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**ETH**

**Search for High-Mass Diphoton  
Resonances in Proton-Proton  
Collisions at 13 TeV  
and  
Radiation Studies for Calorimetry at  
the High-Luminosity LHC**

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PRESENTED BY:

**Milena Eleonore Quittnat**

M. Sc. RWTH Aachen University  
born on June 17<sup>th</sup>, 1988  
citizen of Germany

ACCEPTED ON THE RECOMMENDATION OF

EXAMINER:

**Prof. Günther Dissertori**

CO-EXAMINER:

**Prof. Rainer Wallny**

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# Abstract

In this dissertation, two different topics are addressed which are part of the main areas of research of modern high-energy physics experiments at the Large Hadron Collider (LHC): a search for new physics and the development of new detectors.

The first part of this dissertation presents the search for high mass diphoton resonances in proton-proton collisions at a center-of-mass energy of 13 TeV with the Compact Muon Solenoid (CMS) experiment. Particular attention is paid to the assessment of the background. The results are interpreted in terms of spin-0 and spin-2 resonances with masses between 0.5 and 4.5 TeV and widths, relative to the mass, between  $1.4 \times 10^{-4}$  and  $5.6 \times 10^{-2}$ . Limits are set on scalar resonances produced through gluon-gluon fusion, and on Randall–Sundrum gravitons. Two results are presented, both following the same search strategy, but one employing a dataset of  $3.3 \text{ fb}^{-1}$ , the other  $16.2 \text{ fb}^{-1}$ . Both are statistically combined with results obtained by the CMS collaboration at 8 TeV with  $19.7 \text{ fb}^{-1}$ . For the combination with the dataset of  $3.3 \text{ fb}^{-1}$ , a modest excess of events compatible with a narrow resonance with a mass of about 750 GeV and a global significance of 1.6 standard deviations is observed. This excess could not be confirmed with the larger dataset of  $16.2 \text{ fb}^{-1}$ . The production of RS-gravitons is excluded at leading order at a 95 % CL<sub>s</sub> up to 3.85 and 4.45 TeV for coupling parameters of 0.1 and 0.2, respectively. These are the most stringent limits on Randall-Sundrum graviton production to date.

For the High-Luminosity LHC (HL-LHC), the forward electromagnetic calorimeter (ECAL) of CMS has to be replaced. A sampling calorimeter, using an inorganic scintillator as an active medium, was one suitable option. In the second part of this dissertation, Monte-Carlo simulations with the particle-physics toolkit FLUKA determine aspects of the behavior of such a sampling calorimeter in the radiation environment of the upgraded CMS detector at the HL-LHC. Measurements performed for LYSO, YSO and cerium fluoride crystals, exposed to a proton fluence of up to  $5 \times 10^{14} \text{ cm}^{-2}$ , are compared to dedicated FLUKA simulations. The main drivers of their residual dose are determined. It is found that LYSO and cerium fluoride crystals show similar levels of residual dose as lead-tungstate. Based on these results, an extrapolation to the behavior of the sampling calorimeter, located in the CMS detector, is performed. Characteristic parameters such as the induced ambient dose, fluence spectra for different particle types and the residual nuclei are studied, and the suitability of these materials for a future calorimeter is surveyed. Particular attention is given to the creation of isotopes in an LYSO-tungsten calorimeter that might contribute a prohibitive background to the measured signal.

The harsh radiation environment in CMS induces high levels of radioactivity in the exposed materials. The radiological hazard to personnel during the upgrade of the electronic system of the central part of ECAL for the HL-LHC is quantified.

# Zusammenfassung

In der vorliegenden Dissertation werden zwei Themenkomplexe behandelt, die von zentraler Bedeutung für die moderne Hochenergie-Teilchenphysik und die Forschung an Beschleunigern wie dem Large Hadron Collider (LHC) sind: die Suche nach Anzeichen von Physik jenseits des Standardmodells sowie die Entwicklung von neuen Detektoren für den Teilchennachweis.

Der erste Teil dieser Arbeit befasst sich mit der Suche nach Diphoton-Resonanzen mit hohen Massen. Hierfür werden Daten verwendet, die das Compact Muon Solenoid (CMS) Experiment in Proton-Proton-Kollisionen bei einer Schwerpunktsenergie von 13 TeV aufgenommen hat. Ein besonderes Augenmerk wird hierbei auf die Bestimmung des Untergrundes von bekannten Prozessen gelegt.

Die Ergebnisse werden hinsichtlich möglicher Spin-0 und Spin-2 Resonanzen mit Massen zwischen 0.5 und 4.5 TeV sowie mit relativen Zerfallsbreiten von  $1.4 \times 10^{-4}$  und  $5.6 \times 10^{-2}$  interpretiert. Grenzwerte für durch Gluon-Gluon-Fusion produzierte skalare Resonanzen sowie für Randall-Sundrum-Gravitonen werden bestimmt. Es werden zwei Endergebnisse präsentiert, die derselben Analysestrategie folgen, jedoch verschiedene Datensätze mit integrierten Luminositäten von  $3.3 \text{ fb}^{-1}$  sowie  $16.2 \text{ fb}^{-1}$  verwenden. Beide Resultate werden statistisch mit den Ergebnissen der vorausgegangenen CMS-Studie bei 8 TeV mit  $19.7 \text{ fb}^{-1}$  kombiniert. Für die Kombination mit dem Datensatz von  $3.3 \text{ fb}^{-1}$  ergibt sich ein leichter Überschuss an gemessenen Events, die durch eine schmale Resonanz mit einer Masse von etwa 750 GeV erklärt werden könnte. Die beobachtete globale Signifikanz beträgt 1.6 Standardabweichungen.

