕ_η^* versus $\pi - \Delta\phi_{\gamma\gamma}$ and $a_{T,\gamma\gamma}$ versus $\pi - \Delta\phi_{\gamma\gamma}$ are depicted in Fig. 7.39. As described in Section 7.4 these observables are strongly correlated.

The full correlation matrices between the statistical uncertainty of the results of all bins of all observables are provided as part of the detailed results published on the HEPData portal [162] and need to be taken into account if the spectra of multiple observables are interpreted together e.g. in a combined fit.

The uncertainty from limited MC statistics are also estimated with the bootstrapping method. The toys are used to estimate the input parameters for the background estimation and for the unfolding to take the correlations between the different steps into account. As shown in Fig. 7.38 for $m_{\gamma\gamma}$, the

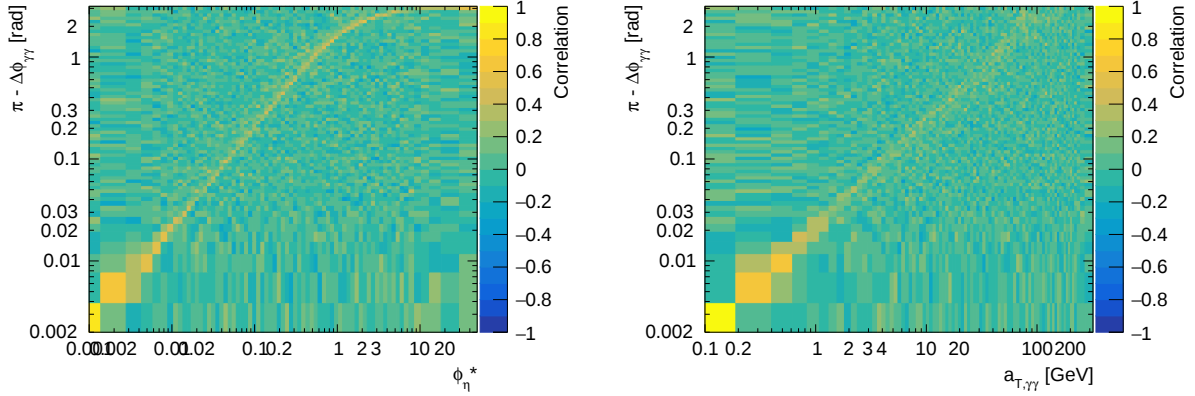


Figure 7.39.: Correlation of the uncertainty from data statistics between bins of different observables.

MC statistical uncertainty is negligible in comparison to the data statistical uncertainty.

7.8. Theory predictions

The different predictions which are compared to the measured results in the following Section 7.9 are described in this section.

SHERPA

The SHERPA signal prediction is described in Section 7.2.1 already. Different uncertainties on the prediction are evaluated:

- A 7-point variation of the factorisation and renormalisation scale μ_F and μ_R is applied as described in Section 2.2 to estimate the perturbative uncertainties.
- The uncertainties of the NNPDF3.0NNLO PDF set [137] are considered by using the varied PDF sets.
- The sensitivity to the strong coupling constant is evaluated by varying $\alpha_s(m_Z)$ in the range between 0.117-0.119 and varying a PDF set correspondingly.

The uncertainties are evaluated using event reweighting [168] and are completely dominated by the scale variations.

NNLOJET

The NNLOJET program [49] is used to create fixed-order predictions at NNLO for diphoton production. The $gg \rightarrow \gamma\gamma$ loop process is included at LO in these NNLO calculations. The same program with a similar setup is also used to calculate the LO and NLO predictions to study the convergence of the perturbative series. The factorisation and renormalisation scales are set to $\mu_R = \mu_F = m_{\gamma\gamma}$ and a 7-point variation is used to estimate the uncertainties from the scale choice. The studies in Ref. [50]

indicate that using the average of the two photon transverse momenta as a scale choice improves the prediction. The NNPDF3.0NNLO PDF set [137] is used.

The calculations rely on a hybrid isolation scheme [40, 169, 170] combining a very loose smooth-cone isolation [45] with $n = 2$, $\delta_0 = 0.1$, $\varepsilon = 0.1$ (cf. Section 2.3) with the experimental isolation criterion of the fiducial phase space definition in Table 7.2. The smooth-cone isolation is required to avoid divergences of collinear photon emissions. The combination of the loose smooth-cone isolation with the tight experimental criterion reduces the possible bias introduced by different isolation cuts in theory and experiment.

DIPHOX

DIPHOX [41] is used to calculate fixed-order predictions at NLO taking into account the photon fragmentation and therefore not relying on a smooth-cone isolation criterion. The CT10 NLO PDF set [171] is used for the calculations. The factorisation, renormalisation and fragmentation scales are set to $\mu_R = \mu_F = \mu_{\text{frag}} = m_{\gamma\gamma}$. The renormalisation and factorisation scale are varied according to the 7-point scheme. The fragmentation scale is varied by a factor of 2 and 1/2. The calculations are redone using the PDF sets MSTW2008 [172] and NNPDF2.3 [120] as variations. The renormalisation and factorisation scale are again the dominant variations.

7.9. Results

7.9.1. Integrated fiducial cross section

The differential cross sections resulting from the measurement are integrated to calculate the integrated fiducial cross section. This has the advantage over a one-bin analysis of avoiding possible biases from the modelling of the kinematic distribution in the MC sample, because e.g. the efficiency corrections depend on the kinematics as shown in Section 7.6.3. The values integrated over the different observables are compatible within 0.1 pb and the value from integrating over p_{T,γ_1} is reported as result, because the efficiency corrections vary most strongly for this observable. The measured integrated fiducial cross section is:

$$\sigma_{\gamma\gamma} = 31.4 \pm 0.1 \text{ (stat.)} \pm 2.4 \text{ (syst.) pb.}$$

The relative uncertainties of different sources were summarized in Table 7.3. The measured values are compared to the different theory predictions in Fig. 7.40 and Table 7.4. Only the NNLO and the SHERPA prediction agree with the measured values within uncertainties. The LO and NLO values severely underestimate the cross-section indicating the importance of the qg and gg initiated production channels with fragmentation photons opening up at NLO and NNLO. The scale variation uncertainties of the LO and NLO predictions are much smaller than the difference to the measured values, which is a prime example of the insufficiency of scale variations for the estimation of missing higher-order corrections. The DIPHOX NLO values are slightly higher than the NNLOJET NLO values, but compatible within uncertainties, which means the resummation of fragmentation photons in DIPHOX yields similar results as the hybrid isolation scheme used for NNLOJET in the isolated fiducial phase space measured here. The uncertainties of the NNLO predictions are smaller than the SHERPA

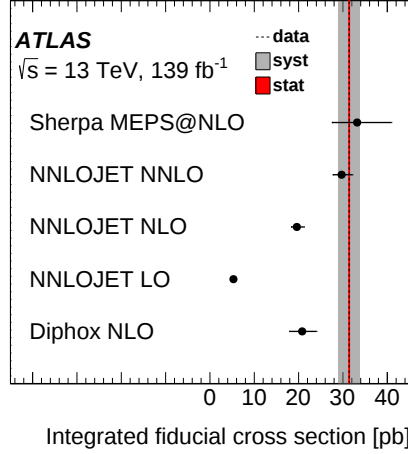


Figure 7.40.: Integrated fiducial cross-section comparison between ATLAS data and theory predictions [38].

uncertainty and are of similar size as the experimental uncertainties on the measured values. The large uncertainty of SHERPA is caused by the high jet multiplicities included through LO matrix elements, which exhibit a larger sensitivity to the renormalisation scale uncertainty.

Table 7.4.: Integrated fiducial cross section from ATLAS data compared to theory predictions with their systematic uncertainties from QCD scale variations [38].

Fiducial cross section [pb]	$\sigma_{\gamma\gamma}$	$\pm$ unc.
SHERPA MEPS@NLO	33.2	+7.7 -5.6
NNLOJET NNLO	29.7	+2.4 -2.0
NLO	19.6	+1.6 -1.3
LO	5.3	+0.5 -0.5
DIPHOX NLO	20.8	+3.2 -2.9
Data	31.4	2.4

7.9.2. Differential cross sections

The measured differential cross sections as a function of the 8 analysed observables are compared to the DIPHOX NLO, NNLOJET NNLO and the SHERPA predictions in Figs. 7.41 and 7.42.

The measured differential cross-section values usually span more than four orders of magnitude showcasing the rich statistics of the LHC Run-2 data. The cross sections are measured up to very high values of $m_{\gamma\gamma} \sim 1$ TeV and $p_{T,\gamma\gamma} \sim 500$ GeV. The fine binning in the high statistics region reflects the excellent detector resolution for photons enabling e.g. measurements of very low $p_{T,\gamma\gamma} \sim 5$ GeV

configurations in bins of $\Delta p_{T,\gamma\gamma} \sim 3$ GeV. The momentum with respect to the direction transverse to the diphoton trust $a_{T,\gamma\gamma}$ can be resolved with even higher precision down to the sub-GeV regime.

The p_{T,γ_1} spectrum is described well by the NNLOJET NNLO and SHERPA predictions within the uncertainties. The DIPHOX NLO prediction describes the exponentially decreasing spectrum qualitatively, but underestimates the normalisation by around 30% as seen for the integrated values. For p_{T,γ_2} the NNLOJET NNLO and SHERPA predictions perform similarly well, whereas the DIPHOX NLO values exhibit a larger deviation at low values $p_{T,\gamma_2} < 40$ GeV, which indicates important contributions of $\gamma\gamma+2$ jet configurations in this regime.

The differential cross section as a function of $m_{\gamma\gamma}$ shows relatively low rates at $m_{\gamma\gamma} < 70$ GeV followed by a sharp rise peaking around $m_{\gamma\gamma} \sim 90$ GeV and turning into an exponential decrease towards high $m_{\gamma\gamma}$. The values of $m_{\gamma\gamma} < 70$ GeV require additional jets in the event causing the necessary boost of the photon-pair system given the thresholds of $p_{T,\gamma_1}(p_{T,\gamma_2}) > 40(30)$ GeV of the measurement. The spectrum is described well by SHERPA and NNLOJET NNLO. The low $m_{\gamma\gamma} < 70$ GeV region is severely underestimated by the DIPHOX prediction whereas the values at higher $m_{\gamma\gamma}$ show mainly the inclusive normalisation offset.

The $|\cos\theta^*|^{(\text{CS})}$ observable is an angular variable correlated with the pseudo-rapidity gap $\Delta\eta_{\gamma\gamma}$ between the photons (cf. Section 7.4). The $|\cos\theta^*|^{(\text{CS})}$ spectrum is relatively flat monotonically decreasing towards $|\cos\theta^*|^{(\text{CS})} \sim 1$. The shape is well described by all predictions up to $|\cos\theta^*|^{(\text{CS})} < 0.8$, with larger discrepancies in particular for the DIPHOX NLO and NNLOJET NNLO predictions towards $|\cos\theta^*|^{(\text{CS})} \sim 1$. This region of photon pairs with a large rapidity gap $\Delta\eta_{\gamma\gamma}$ is characterized by multiple additional jets responsible for the decorrelation of the photons.

The observables ϕ_η^* , $\pi - \Delta\phi_{\gamma\gamma}$, $p_{T,\gamma\gamma}$ and $a_{T,\gamma\gamma}$ share some common features. They are all trivially fixed at 0 in the absence of additional emissions to the photon pair, which corresponds to the LO description of the process. This means the (N)NLO fixed-order calculations of this spectrum are effectively (N)LO. Low values of these observable are associated to soft wide-angle or collinear emissions, which are only contained in resummed predictions e.g. utilizing parton-shower algorithms like the SHERPA samples and can not be described by fixed-order calculations. This justifies the fact, that only the SHERPA predictions give an excellent description of the full spectra, whereas the DIPHOX NLO and the NNLOJET NNLO predictions are not valid at the lower end of the spectra.

The $p_{T,\gamma\gamma}$ spectrum shows a peak around $p_{T,\gamma\gamma} \sim 10$ GeV which is the difference of the p_{T,γ_1} and p_{T,γ_2} thresholds and corresponds e.g. to back-to-back configurations with close to minimal p_{T,γ_1} and p_{T,γ_2} . The ‘shoulder’ in the spectrum around $p_{T,\gamma\gamma} \sim 70$ GeV indicates the onset of $\Delta\phi_{\gamma\gamma} < \pi/2$ configurations and is again a consequence of the $p_{T,\gamma}$ thresholds [173]. A similar feature can be observed for $a_{T,\gamma\gamma} \sim 60$ GeV. As shown in Fig. 7.3, $a_{T,\gamma\gamma}$ and $p_{T,\gamma\gamma}$ are similar for low $\Delta\phi_{\gamma\gamma} < \pi/2$ and approximately symmetric $p_{T,\gamma_1}/p_{T,\gamma_2} \sim 1$ configurations. The shifted position of the feature for $a_{T,\gamma\gamma}$ with respect to $p_{T,\gamma\gamma}$ can be explained by the asymmetry of the thresholds reducing the values of $a_{T,\gamma\gamma}$ with respect to the corresponding $p_{T,\gamma\gamma}$. These regions of $p_{T,\gamma\gamma} > 70$ GeV and $a_{T,\gamma\gamma} > 60$ GeV are well described by the SHERPA and the NNLOJET NNLO predictions within their respective uncertainties. The DIPHOX NLO prediction also exhibits the shoulder in the spectrum, but underestimates the normalisation.