Mit dem größeren Datensatz kann die Abweichung nicht bestätigt werden. Die Produktion von Randall-Sundrum-Gravitonen wird mit einem Konfidenzniveau von 95% in führender Ordnung der Störungstheorie ausgeschlossen für Massen bis 3.85 TeV bzw. 4.45 TeV für Kopplungskonstanten von 0.1 bzw. 0.2. Diese Ergebnisse stellen die bislang höchsten Grenzwerte für die Produktion von Randall-Sundrum-Gravitonen dar.

Im zweiten Teil der Dissertation werden Monte-Carlo-Studien zum Design eines neuen CMS-Kalorimeters vorgestellt. Die Endkappen des elektromagnetischen Kalorimeters des CMS-Experiments müssen für einen Betrieb am High-Luminosity-LHC (HL-LHC) ersetzt werden. Eine der vorgeschlagenen Optionen ist ein Samplingkalorimeter mit anorganischen Szintillatoren als sensitive Detektorschicht.

Mithilfe der Monte-Carlo Simulationssoftware FLUKA wurden Studien zum Verhalten des Samplingkalorimeters in der hohen Strahlungsumgebung von CMS durchgeführt. Messungen von LYSO, YSO und Cerium-Fluorid-Kristallen bei Proton-Fluenzen von bis zu  $5 \times 10^{14} \text{ cm}^{-2}$  werden mit entsprechenden FLUKA-Simulationen verglichen und die Umgebungs-Äquivalentdosisraten und deren Hauptursachen bestimmt. Die Studie

zeigt, dass LYSO und Cerium-Fluorid Kristalle ähnliche verbleibende Umgebungs-Äquivalentdosisraten aufweisen wie Blei-Wolframat Kristalle.

Eine Extrapolierung des Verhaltens eines Samplingkalorimeters im CMS-Experiment, basierend auf diesen Ergebnissen, wird durchgeführt. Charakteristische Parameter wie Umgebungsdosis, Fluenzspektren für verschiedene Teilchentypen sowie die radioaktiven Zerfälle an sich werden untersucht und die Eignung der entsprechenden Materialien für ein zukünftiges Kalorimeter werden beurteilt. Besondere Aufmerksamkeit wird hierbei der Produktion von Isotopen in einem LYSO-Wolfram-Kalorimeter gewidmet, die durch radioaktive Zerfälle ein Störsignal im Detektor bewirken könnten.

Die starke Strahlenbelastung der Materialien im CMS-Experiment führt zu hohen Radioaktivitätslevel im Inneren des Detektors. Deshalb wird in einer weiteren Studie die Strahlenbelastung bestimmt, der das technische Personal während den Upgradearbeiten der elektronischen Systeme des zentralen Kalorimeters für den HL-LHC ausgesetzt sein wird.

Some results presented in this thesis have been shown previously in the following publications:

- [1] CMS Collaboration, “Search for high-mass diphoton resonances in proton-proton collisions at 13 TeV and combination with 8 TeV search”, (2016). Accepted by *Phys.Lett.B*, arXiv:1609.02507. This paper is based on the results of EXO-PAS-16-027.
- [2] CMS Collaboration, “Search for Resonant Production of High-Mass Photon Pairs in Proton-Proton Collisions at  $\sqrt{s} = 8$  and 13 TeV”, *Phys.Rev.Lett.*117:051802, (2016). doi:10.1103/PhysRevLett.117.051802. This paper is based on the results of arXiv:1606.04093 and EXO-PAS-15-004.
- [3] R. Becker and others, “Proof-of-principle of a new geometry for sampling calorimetry using inorganic scintillator plates”, *Journal of Physics Conference Series*, 587(1):012039, (2015). doi:10.1088/1742-6596/587/1/012039.
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- [6] F. Nessi-Tedaldi and M. Quittnat, “Irradiations with 24 GeV/c protons of Lead Tungstate, LYSO and Cerium Fluoride crystals: a comparison to CMS running conditions”, *ETH-ZURICH-PREPRINT-ETHZ-IPP-2014-02*, (2014). doi:10.3929/ethz-a-010336890.



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# 1

## CHAPTER

# Introduction

Max Planck was one of the leading minds of an era of modern physics. His development of the quantum theory revolutionized not only the understanding of subatomic processes, but the human understanding of the world. The Nobel Laureate was however discouraged by the physics professor Philipp von Jolly to study physics in the beginning: "in this field, almost everything is already discovered and all that remains is to fill a few holes." [7]. Roughly 140 years later, modern physics comprises fields like general relativity and quantum physics, which were unknown back then. Areas of research like dark matter, dark energy, and elementary particle physics show that we only have a limited knowledge of about 4 % of our universe [8].

In the last century most elementary particles and fundamental forces were discovered. The standard model of particle physics [8] predicted many of these discoveries and summarizes our current understanding of physics at the smallest scale. During the last 60 years the research in particle physics was dominated by projects employing the highest energies. Many discoveries were only possible with the help of accelerators and state-of-the-art detectors. The LHC accelerator [9, 10] at CERN currently collides protons with an unprecedented energy of 13 TeV. This collision energy enables us to reproduce the state of the universe shortly after the Big-Bang under laboratory conditions. The decay particles from these collisions are detected with experiments such as the Compact Muon Solenoid (CMS) detector [11]. With the recordings of the decay products, the particle interaction during the collision can be reconstructed.

The standard model of particle physics is an incomplete theory and leaves many unanswered questions. Still, part of the particle physics community is disenchanted about the discovery potential of particle physics these days. New physics might be hidden at an energy scale which is inaccessible with our current instruments. It might however also be just around the corner.