The $\pi - \Delta\phi_{\gamma\gamma}$ spectrum shows the high prevalence of back-to-back $\Delta\phi_{\gamma\gamma} > \pi/2$ configurations. Although the dominance of these events is reflected in the fixed-order DIPHOX and NNLOJET predictions, the exact shape of the spectrum is sensitive to wide-angle radiation, which is very well

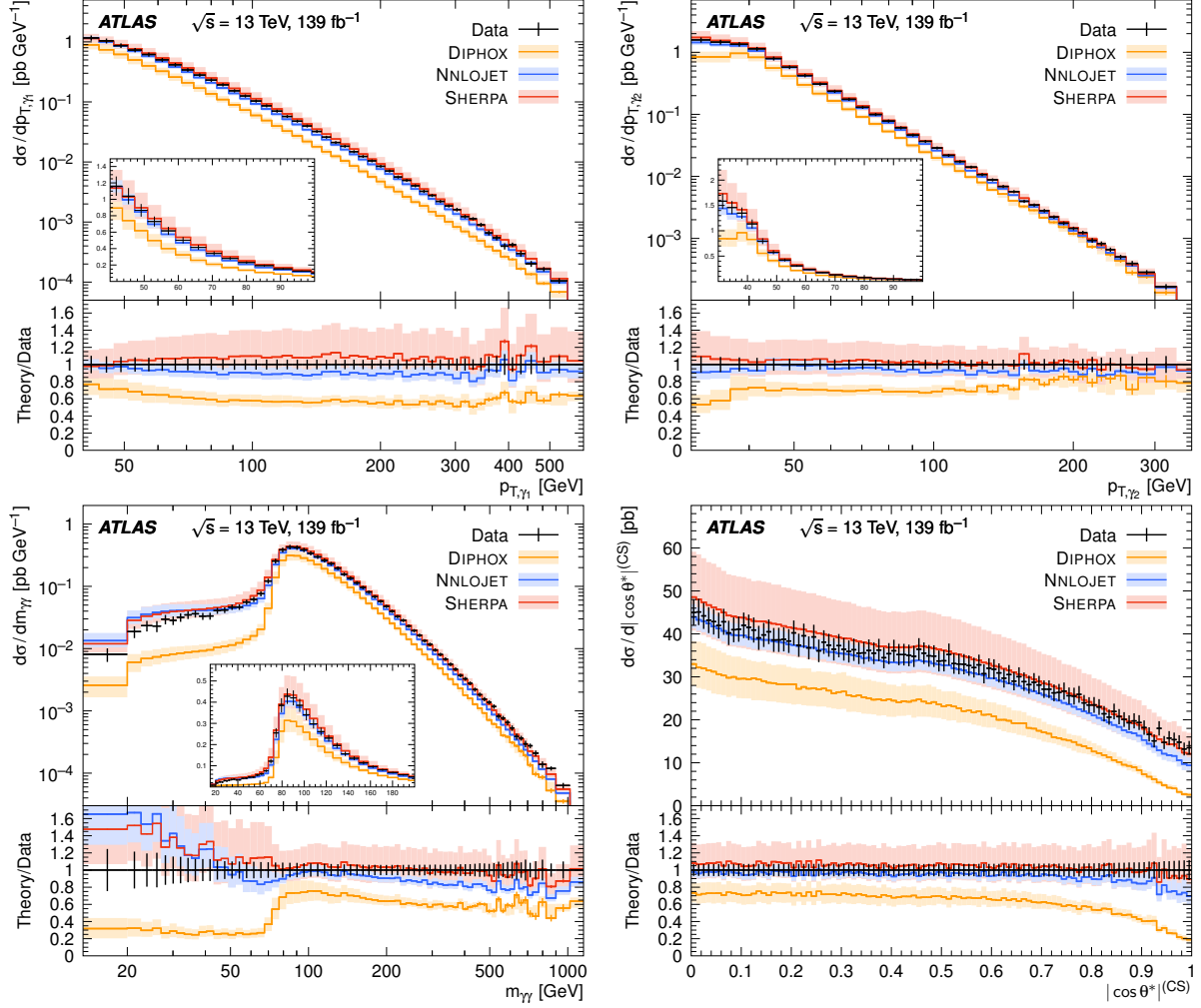


Figure 7.41.: Differential cross sections measured as functions of p_{T,γ_1} , p_{T,γ_2} , $m_{\gamma\gamma}$ and $|\cos \theta^*|^{(CS)}$ (black error bars) compared with the predictions from DIPHOX NLO, NNLOJET NNLO and SHERPA MEPS@NLO (lines with coloured bands). At the bottom of each plot, the ratio of the prediction to the data is shown. Uncertainty bars on the data represent the total uncertainty, while uncertainty bands (bars) on the predictions represent perturbative scale (statistical) uncertainties. Inset plots show the core of each distribution on a linear scale. For p_{T,γ_1} , p_{T,γ_2} and $m_{\gamma\gamma}$ the last bin is only visible in the ratio inset and includes the overflow events [38].

modelled by SHERPA as shown by the impressive agreement with the measured spectrum. The ϕ_η^* spectrum shows similar features as the $\pi - \Delta\phi_{\gamma\gamma}$ as it is mostly given by a transformation of $\Delta\phi_{\gamma\gamma}$ with slight influences of $\Delta\eta_{\gamma\gamma}$ (cf. Section 7.4). The region of very low azimuthal separation of the photons $\pi - \Delta\phi_{\gamma\gamma} > 2.7$ is highlighted by the high $\phi_\eta^* > 5$ region and is only possible with $\Delta\eta_{\gamma\gamma} > 0$, because of the $\Delta R_{\gamma\gamma} > 0.4$ requirement. This region is well described by the NNLOJET NNLO and by the SHERPA prediction.

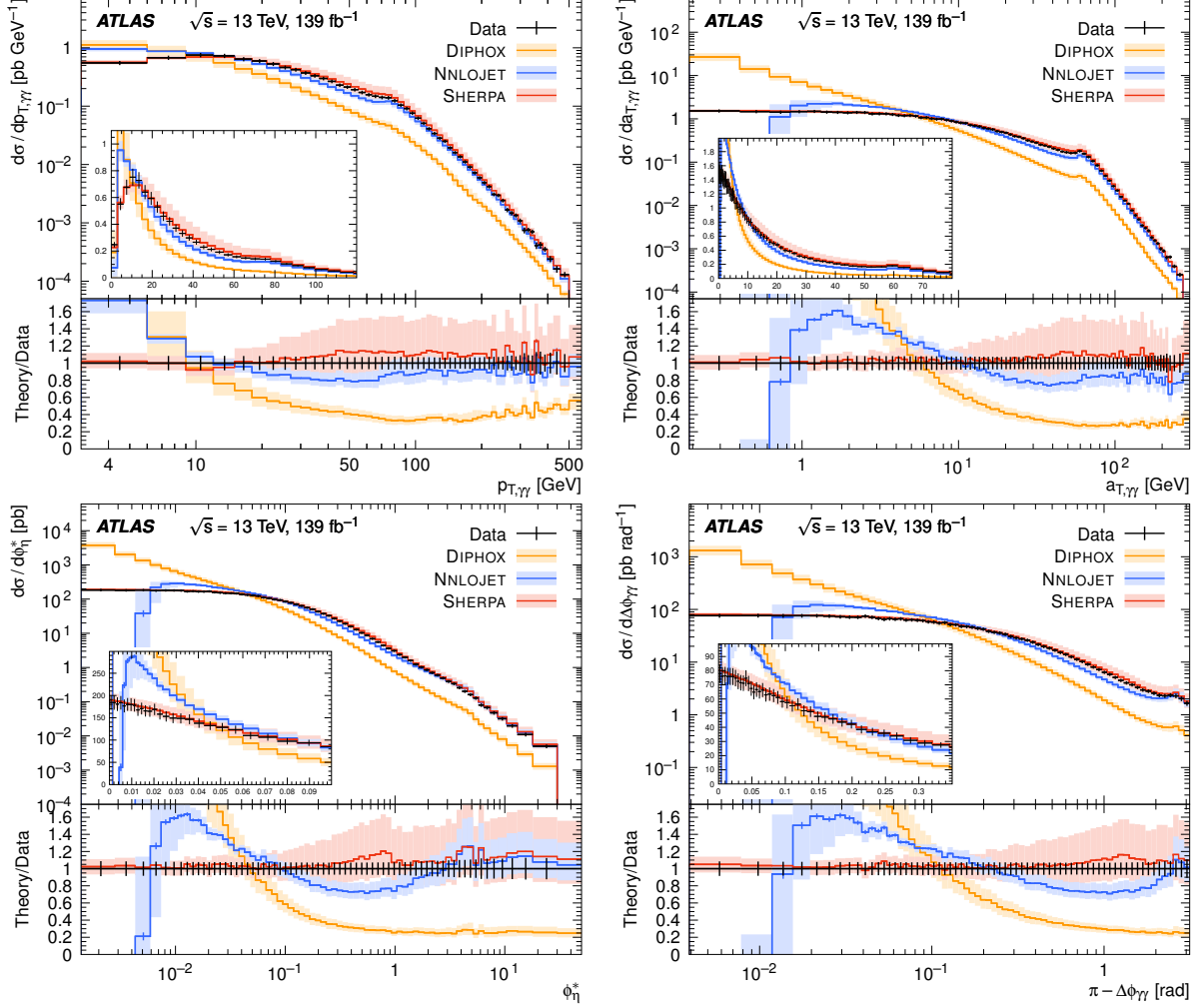


Figure 7.42.: Differential cross sections measured as functions of $p_{T,\gamma\gamma}$, $a_{T,\gamma\gamma}$, ϕ_η^* and $\pi - \Delta\phi_{\gamma\gamma}$ (black error bars) compared with the predictions from DIPHOX NLO, NNLOJET NNLO and SHERPA MEPS@NLO (lines with coloured bands). At the bottom of each plot, the ratio of the prediction to the data is shown. Uncertainty bars on the data represent the total uncertainty, while uncertainty bands (bars) on the predictions represent perturbative scale (statistical) uncertainties. Inset plots show the core of each distribution on a linear scale. For ϕ_η^* , $p_{T,\gamma\gamma}$ and $a_{T,\gamma\gamma}$ the last bin is only visible in the ratio inset and includes the overflow events [38].

Chapter 8.

Summary and Outlook

8.1. Summary

The data-driven validation and correction of simulated samples is indispensable for reliable and precise measurements, because simulations are instrumental in the interpretation of the detector-level data. In Chapters 5 and 6 the performance of the detector simulation was studied with respect to important quantities relevant to the photon-pair measurement presented in Chapter 7.

In Chapter 5 isolation variables were scrutinized, which are used ubiquitously by almost all ATLAS measurements involving photons, electrons or muons. The calorimetric isolation variables were studied as a function of pileup providing insights which will gain additional importance with the ever increasing pileup of future runs of the LHC. The studies were performed data-driven in a pure sample of $Z \rightarrow ee$ events. An improved pileup subtraction was proposed which stabilises the isolation variables as a function of η and will be part of the ATLAS wide recommendations for future measurements with electrons and photons using the calorimetric isolation. The peak position and width of the isolation distribution as a function of pileup was studied and compared between data and MC. A pileup dependent shift to the MC distribution is derived to match the peak position with data. A large overestimation of the pileup noise in MC was observed, which leads to an increased width of the isolation distribution in MC with respect to data. The pileup noise in MC depends on the modelling of the simulated minimum-bias events with which the MC samples are overlayed. The isolation distributions using different minimum-bias generators were compared and the results were taken into account for the choice of the new improved minimum-bias overlay which will be used for the production of a new collection of MC samples by ATLAS. An intermediate fix for the isolation distributions was derived by reducing the amount of pileup in MC samples and was used to correct the photon isolation related quantities in the photon pair measurement presented in Chapter 7.

In Chapter 6 a measurement of photon selection efficiencies in $Z \rightarrow \mu\mu\gamma$ events was performed. The approach of the measurement enabled the simultaneous measurement of the isolation efficiency, the identification efficiency, the reconstructed photon conversion fraction and most importantly the photon-to-electron ambiguity resolution efficiency. The photon-to-electron ambiguity resolution is part of the photon reconstruction and removes around 4% of electron-like photon candidates. Previously no correction to this efficiency was applied assuming that it is well modelled in the simulation. The measurements performed in Chapter 6 showed that the photon-to-electron losses are underestimated in MC especially at high $|\eta|$ of the photon candidate. The corresponding correction is applied for

the photon-pair measurement in Chapter 7 and increases the nominal cross-section result by 1.8%. Furthermore, the measurement was repeated separately for subsamples corresponding to different data-taking years, and it was found that slightly different MC corrections are needed for the different years. This could hint to changing experimental conditions between the different data-taking years which are not taken into account in the respective simulated samples.

In Chapter 7 the first measurement of the production of pairs of isolated photons in proton–proton collisions at $\sqrt{s} = 13$ TeV has been presented which was also published in [38]. The full LHC Run-2 data recorded by ATLAS corresponding to an integrated luminosity of $\mathcal{L} = 139 \text{ fb}^{-1}$ has been used. This large dataset provides unprecedented statistics for a photon-pair measurement in hadron collisions. Differential cross sections in several kinematic variables of the photon pairs were measured in a fiducial phase space characterised by a good detector performance. The signal yields were corrected for background, detector resolution effects and detector inefficiencies. The particle-level results of this analysis provide a valuable precise benchmark for QCD predictions underpinning LHC physics. The results are provided easily accessible on the HEPData portal and as a Rivet implementation [161, 162, 174, 175]. The influence of various uncertainties on the result were evaluated and the leading uncertainties are related to the photon isolation efficiencies and the background estimation. In the bulk of the kinematic distributions the precision is limited by the systematic uncertainties with relative uncertainties around 7.5% which is smaller than or at the same level as the uncertainties of current state-of-the-art theory predictions. One particular test comparing the measured cross sections between different years showed differences in the results which are larger than the uncertainties considered as uncorrelated between the years. Various studies were launched including the measurement in Chapter 6 to understand these differences, but the reason could not be identified, thus yielding an additional uncertainty covering the discrepancies between the individual years and the full result which amounts to around 3%. An integrated fiducial cross section of $\sigma_{\gamma\gamma} = 31.4 \pm 0.1 \text{ (stat.)} \pm 2.4 \text{ (syst.) pb}$ has been measured. The integrated and differential cross-sections were compared to state-of-the-art QCD predictions and showed good agreement within uncertainties with fixed-order NNLO calculations and for NLO calculations merged with Monte Carlo parton showers.

The presented measurement is part of the large program of ATLAS cross-section measurements (cf. Fig. 8.1) which probe the range of validity of SM predictions from the most common to even the rarest processes. Because significant deviations of the measured values from the SM prediction would be an indication of BSM physics, cross-section measurements provide a complementary approach to searches for specific BSM signatures.

8.2. Outlook

In the upcoming LHC Run-3 the centre-of-mass energy will increase slightly, potentially to $\sqrt{s} = 13.6$ TeV, and the integrated luminosity is expected to be of similar size as the one collected in LHC Run-2. This means the kinematic reach and statistical sensitivity e.g. for rare highly-energetic BSM processes will only be extended moderately, further shifting the focus of the LHC physics program to precision measurements.

The systematic uncertainties of the photon-pair measurement is currently at the same level as the scale uncertainties of NNLO calculations to which the results have been compared. With the upcoming more precise calculations, e.g. the new $pp \rightarrow \gamma\gamma + \text{jet}$ calculations at NNLO [55] or resummed

$N^3\text{LL} + \text{NNLO}$ calculations [53, 54], the experimental uncertainties might be challenged and the leading experimental uncertainties related to the photon isolation and background estimation could be revisited. The background estimation could be improved by deriving more detailed knowledge about the background of relatively isolated neutral hadron decays like $\pi^0 \rightarrow \gamma\gamma$. The distribution of photon identification variables for such background events could be measured e.g. in events with hadronic tau decays $\tau^\pm \rightarrow h^\pm + \pi^0 + \nu$ from W - or Z -decays requiring a large enough separation between the neutral electromagnetic cluster and the track. MC samples with sufficient statistics of isolated and mis-identified photon candidates in di-jet and γ +jet events would also represent an improvement. Ref. [64] mentions the option to achieve this by placing constraints at generator level. The isolation uncertainties are dominantly related to the overestimation of the pileup noise in the MC samples. This uncertainty could be reduced correcting the detector-level MC isolation variables by rescaling them based on the particle-level values. Furthermore, improvements to the isolation variables to reduce their sensitivity to pileup could be investigated, e.g. using promising approaches originally developed for jet measurements. Particle-flow objects [177] could be used, which are created by combining tracking information and calorimeter clusters and remove clusters matched to tracks from pileup vertices. The pileup subtraction could be applied on constituent level [178], which refers to the momenta of the individual clusters or particle-flow objects. Applying these algorithms to the isolation variables needs careful performance studies, e.g. because the low isolation energy regime of up to a few GeV is most important while jet measurements usually start only at 20 GeV, such that the improvements for jets can easily deteriorate the isolation variables.

In future photon-pair measurements the isolation distribution of the photons could be measured and unfolded, which could be used to scrutinise predictions for fragmentation photons. On the experimental side this measurement would benefit from a calibrated isolation energy more closely matching the particle-level quantity e.g. by applying the local hadronic calibration (LCW) [104] to the input clusters or even novel deep-learning based calibration strategies [179].

With the excellent statistics of the photon-pair dataset it would be possible to measure double-differential cross sections especially in the low p_T -regime. As multi-dimensional binned approaches quickly run into problems with too many bins to still have sufficient statistics in all of them, and with being comprehensible by humans, a novel unbinned multidimensional unfolding approach could be used [180].

The photon-pair analysis could be extended by measuring also the jets in the event directly. The diphoton + 2 jet category could be used for a first measurement of electroweak production of photon pairs by requiring a large rapidity gap between the jets [39]. The zero jet category might be sensitive to the top-loop contribution of gluon-gluon initiated photon-pair production enabling a top-mass measurement [181, 182]. In the inclusive measurement presented here these contributions are expected to be at the sub-percent level even for $m_{\gamma\gamma} > 2m_t$.

Finally, also the number of measured photons could be increased. A first measurement of three photon final states has been performed at $\sqrt{s} = 8$ TeV by ATLAS [183]. Four photon production has not been measured yet and has an expected cross-section of around 50 ab at $\sqrt{s} = 13$ TeV in a fiducial phase space accessible by ATLAS [184]. Such a low cross section would be very challenging to measure, but it might be achievable in the future e.g. by including the data from the coming LHC Run-3 or even from the high luminosity LHC [83].

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Appendix A.

SHERPA-to-PYTHIA particle-level isolation reweighting

The accuracy of the SHERPA and PYTHIA samples will vary in different regions of phase space. Fragmentation photons produced in PYTHIA parton shower are a good description for collinear (non-isolated) configurations, while the NLO matrix elements used in the SHERPA description gives a better modelling of well-separated (isolated) configurations. Furthermore, also the kinematic range will be different: the photon isolation distribution will be completely inclusive in the PYTHIA sample, while it is cut off with a very loose smooth-cone isolation in the higher-order matrix elements of the SHERPA sample. In summary, their approaches for the modelling of prompt photon production should be different enough to give a good estimate of uncertainties induced by modelling.

SHERPA is used as the nominal event generator in this analysis, and one could repeat the whole analysis chain with the PYTHIA sample to estimate the uncertainty. The available PYTHIA sample is severely affected by duplicated events. Thus, instead of using the sample directly, a reweighting is derived from SHERPA to PYTHIA based on the PL isolation distribution of the photons, which is described in more detail in the following. The duplicated events in the Pythia sample can not easily be removed and are kept for this study. To minimize the influence of these duplicated events, which mostly affect the results of the following studies by enhancing statistical fluctuations over their estimate, the reweighting is smoothed.

The two dimensional relative PL isolation distribution of the leading and subleading photon $E_{T,PL}^{\text{cone20}}/p_{T,\gamma}$ are compared in the two samples (cf. Fig. A.1). As expected the photons in the Sherpa sample tend to be more isolated. A ratio PYTHIA/SHERPA is calculated which is applied as a weight to SHERPA (cf. Fig. A.2). The ratio is smoothed to minimize fluctuations of the weight. A comparison between the 2D relative PL isolation in PYTHIA and the reweighted one in SHERPA is depicted in Fig. A.3. As closure test the weight is applied to SHERPA and the 1D relative PL isolation distributions are plotted (cf Fig. A.4). Good agreement can be observed. The residual difference is due to the smoothing. The influence of the reweighting on the DL isolation efficiency is shown in Fig. A.5 as a function of the mass of the diphoton system. As expected the isolation efficiencies are lowered. The reweighting scheme is used to estimate the uncertainty associated with theoretical modelling of the photon isolation in the absence of a usable PYTHIA sample. For all relevant quantities calculated from the MC samples for the analysis (e.g. efficiency corrections) some isolation criterion is always applied: either the DL requirement, the PL requirement or both.

Appendix A. SHERPA-to-PYTHIA particle-level isolation reweighting

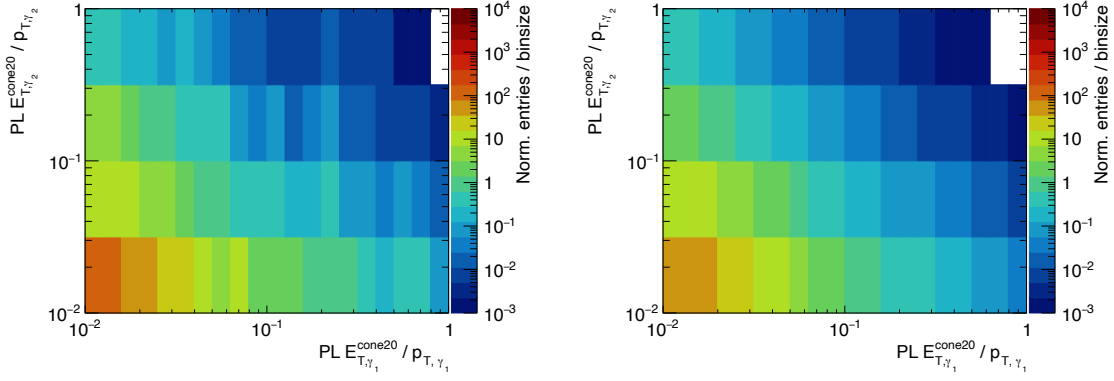


Figure A.1.: Distribution of the relative PL isolation of the leading and subleading photon for PYTHIA (left) and SHERPA (right).

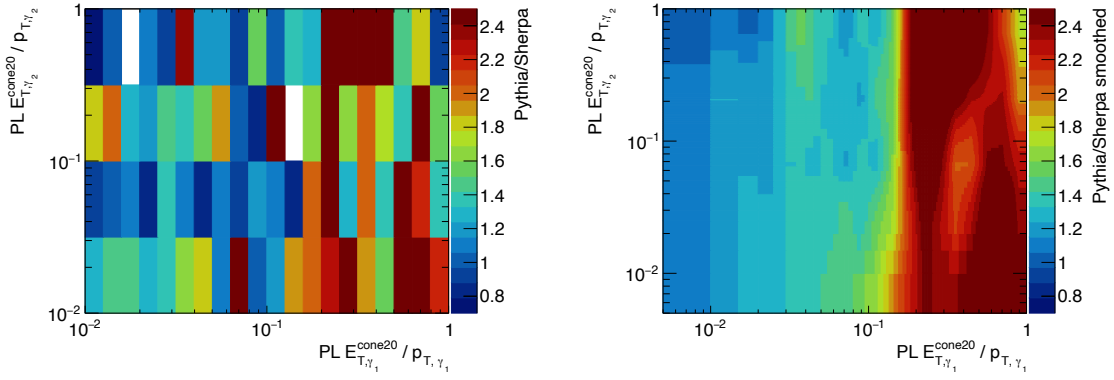


Figure A.2.: Ratio PYTHIA/SHERPA as a function of the relative PL isolation of the two photons unsmoothed (left) and smoothed (right). The smoothed ratio is used for the reweighting.

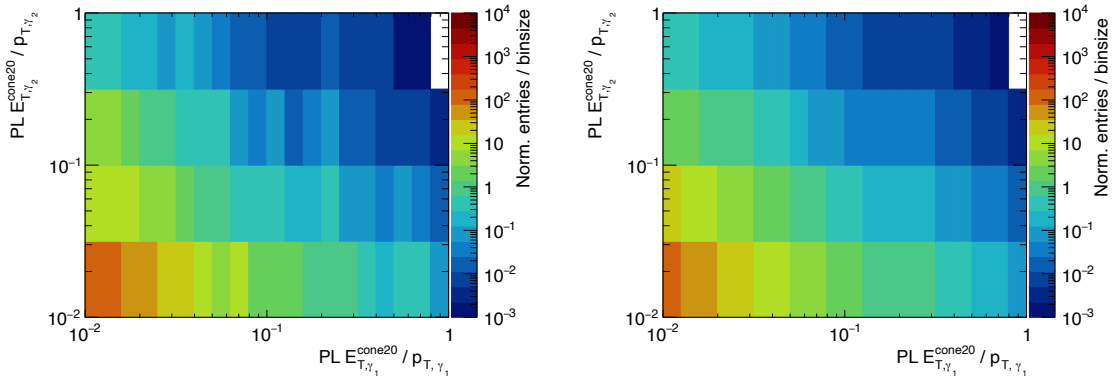


Figure A.3.: Comparison of the 2D relative PL isolation distributions of PYTHIA (left) and SHERPA after reweighting (right).