This dissertation discusses the quest for new physics on the example of an analysis searching for a resonance, decaying to a photon pair. In the context of this search, key aspects of the standard model of particle physics are highlighted in Chapter 2. The search

for the hypothetical signal, which could be new scalar resonances or Randall-Sundrum gravitons, is motivated in Chapter 3. The final introductory Chapter 4 gives a description of the LHC accelerator and the CMS experiment, focusing on the electromagnetic calorimeter (ECAL) and the photon reconstruction.

I was one of the main contributors for a search of new high mass diphoton resonances with the CMS detector. In December 2015, the CMS and ATLAS collaborations presented their results for this search, exploring the new energy range of  $\sqrt{s} = 13$  TeV [12, 13]. Both collaborations observed a modest excess of events compared to the background-only hypothesis, compatible with the production of a resonance with a mass of 750 GeV. This coincidence captured the attention of the particle physics community and over 550 papers interpreted this excess [14]. Since it is unknown if we are able to discover the new physics at the energies of the LHC, physicists were very enthusiastic about this unexpected observation.

During these exciting last two years, we first designed the analysis for the new energy regime and presented the first results of this search in December 2015. The year 2016 was dominated by scrutinizing the analysis, improving the search strategy for resonant signals and updating regularly the results with new collision-data, produced at the CMS detector. Within the analysis group I was concentrating on the assessment of the background components. Due to the excitement of the excess, I was also involved in analysis improvements concentrating on a possible resonant signal. I worked on the accuracy of the background model and alternative models and estimated the significance of the excess in the context of our overall search spectrum.

The analysis strategy is detailed in Chapter 5-8 and Chapter 9 focuses on the determination of the background components. The statistical interpretation, the background and signal model and their systematic uncertainties are discussed in Chapter 10, Chapter 11, Chapter 12 and Chapter 13 respectively.

The analysis of a recent larger dataset, presented at the ICHEP16 conference in August 2016, showed however that the diphoton excess could not be confirmed for both collaborations [1, 15]. Chapter 14 details the findings and concludes with an outlook based on these results.

The particle physicists community went through the different states of grief [16] and disillusionment concerning the discovery potential of high energy particle physics after these recent results. I personally hope that the presentation of new results from the particle physics experiments at the Moriond conference 2017 reflects the fourth stage of grieve for the particle physics community: "on the way to new horizons".

Apart from the analysis of particle physics processes, the high energy physics discipline also includes the interesting and challenging field of the development of the detection instruments. To further uncover the mysteries of the universe, the LHC will

be upgraded in the year 2024 to the High-Luminosity LHC [17]. For this project, the detectors have to operate in a harsh radiation environment. The CMS detector has to be upgraded to allow the same or improved reconstruction of the decay products. The electromagnetic calorimeter (ECAL), mainly used for the energy reconstruction of electromagnetic particles, faces two upgrade projects: the upgrade of the readout electronics of the central part and a completely new forward part. These upgrades are motivated in Chapter 16.

During my PhD, I was the ECAL expert for FLUKA radiation simulations. This Monte-Carlo simulation program is introduced in Chapter 17. In this role, I collaborated with the BRIL (Beam conditions, RadIation and Luminosity) project of CMS and the radiation-protection group to estimate the radiological hazard for personnel during the upgrade of the ECAL for the HL-LHC. This was crucial for the planning of the upgrade and the protection of the personnel and is detailed in Chapter 18.

Since the current forward ECAL will not perform well under HL-LHC running conditions, the ETH Zürich (ETHZ) group collaborates since many years with other universities and companies to develop new materials for the new forward ECAL [18]. The ETHZ group and collaborators designed in this context a new scintillating sampling ECAL. The focus of my work was the simulation of the impact of the CMS radiation environment on this 'Shashlik' sampling calorimeter, concentrating on the created fluence inside of the material, possible material damage and radioactivity studies. First, the residual dose rate of proton-irradiated scintillating crystals is discussed in Chapter 19 to determine if a constant background of decaying isotopes could lead to a prohibitive background in the ECAL readout. I then describe in Chapter 20 the extrapolation from the fluence induced by these proton-irradiations to the CMS environment. The final studies of the behavior of a Shashlik calorimeter in the CMS environment at the HL-LHC are discussed thereafter. The main causes of the absorbed dose are studied and it is determined if they lead to a constant background noise in the ECAL readout. This part of the dissertation concludes with a summary of the results and an outlook of the ECAL CMS upgrade for the HL-LHC.

In conclusion, this dissertation addresses with the 'search for high-mass diphoton resonances in proton-proton collisions at 13 TeV' and 'radiation studies for calorimetry at the HL-LHC' two different topics which are part of the main areas of research of modern high-energy physics experiments.



## 2

# Theoretical framework for diphoton production in the standard model

This chapter highlights the key elements of particle physics, which are necessary for the understanding of the research presented in part I of this dissertation. It gives an overview of the standard model of particle physics, the underlying physics processes of a proton-proton collision and the diphoton production. This chapter is not aimed at providing a comprehensive description of the theoretical concepts. These can be found in the respective references. In this dissertation, most formulas and numerical values follow the notation of natural units ( $\hbar = c = 1$ ).