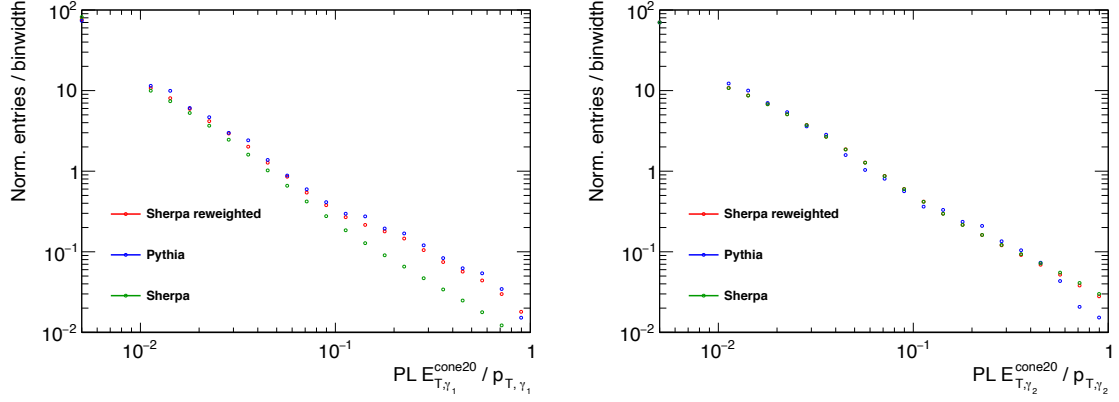


Figure A.4.: Comparison of the relative PL isolation distribution for SHERPA (green), reweighted SHERPA (red) and PYTHIA (blue) for the leading (left) and subleading (right) photon. The closure is not perfect because of the smoothing. In general the photons in the PYTHIA sample are less isolated than in the SHERPA samples. The lowest bins extend to 0.

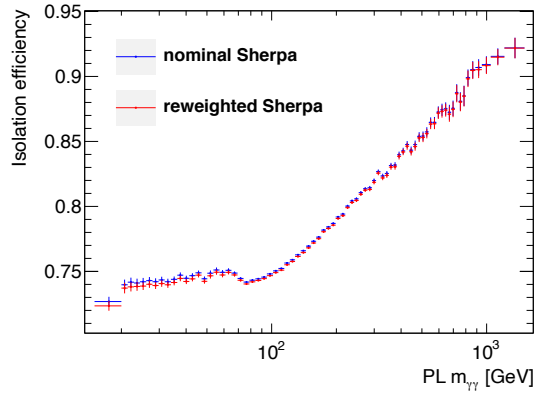


Figure A.5.: Efficiencies for both photons to fulfill the DL isolation requirement as a function of the mass for the nominal (blue) and reweighted (red) SHERPA sample. As expected the reweighting is decreasing the isolation efficiencies. Note that the efficiencies are calculated with respect to events which fulfill the DL isolation described in Section 7.6.5.

Appendix B.

Optimization of the detector-level isolation requirement

The DL isolation cut has been optimised by repeating the whole analysis chain including the background estimation and the unfolding for different isolation requirements and comparing the uncertainties. The relative and absolute values of the isolation requirement are varied and two different cone sizes E_T^{cone40} and E_T^{cone20} are tested. For each DL isolation configuration the closest PL isolation cut is computed as described in Section 7.6.5. The only sizeable impact of the PL isolation working point on the uncertainties is visible for the uncertainty related to the theory modelling of the isolation derived by applying the PYTHIA-to-SHERPA reweighting.

The different options are summarized in Fig. B.1. In Fig. B.2 the uncertainties of the data-driven shifts from the isolation and from the pileup reweighting (cf. Section 7.7.4) are compared between the different working points. Looser isolation cuts and the smaller cone size yield smaller uncertainties.

In Fig. B.3 the uncertainties from the PYTHIA-to-SHERPA reweighting and from the isolation–identification correlation in the background estimation are compared. The PYTHIA-to-SHERPA uncertainty is decreased by switching to the narrow cone of $\Delta R = 0.2$, because the PYTHIA and SHERPA PL isolation distributions match more closely for this smaller cone compared to $\Delta R = 0.4$. In general the isolation–identification correlation uncertainty is reduced for looser isolation cuts, although for very loose requirements the uncertainty is increasing again.

In Fig. B.4 the uncertainty from limited statistics and the total uncertainty of the different DL isolation requirements are depicted. For looser isolation cuts the statistical uncertainty is increased due to the decrease in purity in the signal region. The total uncertainty is optimal for:

$$E_T^{\text{cone20}} < 0.05 \cdot E_T$$

Appendix B. Optimization of the detector-level isolation requirement

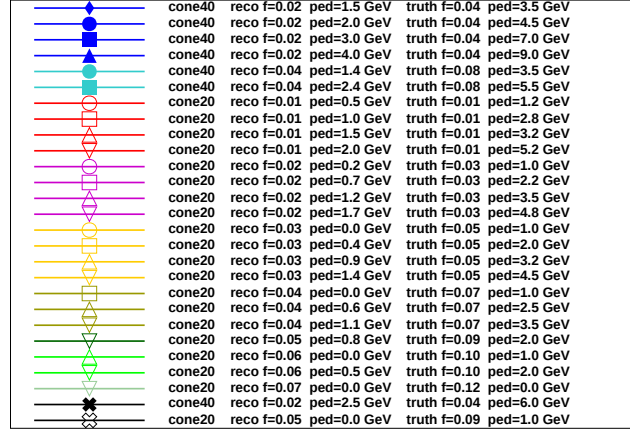


Figure B.1.: Legend of different PL isolation working point configurations. Different colors indicate different fractional isolation cuts and different markers different pedestal values. Empty markers correspond to an isolation cone with $\Delta R = 0.2$ and filled markers to an isolation cone with $\Delta R = 0.4$.

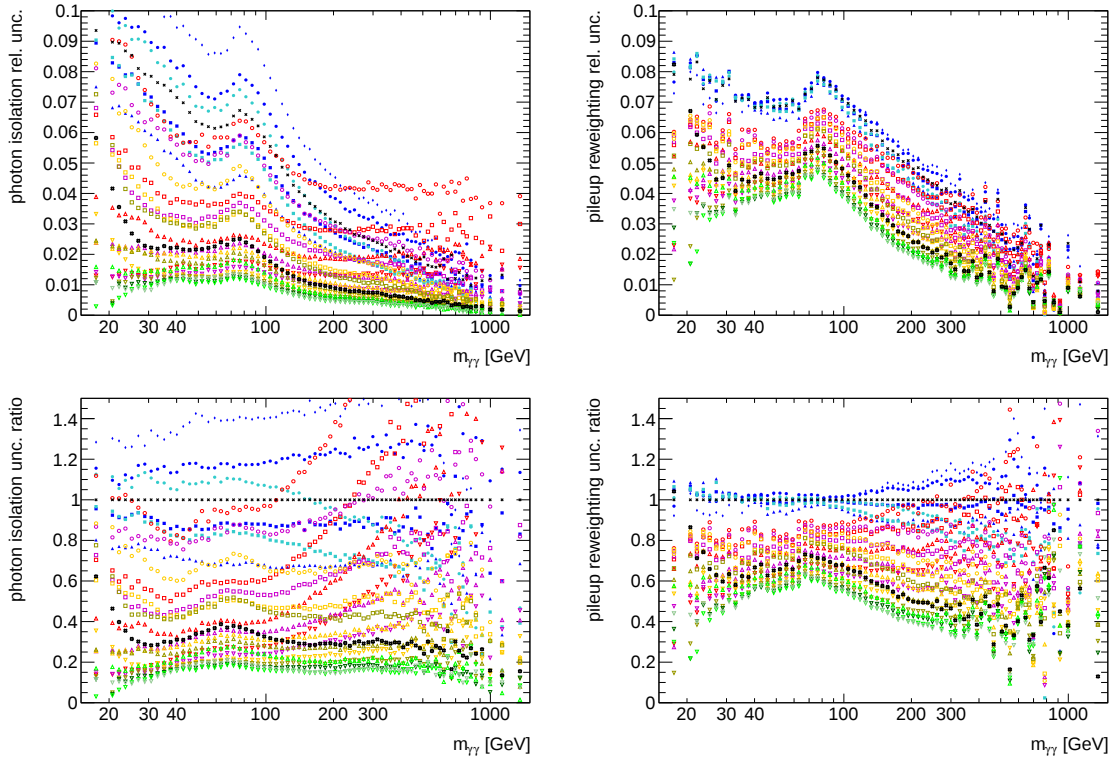


Figure B.2.: Relative uncertainty on the final result due to the variation of the data-driven shift of the isolation variables (left) and pileup reweighting variation (right) as a function of $m_{\gamma\gamma}$ (top). Ratio of the relative uncertainty with respect to the DL requirement: $E_T^{\text{cone40}} < (0.022 \cdot p_{T,\gamma} - 2.45 \text{ GeV})$ (bottom).

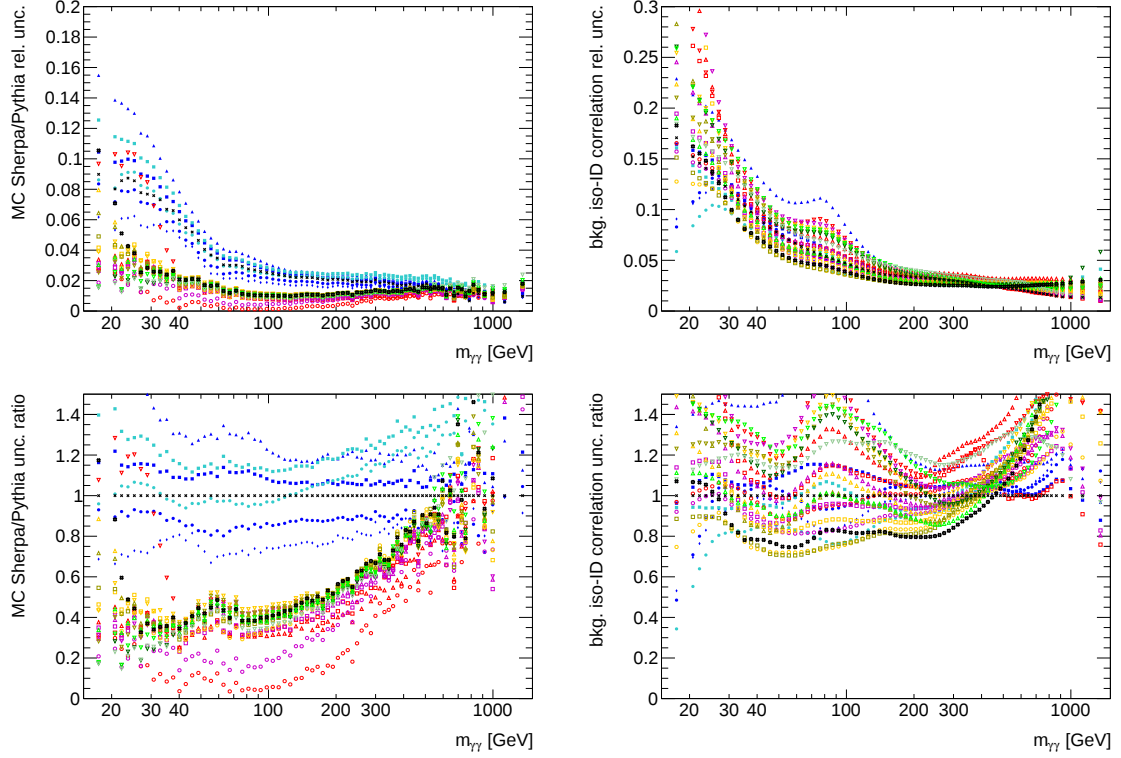


Figure B.3.: Relative uncertainty on the final result from the theory isolation modelling uncertainty (left) and from the isolation–identification correlation of mis-identified photons (right) as a function of $m_{\gamma\gamma}$ (top). Ratio of the relative uncertainty with respect to the DL requirement: $E_T^{\text{cone40}} < (0.022 \cdot p_{T,\gamma} - 2.45 \text{ GeV})$ (bottom).