## 2.1 Selected aspects of the standard model of particle physics

The standard model of particle physics (SM) is a quantum-field theory, summarizing our current understanding of elementary particle physics. It describes all observed elementary particles, the fundamental structure of matter and all fundamental forces with the exception of gravity. A detailed overview of the key concepts of the SM and several experimental measurements are given in Ref. [8]. The SM is a renormalizable and locally invariant gauge theory [19]. The structure of the gauge symmetry group is  $SU(3)_C \otimes SU(2)_L \otimes U(1)_Y$ , with the index 'C' for the color-charge, 'L' for the left-handed nature of weak interactions, and 'Y' for the weak hypercharge. The SM categorizes the elementary particles in fermions, gauge bosons and the Higgs boson, which are spin-1/2, spin-1 and a spin-0 particle(s), respectively.

The fermions follow the Pauli exclusion principle and each fermion has its own antiparticle, with the exception of neutrinos which could also be Majorana particles. They are grouped in three generations of leptons  $e, \mu, \tau$  and their corresponding neutrinos

$\nu_e, \nu_\mu, \nu_\tau$  and three generations of quarks (u,d);(c,s);(t,b). All fermions, except for the neutrinos, carry an electromagnetic charge, which is listed in Figure 2.1, together with its mass and spin value.

The gauge bosons are the carriers of fundamental forces. The electroweak force is mediated by (virtual)  $\gamma, W^\pm$  and Z bosons, the strong force by (virtual) gluons (g). Their interaction with the respective fermions is highlighted in beige in Figure 2.1.

A key feature of the SM is quantum chromodynamics (QCD) [20–24]. It describes the strong force between color-charged particles, the quarks. The strong force is mediated by eight self-interacting gluons, carrying quantum states of color and anti-color. These are related to the eight generators of the  $SU(3)_C$  group. The 'confinement' in QCD refers to the phenomenon that no free color charges are observed in nature, which means that quarks and gluons are only found in bound states as hadrons or mesons. The interaction of color-charged particles is dependent on the strong coupling 'constant'  $\alpha_s$ , which depends on the momentum transfer  $\mu^2$  to one of the interaction partners. The strong coupling constant decreases towards higher  $\mu^2$ , leading to an 'asymptotic freedom' of the quarks and gluons [25]. For short-distances and large energies, these particles can be treated as quasi-free and are described by perturbative theories. The QCD is the main underlying theory of proton-proton collisions, which is subject to the following Section 2.2.

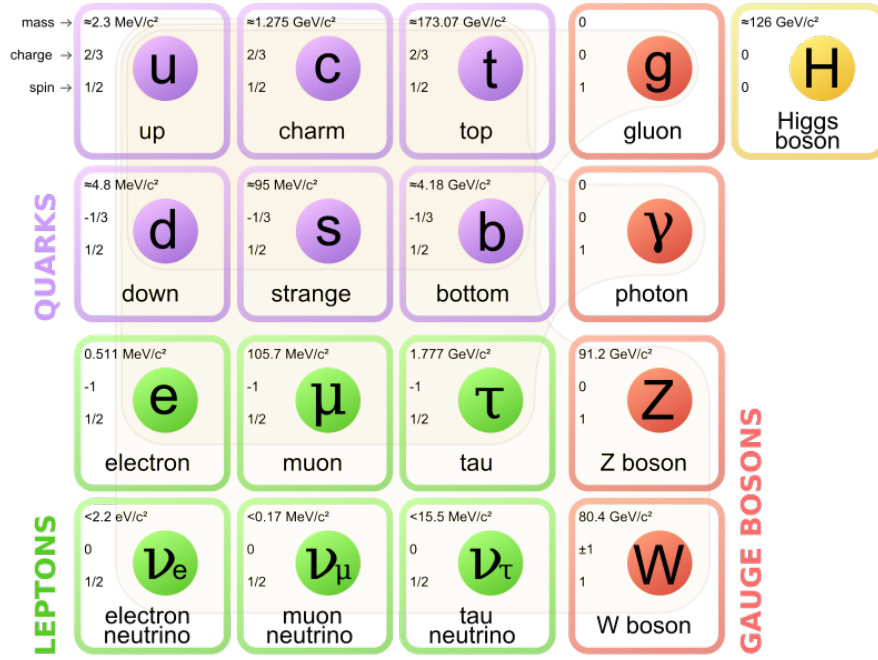
A great accomplishment of the SM theory was the unification of electromagnetic and weak forces in a local gauge theory of electroweak interactions  $(SU(2)_L \otimes U(1)_Y)$  by Glashow [26], Weinberg [27] and Salam [28]. It predicted the existence of the  $W^\pm$  and Z bosons, which were discovered thereafter [29–32]. Historically, this model had the problem that it only predicted massless  $W^\pm$  and Z bosons. The generation of the mass of these gauge bosons breaks the electroweak symmetry and requires in this context the existence of 'Goldstone' bosons [33–35].

### The Higgs mechanism

The spontaneous electroweak symmetry breaking mechanism (EWSB) of a local gauge symmetry was proposed by Englert, Brout [37], Higgs[38–40] and others [41, 42] and it is shortly outlined in the following. In a renormalizable quantum field theory, the mass of the gauge bosons can be generated by a scalar field. The chosen doublet of complex scalar fields ( $SU(2)_L$ ) is of the form:

$$\phi = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{2}\phi^+ \\ \phi^0 + ia^0 \end{pmatrix} \quad (2.1)$$

with  $\phi^0$  and  $a^0$  being the CP-even and CP-odd neutral components, and  $\phi^+$  being the complex charged component of the Higgs doublet. The SM Lagrangian is extended with



**Figure 2.1:** The elementary particles of the standard model of particle physics. The quarks (violet), leptons (green), gauge bosons (red) and the Higgs boson (yellow) are depicted with their mass, electric charge and spin. The interaction of the gauge bosons with the fermions is shown in a beige shade [36].