Appendix B. Optimization of the detector-level isolation requirement

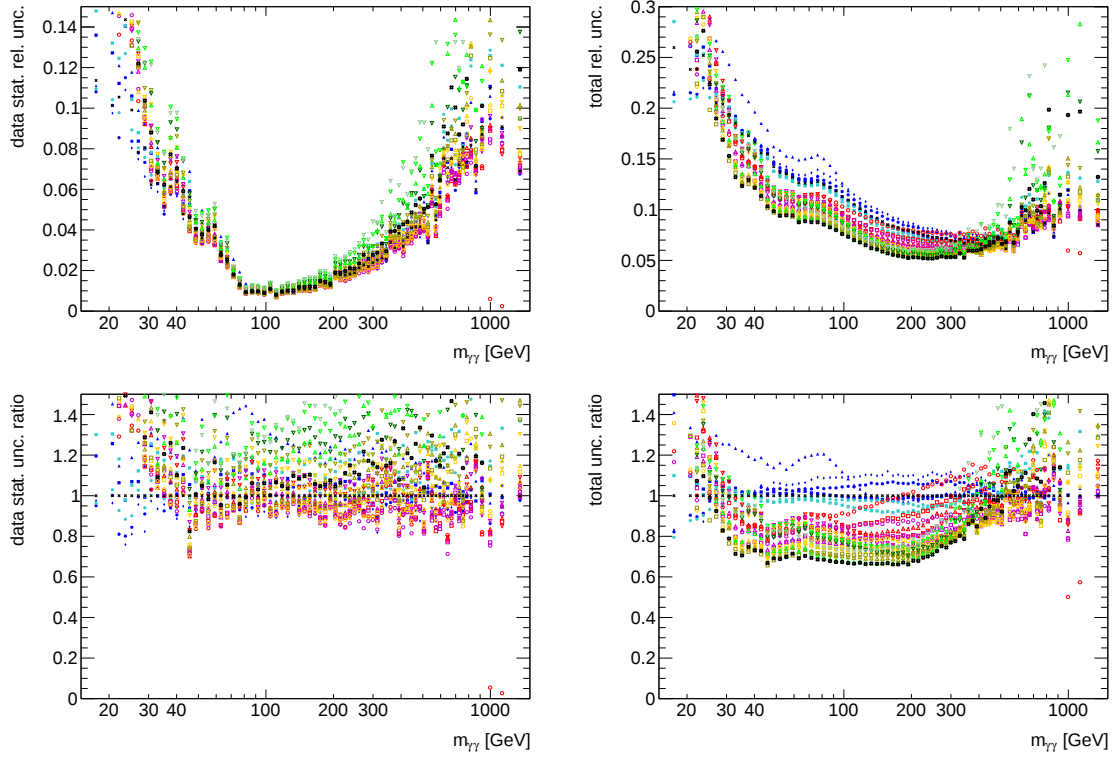


Figure B.4.: Relative uncertainty of the final result due to data statistics (left) and total relative uncertainty (right) as a function of $m_{\gamma\gamma}$ (top). Ratio of the relative uncertainty with respect to the DL requirement: $E_T^{\text{cone40}} < (0.022 \cdot p_{T,\gamma} - 2.45 \text{ GeV})$ (bottom).

Appendix C.

Scale factors and anti-scale factors

In the photon-pair measurement scale factors f are used to correct the modelling of the photon identification efficiencies. These are centrally provided to all ATLAS analysis by measurements as published in Ref. [103]. The most recent Summer 2020 precision recommendations are used¹.

The scale factors are provided in p_T , $|\eta|$ and conversion category bins of the photons and are defined as the ratio of the data $\varepsilon^{\text{data,id}}$ and MC $\varepsilon^{\text{MC,id}}$ identification efficiencies:

$$f_{\gamma_{1(2)}}^{\text{id}}(p_T, \gamma_{1(2)}, |\eta_{\gamma_{1(2)}}|) = \frac{\varepsilon_{\gamma_{1(2)}}^{\text{data,id}}(p_T, \gamma_{1(2)}, |\eta_{\gamma_{1(2)}}|)}{\varepsilon_{\gamma_{1(2)}}^{\text{MC,id}}(p_T, \gamma_{1(2)}, |\eta_{\gamma_{1(2)}}|)}$$

They are applied as an event weight w_{SF} to events where both photons pass the identification requirement:

$$w_{\text{SF}} = f_{\gamma_1}^{\text{id}} f_{\gamma_2}^{\text{id}}.$$

To retain the overall number of events anti-SFs $\bar{f}$ for the photons not passing the identification requirement are calculated:

$$\bar{f} = \frac{1 - f \varepsilon^{\text{MC}}}{1 - \varepsilon^{\text{MC}}}.$$

These diphoton events migrating into the control regions are important for the background estimation. The MC efficiencies ε^{MC} needed for the calculation are estimated on the SHERPA diphoton sample using the leading photon and the same $|\eta|$, p_T and conversion category bins as the provided scale factors. The denominator contains all events where the leading reconstructed photon matches to a PL photon in the fiducial $|\eta|$ and $\Delta R_{\gamma\gamma}$ region. The numerator contains the events where this photon also passes the ID requirement. This means it is assumed that the number of events effectively subtracted from or added to the signal region by the application of the scale factors migrate are still reconstructed. The MC identification efficiencies are depicted in Fig. C.1. The tight identification scale factor map and its up and down variation is depicted in Fig. C.2. The corresponding anti scale factors are shown in Fig. C.3. The scale factors are in general compatible with one and consequently also the anti-scale factors are. The anti-scale factors have much larger variations, because high identification efficiencies cause small relative variations of the efficiencies to yield large relative variations of the inefficiencies.

¹They are retrieved from: `/cvmfs/atlas.cern.ch/repo/sw/database/GroupData/PhotonEfficiencyCorrection/2015_2018/rel21.2/Summer2020_Rec_v1/efficiencySF.offline.Tight.13TeV.rel21.25ns.[u]con.v01.root`

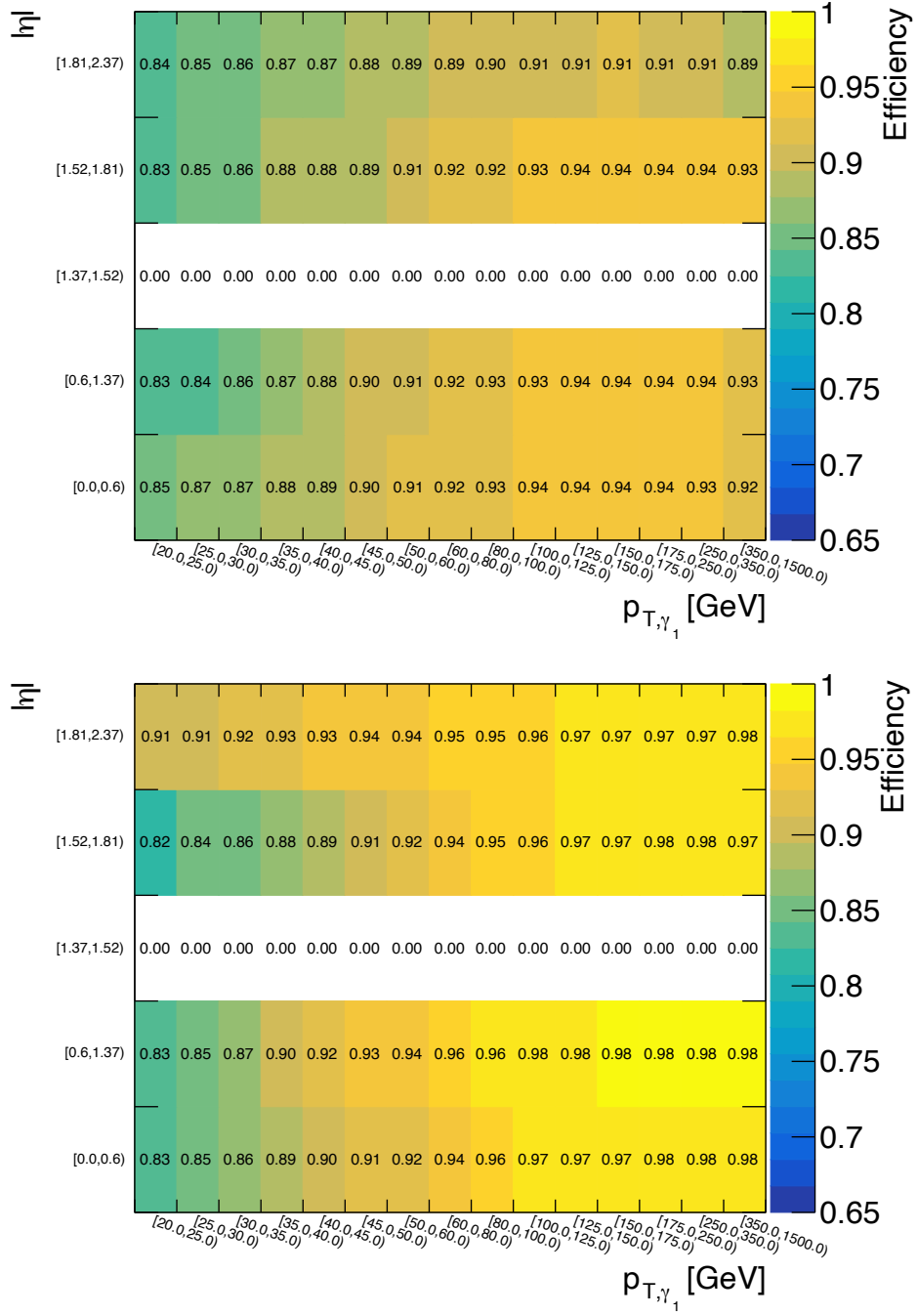


Figure C.1.: The MC identification efficiencies for the leading photon in the SHERPA signal samples for converted (top) and unconverted (bottom) cases are depicted as a function of $|\eta|$ and p_T of the photon.

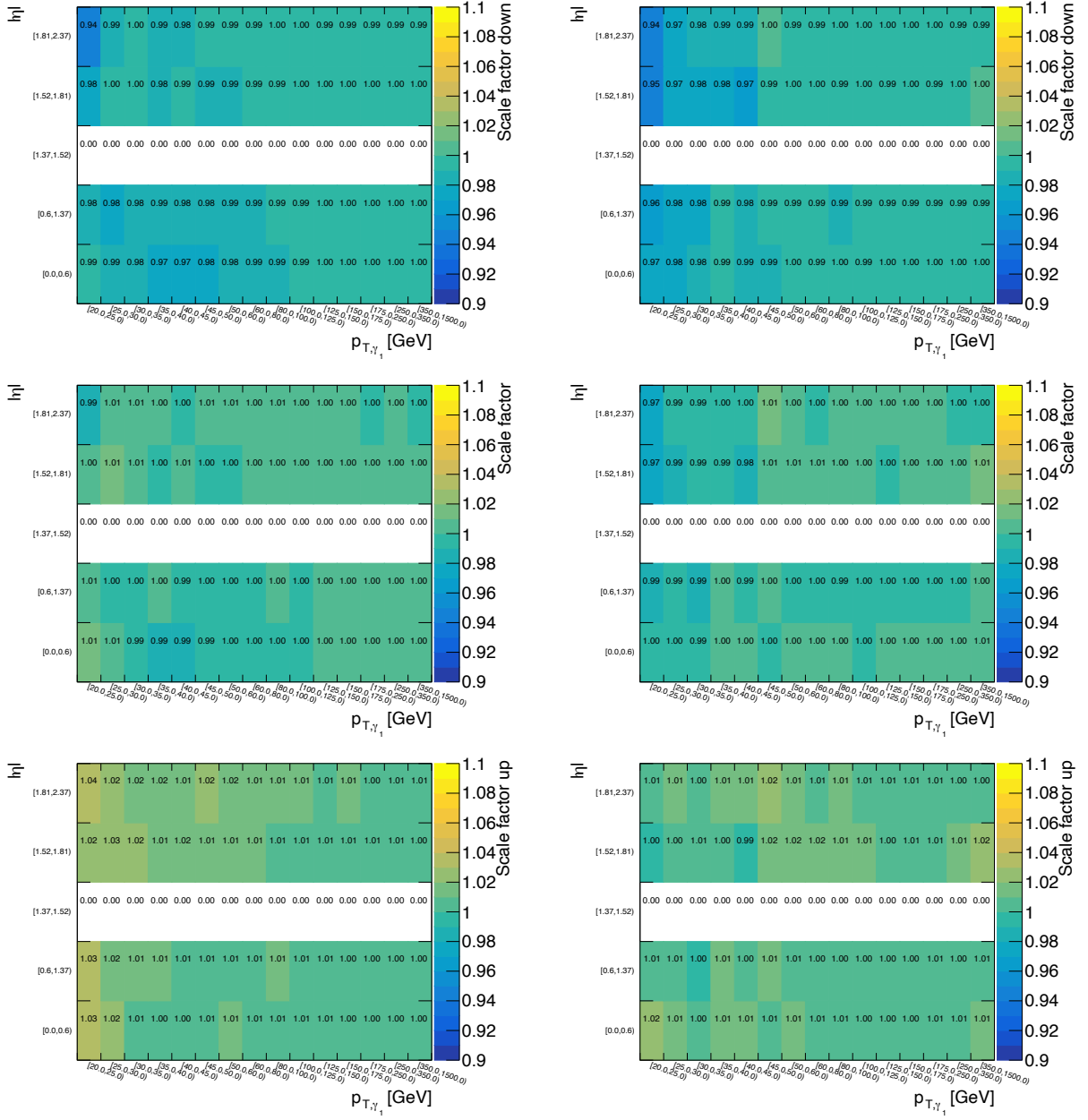


Figure C.2.: Tight photon identification scale factor as a function of $|\eta|$ and p_T . Down variation (top) nominal value (middle) and up variation (bottom) for converted (left) and unconverted (right) photons.