a kinetic term and the so-called Higgs scalar potential:

$$V(\phi) = \mu^2 \phi^\dagger \phi + \frac{\lambda}{2} (\phi^\dagger \phi)^2 \quad (2.2)$$

with the real parameter  $\mu^2$  and quartic coupling  $\lambda$ , the Higgs self-coupling parameter. The minimum of the potential for  $\mu^2 < 0$  and  $\lambda > 0$  is not  $\phi = \vec{0}$ , but:

$$\phi^\dagger \phi = v^2 = \frac{\mu^2}{\lambda} \quad . \quad (2.3)$$

The electroweak symmetry is then said to be spontaneously broken as the SM Lagrangian stays invariant under the symmetry, but the ground state  $\langle \phi \rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v \end{pmatrix}$  of the Higgs potential does not. One component of this scalar field is 'absorbed' by the initially massless gauge boson (in the unitary gauge) and becomes its longitudinal polarization state. With this, the gauge boson has now three degrees of freedom, thus characterizing a massive spin-1 field. The second component denotes a neutral scalar particle, the so-called Higgs boson [43]. The vacuum expectation value can be calculated via:

$$v = \frac{\sqrt{2}|\mu|}{\lambda} \quad . \quad (2.4)$$

It is measured experimentally to be  $v = 246 \text{ GeV}$  [8].

According to the EWSB, the SM particles acquire mass in the following way: three of the four generators of the  $SU(2)_L \otimes U(1)_Y$  gauge group are spontaneously broken, which creates three Goldstone bosons [35]. These Goldstone bosons mix with the gauge fields corresponding to the broken generators of  $SU(2)_L \otimes U(1)_Y$  and become the longitudinal polarizations of the  $W^\pm$  and  $Z$  gauge bosons, which consequently acquire mass [8]. The fourth generator of  $SU(2)_L \otimes U(1)_Y$  is the one of the conserved  $U(1)_{EM}$  gauge symmetry. Its corresponding gauge field, the photon, remains massless [8]. The fermions obtain their masses by their Yukawa interaction with the Higgs field.

The EWSB model does not predict the mass of the Higgs boson  $m_H = \lambda \times v$ . When this parameter is however measured experimentally, the strength of its production cross-sections and decay branching ratios are determined. Recently, a Higgs boson was discovered by the CMS and ATLAS collaborations [44, 45] with a mass of  $m_H = 125.09 \pm 0.21(\text{stat.}) \pm 0.11(\text{syst.}) \text{ GeV}$  [8]. The found Higgs boson does not show yet any significant discrepancies from a standard-model Higgs boson as illustrated in Figure 2.2. The figure shows the current combined best fit values of the cross-section ( $\sigma$ ) and branching fractions ( $\mathcal{B}^f$ ) of the different Higgs-production and decay channels from both collaborations, normalized to the SM expectation.

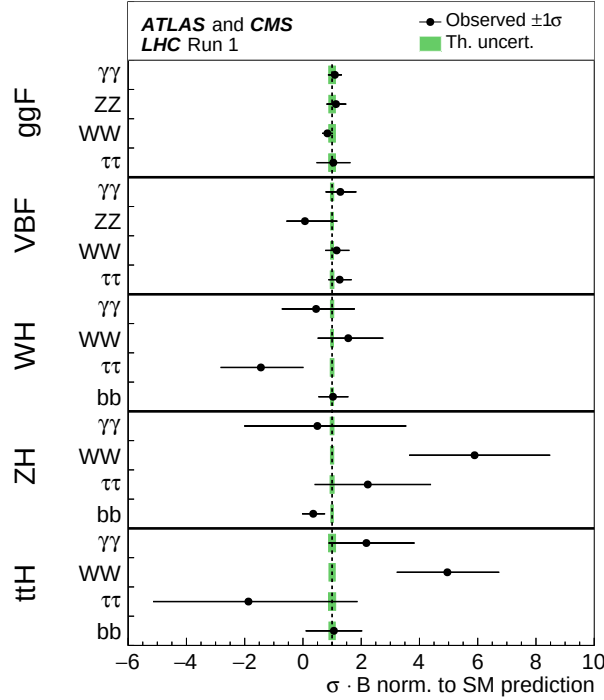
Figure 2.3 presents the expected and measured production cross-section of selected standard model processes. Currently, most channels show a very good agreement with the SM prediction within uncertainties. Disagreements of the SM prediction to observations might be hidden in these uncertainties and more precise results are crucial in the search for new physics. This is highlighted on the example of Higgs boson coupling measurements in Chapter 16 as a motivation for the high-luminosity upgrade of the LHC accelerator.

It is important to note, that the standard model is an incomplete theory. It cannot explain observations like the indirect observation of dark matter and does not include gravity [43]. The need for beyond standard model (BSM) physics motivates searches like the one for high mass diphoton resonances of this dissertation and benchmark models for this specific search are laid out in Chapter 3.

## 2.2 Proton-proton collisions

The main motivations to build a proton-proton (pp) collider were the originally unknown Higgs mass parameter and the search for BSM physics.