Appendix C. Scale factors and anti-scale factors

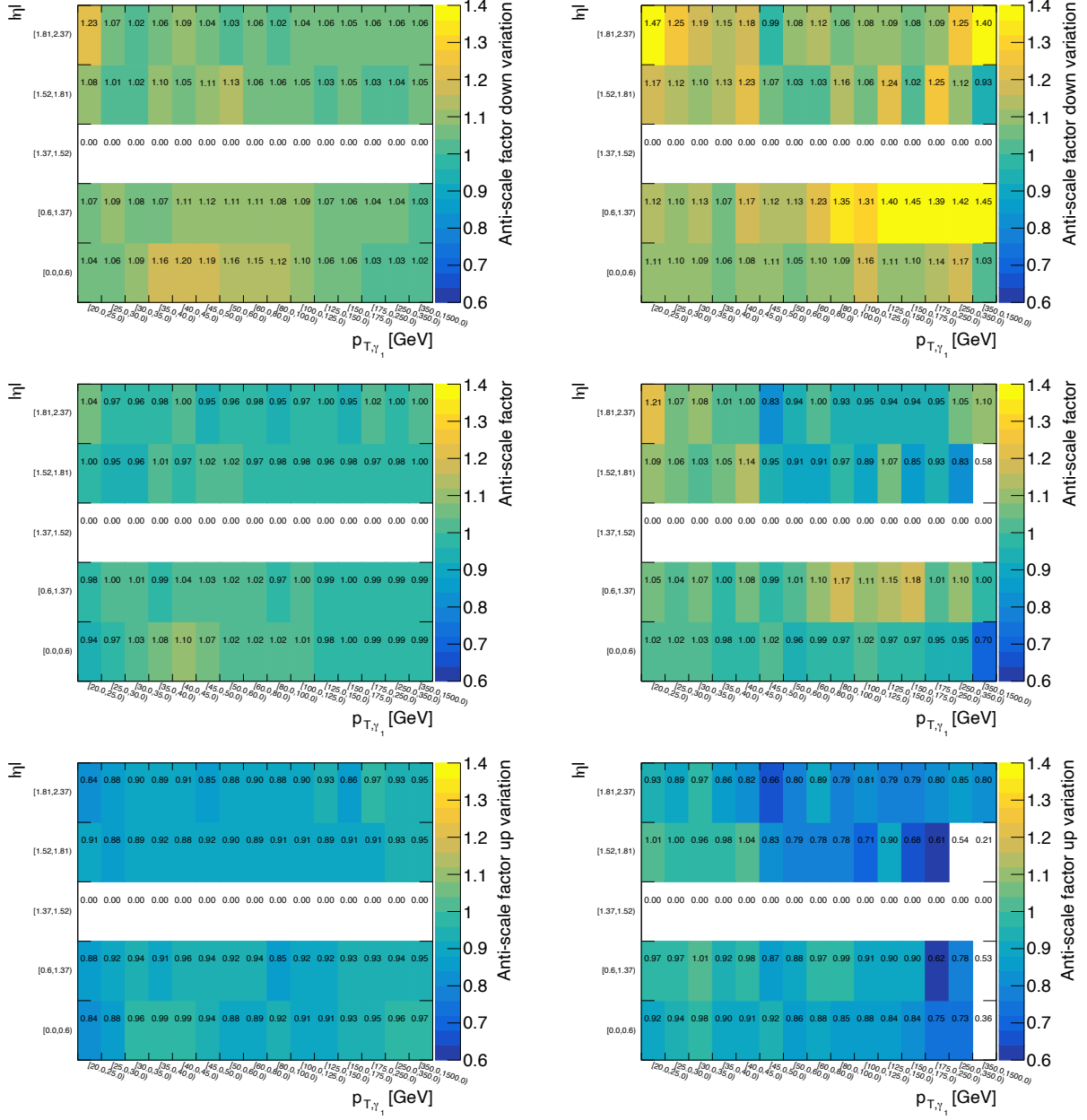


Figure C.3.: Anti-identification scale factor as a function of $|\eta|$ and p_T calculated from the MC identification efficiencies and the scale factors. Down variation (top) nominal value (middle) and up variation (bottom) for converted (left) and unconverted (right) photons.

Appendix D.

Additional figures of the diphoton measurement

In this appendix figures for the complete set of observables in the diphoton measurement are collected. The main features are usually discussed based on reduced sets of observables for which plots are included in the main body.

Appendix D. Additional figures of the diphoton measurement

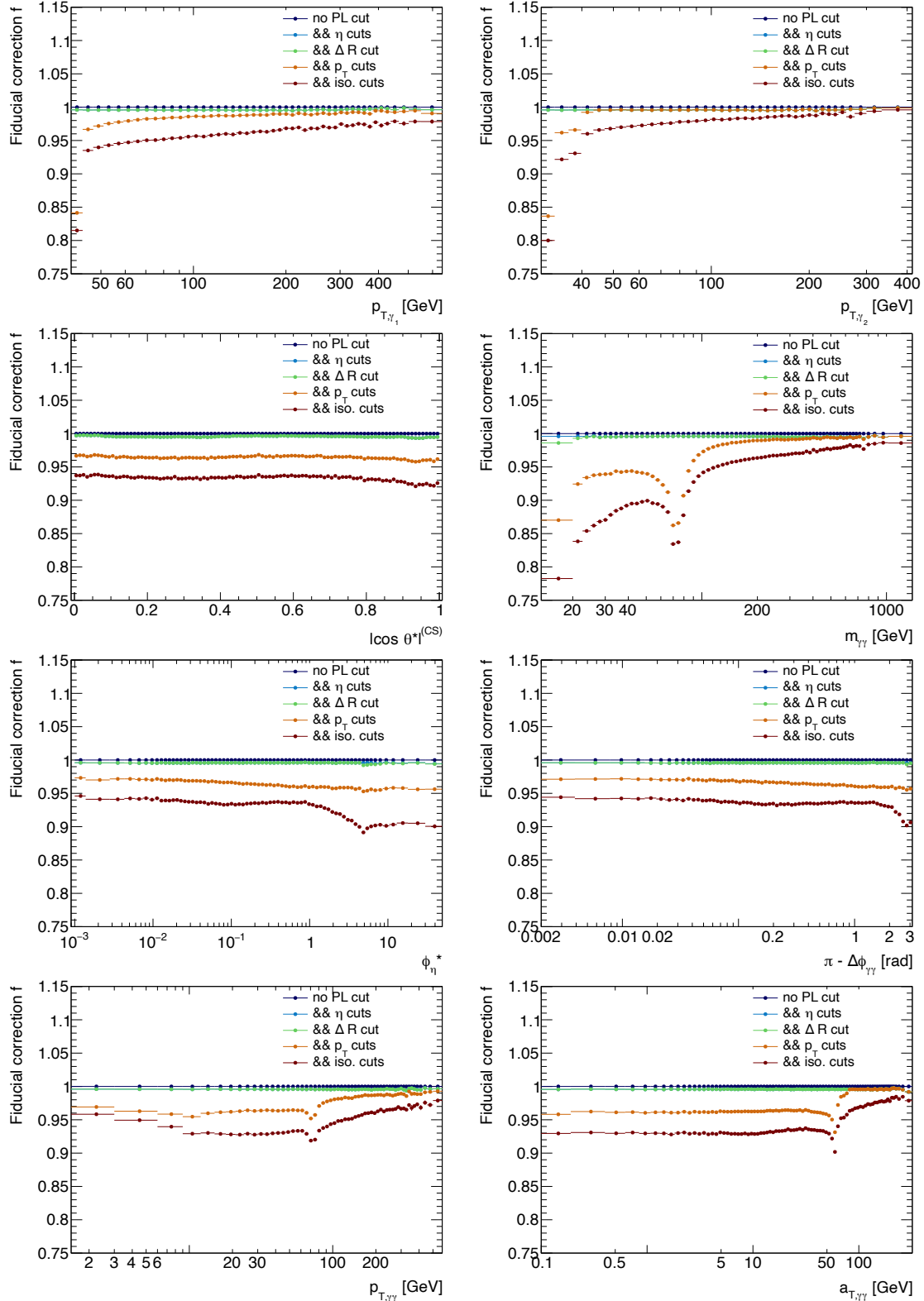


Figure D.1.: The fiducial correction is shown as a function of p_{T,γ_1} , p_{T,γ_2} , $|\cos \theta^*|^{(CS)}$, $m_{\gamma\gamma}$, ϕ_η^* , $\pi - \Delta\phi_{\gamma\gamma}$, $p_{T,\gamma\gamma}$ and $a_{T,\gamma\gamma}$. The different colours indicate different steps in the particle-level selection. The lowest points correspond to the fiducial correction for the full particle-level selection. The denominator for all points is the number of all MC photon pair events which pass the detector level selection.

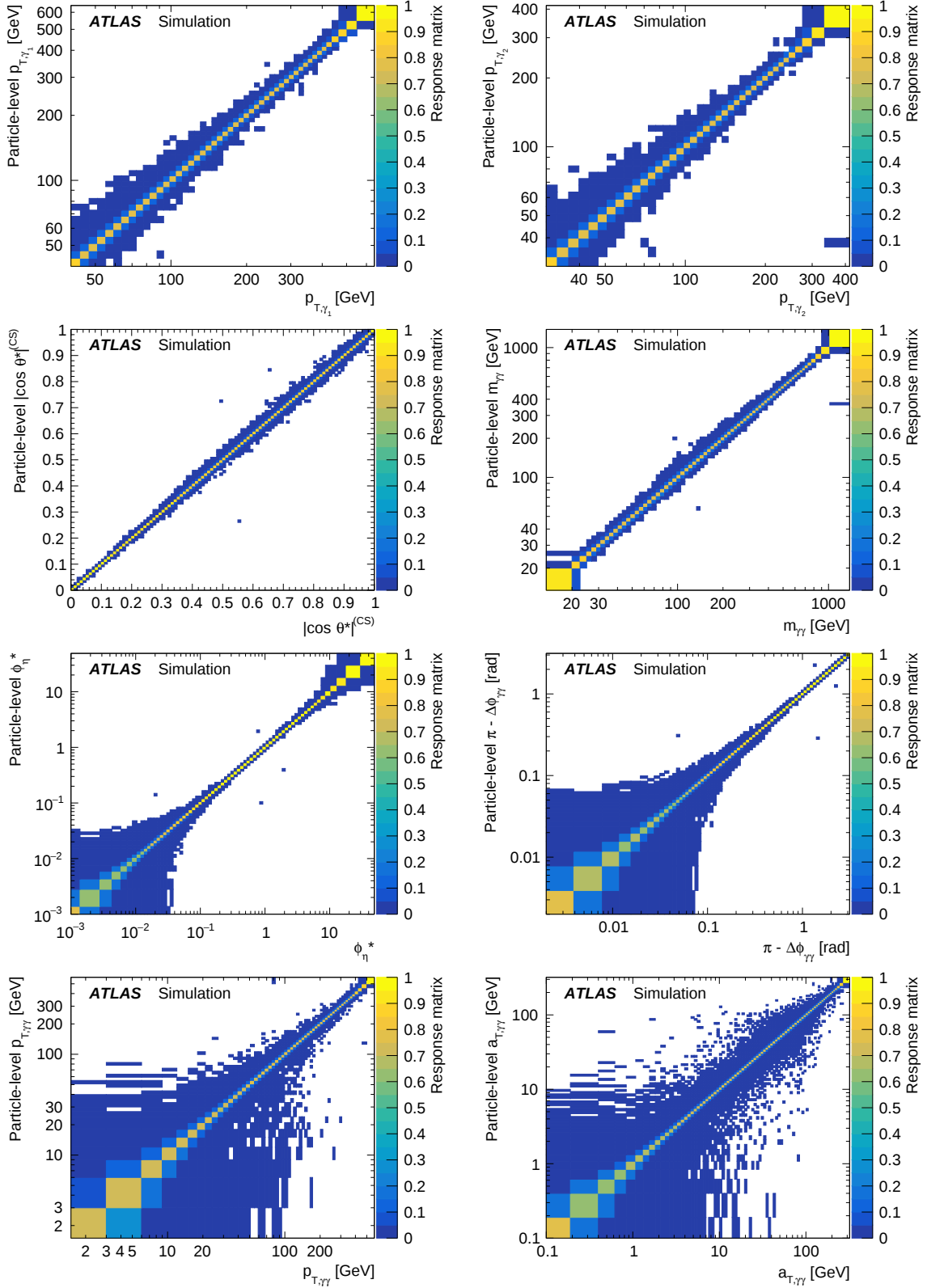


Figure D.2.: Response matrices for p_{T,γ_1} , p_{T,γ_2} , $|\cos \theta^*|^{(CS)}$, $m_{\gamma\gamma}$, ϕ_η^* , $\pi - \Delta\phi_{\gamma\gamma}$, $p_{T,\gamma\gamma}$ and $a_{T,\gamma\gamma}$ containing the conditional probability for a event in a certain particle-level bin to migrate to the different detector-level bins [38].