Because of the composite nature of the proton, the high energy collisions happen at the constituents level with the so-called partons: gluons and quarks. Since the partons carry only part of the overall proton energy, a wide range of interaction energies can be

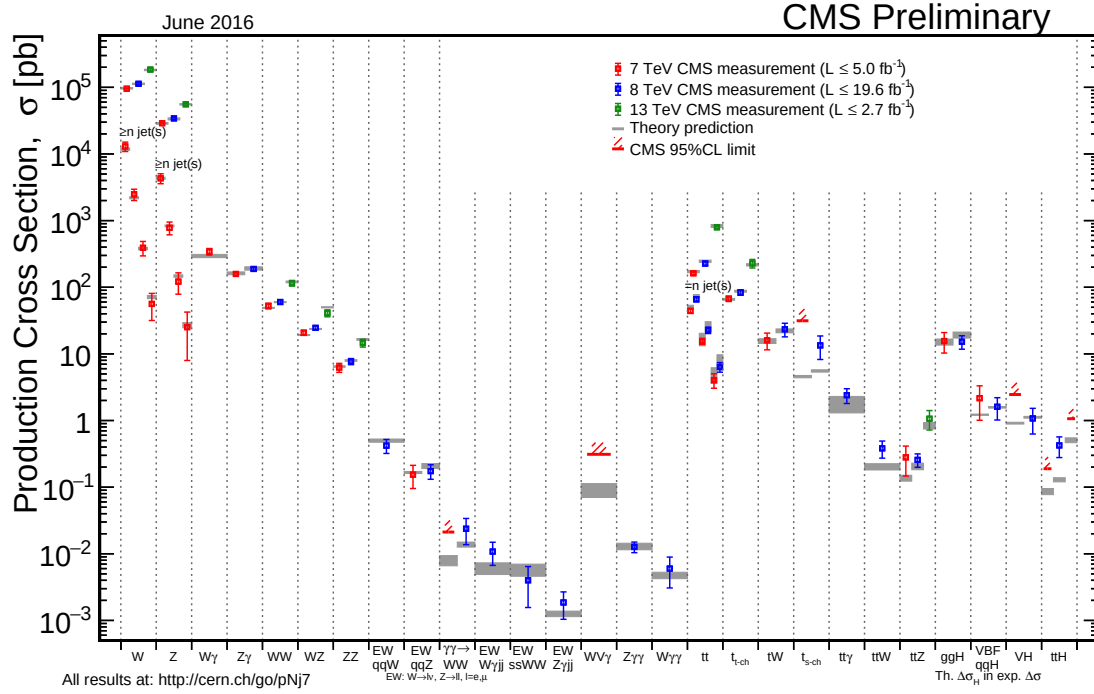


**Figure 2.2:** Best fit values of  $\sigma \cdot B^f$  for each specific channel  $i \rightarrow H \rightarrow X$ , as obtained from the generic parameterization with 23 parameters for the combination of the ATLAS and CMS measurements. The uncertainty bars indicate the  $1\sigma$  intervals. The fit results are normalized to the SM predictions for the various parameters and the shaded bands indicate the theoretical uncertainties in these predictions. Only 20 parameters are shown because some are either not measured with a meaningful precision, in the case of the  $H \rightarrow ZZ$  decay channel for the WH, ZH, and ttH production processes, or not measured at all and therefore fixed to their corresponding SM predictions, in the case of the  $H \rightarrow bb$  decay mode for the ggF and VBF production processes [46].

covered, which translates to a wide search range for masses of new particles. The physics and mathematical concepts of proton-proton collisions are shortly outlined herein.

### The structure of the proton and hard-scattering processes

The precise knowledge of the internal structure of the proton is among others due to the research results produced at the electron-proton HERA collider at DESY in Germany in recent years [48]. The composition of the proton is described by the parton distribution functions (PDF). The evolution of the PDFs is modeled by the DGLAP equations [25, 49, 50]. The fractional momentum of each of these partons to the overall proton momentum is given by the Bjorken scaling variable 'x'. Two exemplary PDFs for two different momenta transfers  $\mu^2$  are shown in Figure 2.4. The proton consists not only of the three valence quarks (u,u,d) and gluons, but also of virtual quarks with low momenta fractions, the 'sea' quarks. These are quantum fluctuations, produced by quark-antiquark annihilation and gluons. The three valence quarks dominate over the sea quarks for momentum fractions of  $x \geq 0.1$ . The momentum transfer of  $\mu^2 = 10 \text{ GeV}^2$



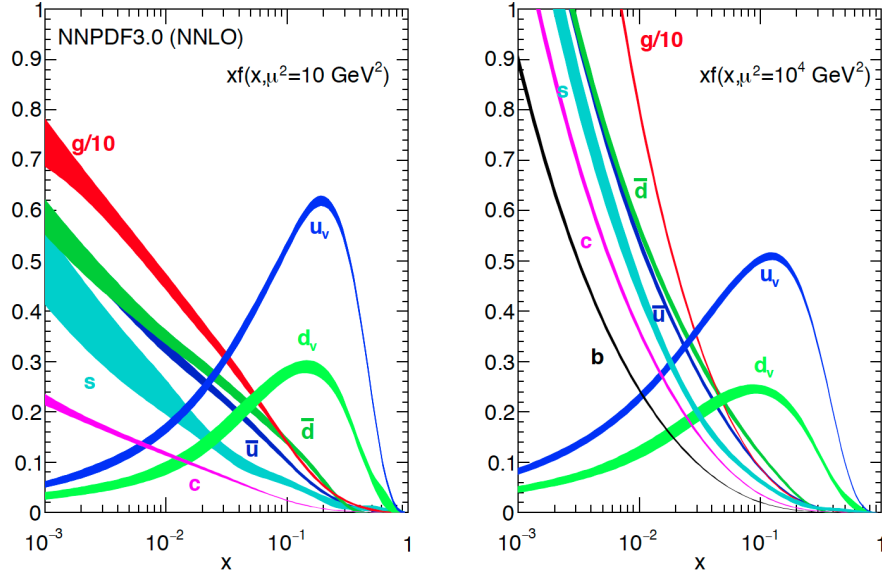
**Figure 2.3:** Selected measurements of standard model production processes compared to their theory prediction for a center-of-mass-energy of 7, 8 and 13 TeV [47].

translates to a resolution of roughly  $1/10$  of the proton radius. In comparison to the higher momentum transfer of  $10^4 \text{ GeV}^2$ , the PDF of the sea quarks and the gluons is lower. This is a consequence of the uncertainty relation, which allows to resolve more quantum fluctuations for a higher momentum transfer. For LHC collisions it is therefore very likely that gluons are the partons colliding in a pp-collision.