Appendix D. Additional figures of the diphoton measurement

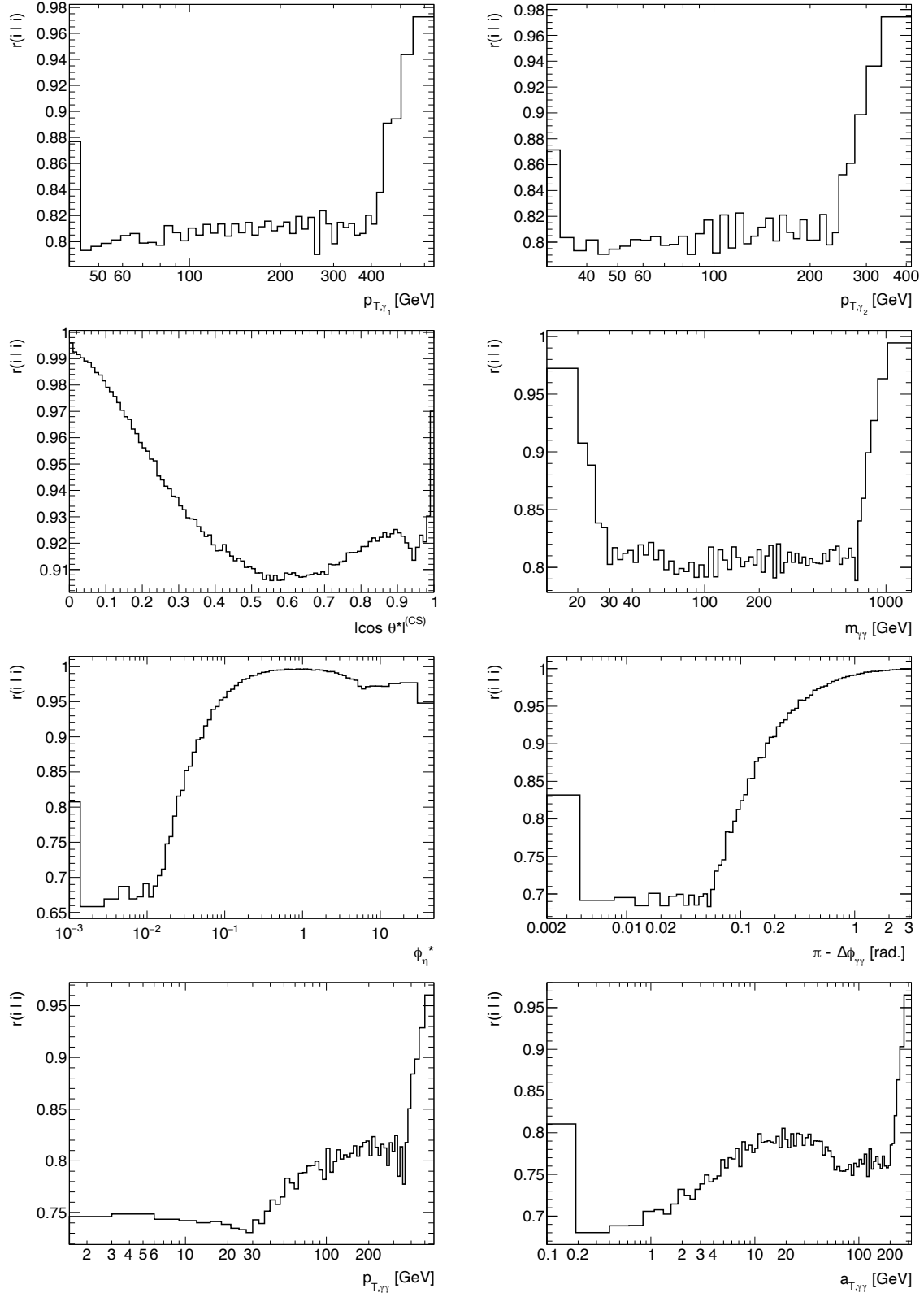


Figure D.3.: Diagonal elements of the response matrices $r(i_{DL} = j_{PL}|j_{PL})$ for p_{T,γ_1} , p_{T,γ_2} , $|\cos \theta^*|^{(CS)}$, $m_{\gamma\gamma}$, ϕ_η^* , $\pi - \Delta\phi_{\gamma\gamma}$, $p_{T,\gamma\gamma}$ and $a_{T,\gamma\gamma}$.

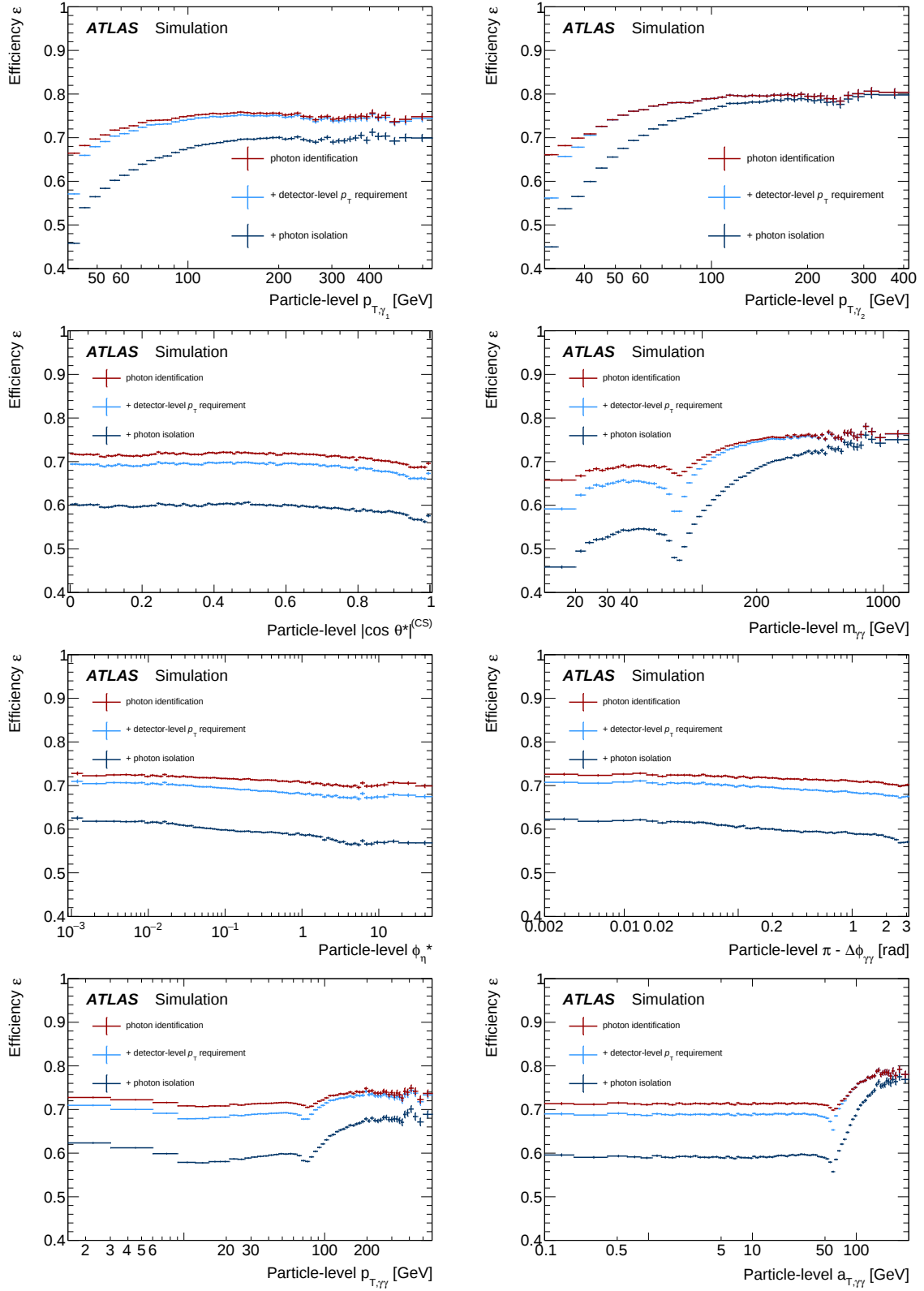


Figure D.4.: Detector efficiency for different steps of the detector-level selection for events passing all particle-level cuts for p_{T,γ_1} and p_{T,γ_2} , $|\cos \theta^*|^{(CS)}$, $m_{\gamma\gamma}$, ϕ_η^* , $\pi - \Delta\phi_{\gamma\gamma}$, $p_{T,\gamma\gamma}$, $a_{T,\gamma\gamma}$ [38].

Appendix D. Additional figures of the diphoton measurement

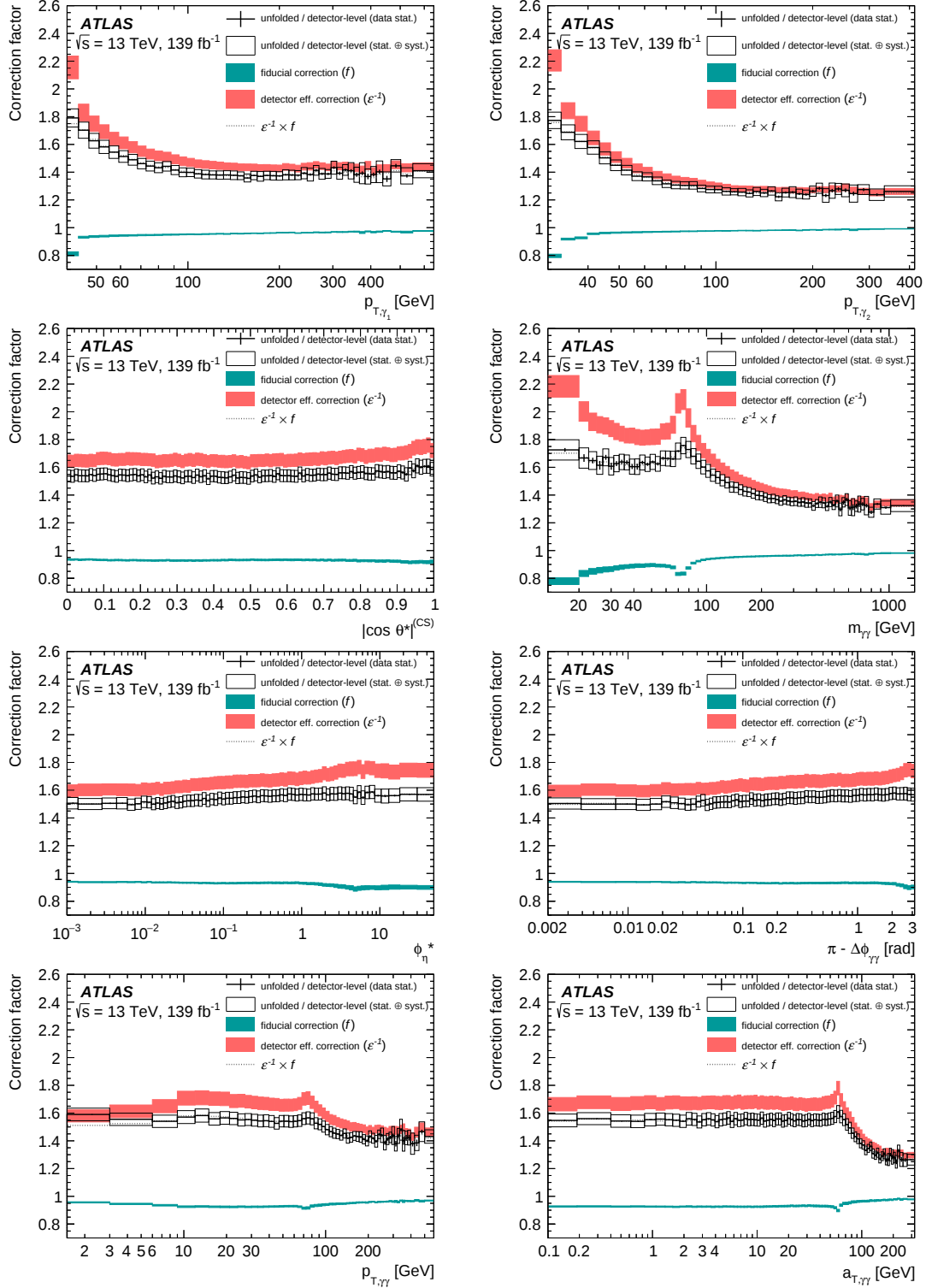


Figure D.5.: Different steps of the unfolding procedure are depicted as a function of the different observables. The green area shows the fiducial correction f and the red area the detector-efficiency correction ε^{-1} . The black line is the ratio of the unfolded result and the detector-level signal yields (the overall unfolding correction). The product $\varepsilon^{-1} \times f$ is depicted with a dashed line. Comparing the dashed line and the black line shows the impact of the resolution corrections [38].