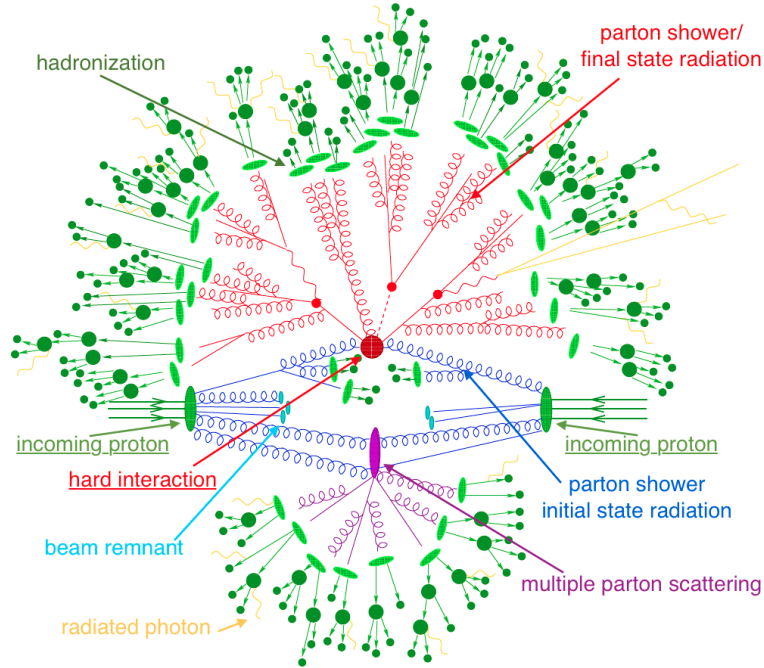
Apart from the hard-scattering process of the partons, the emission of gluons from the interacting partons or the splitting of gluons into quarks is possible. This is named initial or final state radiation, depending if the emission or splitting takes place before or after the hard-scattering process. Figure 2.5 shows an illustration of the hard-interaction (red full circle) of a pp-interaction (green ellipse). The initial and final state radiation is depicted in blue and red, respectively.

### Non-perturbative effects and jet clustering

Because of confinement, the final state particles form color-neutral bound states. The transition between perturbative and the non-perturbative regime is called 'hadronization'. This hadronization (dark green in Figure 2.5) cannot be described by perturbative QCD and is modeled either by a string [52] or cluster model [53, 54]. It is also possible that the residuals of one proton undergo further interactions, the 'multiple parton scattering'. Further detected particles, which are not originating from the primary hard-interaction are named 'underlying event'. These interactions may involve hard and soft, namely interactions with low transverse momentum, processes. The hadronization of boosted



**Figure 2.4:** Distributions of  $x$ -times the unpolarized parton distribution function  $f(x)$  obtained in the NNPDF 3.0 global analysis at the scales of  $\mu^2 = 10 \text{ GeV}^2$  (left) and  $10^4 \text{ GeV}^2$  (right) at  $\alpha_s(M_Z) = 0.118$  [51].



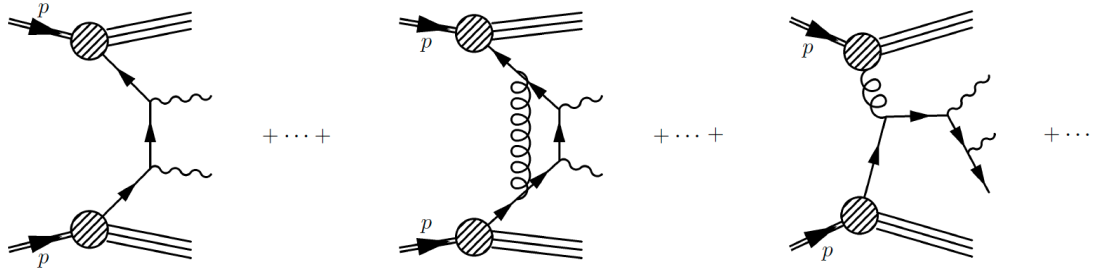
**Figure 2.5:** Sketch of a proton-proton collision and subsequent hadronic shower development. Illustration is taken slightly modified from [60].

quarks and gluons is collimated and the final object, which is measured in the detector, is a so-called 'jet' [55]. The jet reconstruction is described by different algorithms [56–59] and is subject to constant improvements.