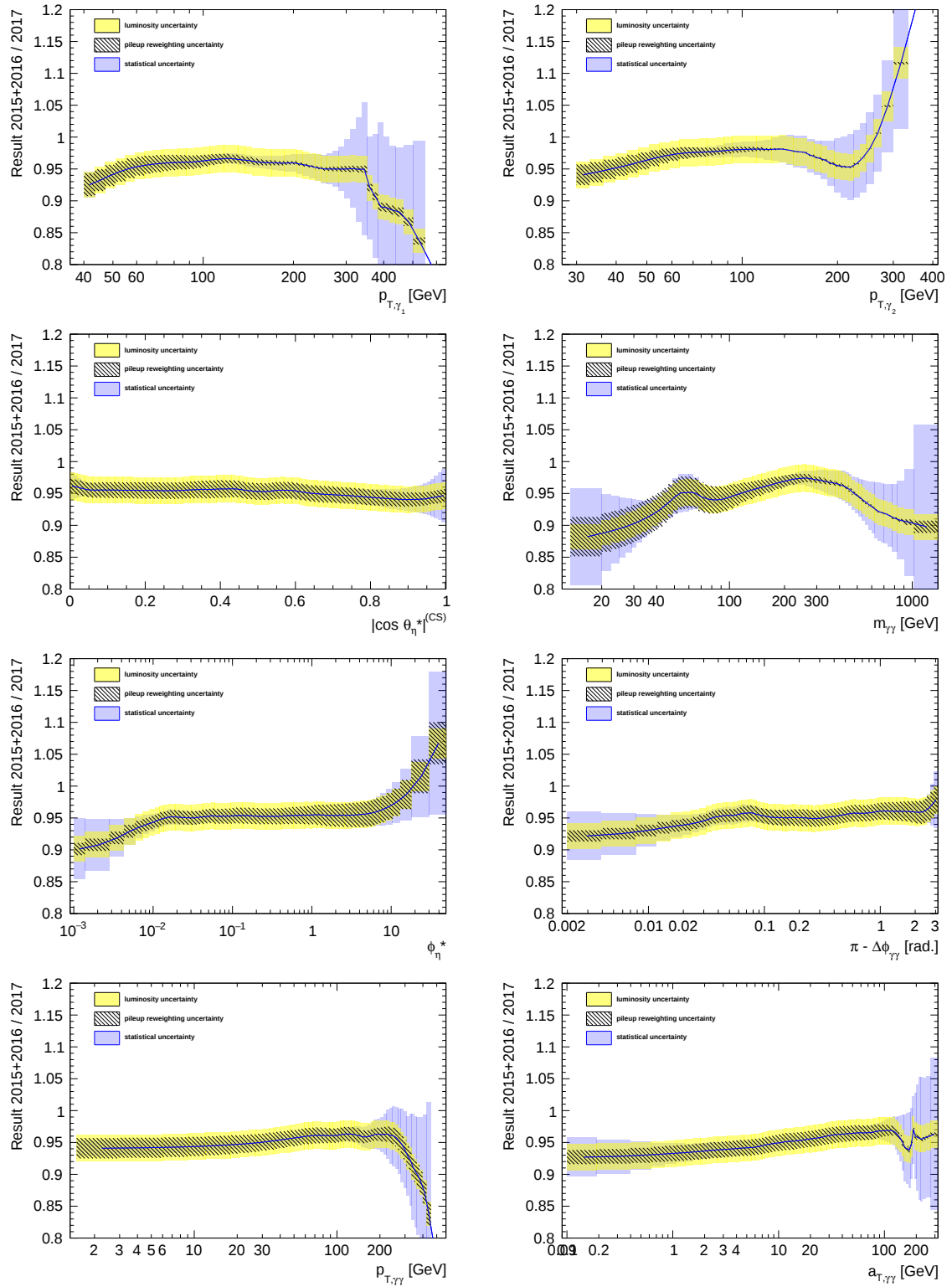


Figure D.6.: Smoothed ratio of the measured cross-sections in 2015+2016 and 2017 data including the statistical uncertainty, the uncertainty from the pileup reweighting and the luminosity uncertainty.

Appendix D. Additional figures of the diphoton measurement

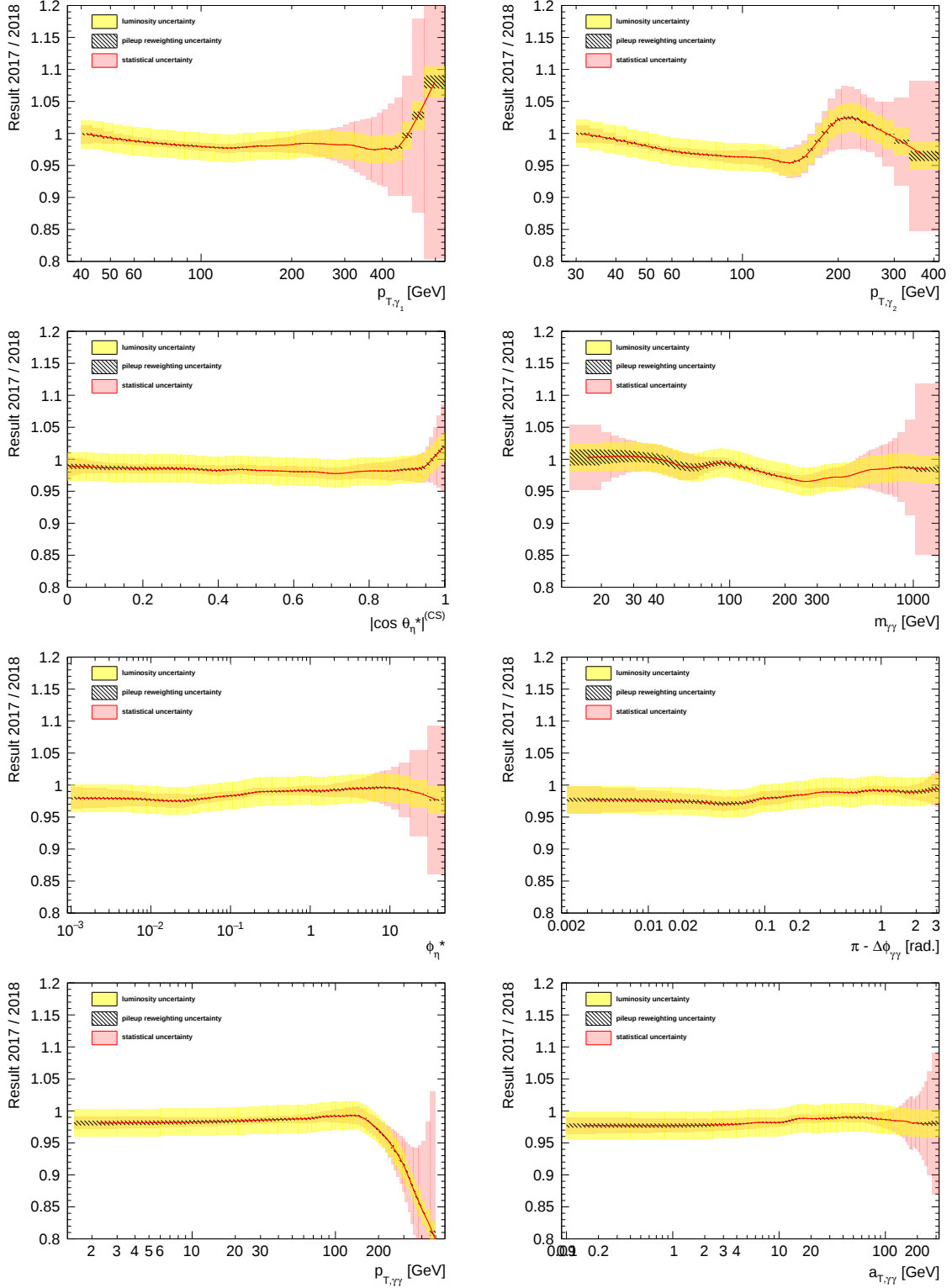


Figure D.7.: Smoothed ratio of the measured cross-sections in 2017 and 2018 data including the statistical uncertainty, the uncertainty from the pileup reweighting and the luminosity uncertainty.

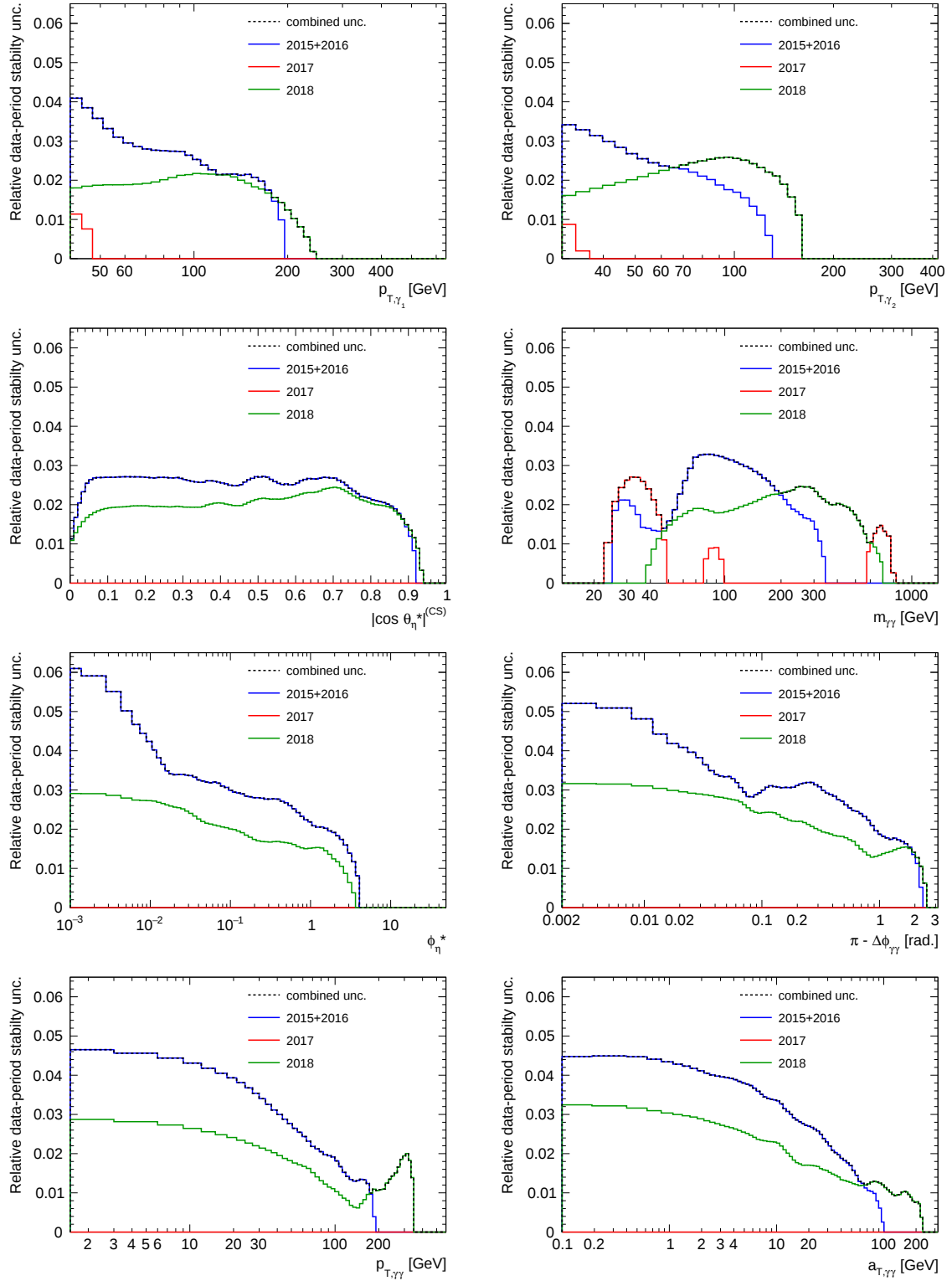


Figure D.8.: Relative data-period stability uncertainty for the separate years and the combined dataset as a function p_{T,γ_1} , p_{T,γ_2} , $|\cos \theta_\eta^{(CS)}|$, $m_{\gamma\gamma}$, ϕ_η^* , $\pi - \Delta\phi_{\gamma\gamma}$, $p_{T,\gamma\gamma}$ and $a_{T,\gamma\gamma}$.

Danksagung

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Last but not least I would like to thank my family for their support and encouragement which enabled me to write this thesis. My special thanks go to my partner Julia who accompanied me during my scientific journey and also became my office partner during the pandemic.

Versicherung

Hiermit versichere ich, dass ich die vorliegende Arbeit ohne unzulässige Hilfe Dritter und ohne Benutzung anderer als der angegebenen Hilfsmittel angefertigt habe; die aus fremden Quellen direkt oder indirekt übernommenen Gedanken sind als solche kenntlich gemacht. Die Arbeit wurde bisher weder im Inland noch im Ausland in gleicher oder ähnlicher Form einer anderen Prüfungsbehörde vorgelegt.

Die Dissertation wurde am Institut für Kern-und Teilchenphysik unter der wissenschaftlichen Betreuung von Dr. Frank Siegert angefertigt.

Christian Wiel
Dresden, den 4.11.2021