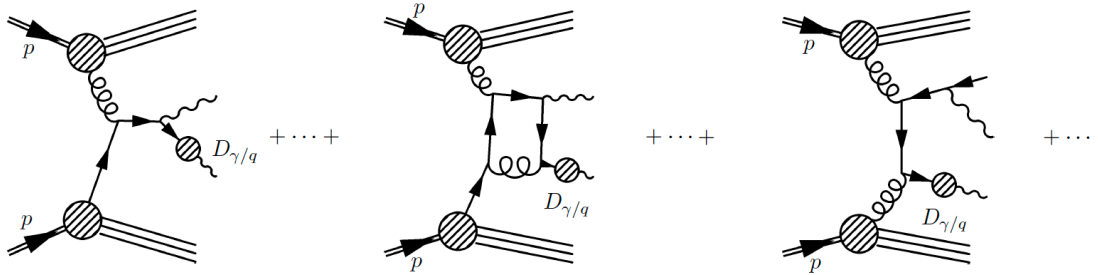
## 2.3 Diphoton production

For the search performed in the context of this dissertation the standard model diphoton production is the main source of background. Diphotons are produced at leading-order via the so-called 'Born process', a quark-antiquark annihilation process  $q\bar{q} \rightarrow \gamma\gamma$ . The corresponding Feynman diagram can be found on the left side of Figure 2.6. The next-to-leading-order (NLO) contributions at  $\mathcal{O}(\alpha_s)$  arise from quark-antiquark annihilation plus an additional gluon ( $q\bar{q} \rightarrow \gamma\gamma g$ ) and  $gq \rightarrow \gamma\gamma q$ , where the quark radiates two photons [61]. The respective Feynman diagrams are illustrated in the middle and on the right side of Figure 2.6. Other subprocesses include photons being produced by final state parton fragmentation. Figure 2.7 shows this process for the case that only one photon is produced via fragmentation, Figure 2.8 for the case of both photons. One next-to-next-to-leading-order (NNLO) subprocess at  $\mathcal{O}(\alpha_s^2)$  is of great importance due to the high gluon-gluon luminosity at the LHC [62]: the Box diagram, which is illustrated in Figure 2.9. A full NNLO calculation for diphoton production at the LHC [63], including contributions at  $\mathcal{O}(\alpha_s^3)$ , was recently published and will further improve the description of the SM diphoton production. In all the diphoton production processes, the photons are produced in association with the proton residuals. Details about the used Monte-Carlo generators for the diphoton background is given in Chapter 5.3 and for higher-order corrections in Chapter 5.3.3.

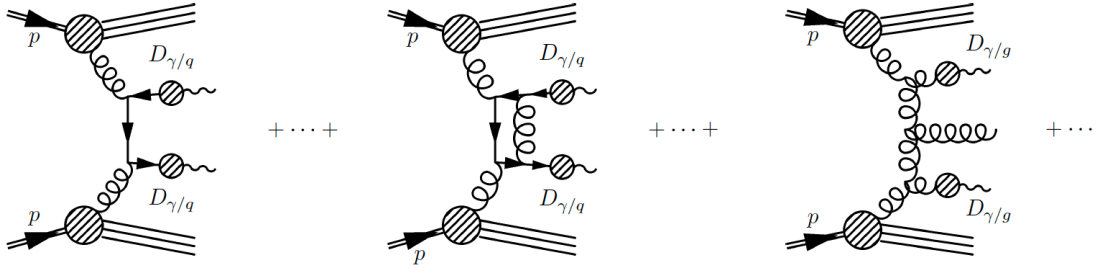
Current measurements of the diphoton production at the LHC agree with the SM prediction. The diphoton final state is however an interesting channel for searches of BSM physics due to its rather unambiguous event signature, which is detailed in the context of the search for high mass diphoton resonances in Chapter 5. Two possible BSM physics scenarios, which could be detected in the diphoton final state, are presented in the following Chapter 3.



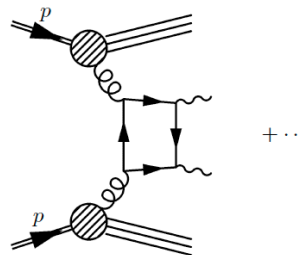
**Figure 2.6:** Feynman diagrams of the diphoton production processes, with the LO Born process  $q\bar{q} \rightarrow \gamma\gamma$  (left), and the NLO contributions  $q\bar{q} \rightarrow \gamma\gamma g$  (middle) and  $gq \rightarrow \gamma\gamma q$  (right) [61] and associated virtual corrections.



**Figure 2.7:** Examples of diphoton production processes with one photon being produced via quark fragmentation [61].



**Figure 2.8:** Examples of diphoton production with both photons being produced via quark fragmentation [61].



**Figure 2.9:** Feynman diagram of the NNLO 'Box' diphoton production process [61].



# BSM theories for high mass resonances decaying into two photons

Part I of this dissertation presents the search for high mass resonances decaying into the diphoton final state at a center-of-mass energy of 13 TeV by the CMS collaboration. This chapter aims to give an insight of two models, motivating this search. A diphoton resonance would need to have a spin of zero or an integer spin of equal or greater than two [64, 65]. The chosen benchmark models were therefore the one of an extradimensional model, predicting spin-2 resonances and detailed in Section 3.1 and the one of the extended Higgs model, predicting spin-0 resonances and detailed in Section 3.2. Besides that, the not-confirmed excess in the diphoton final state at a mass of 750 GeV, seen by the CMS and ATLAS collaborations [12, 13] motivated the publication of over 550 papers, predicting new physics in the diphoton final state [14]. For an overview of the different studied models, Ref. [66] may be consulted.

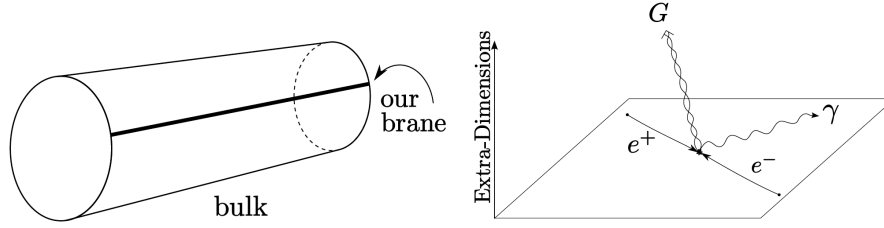
## 3.1 Extradimensions as a solution to the hierarchy problem

### The hierarchy problem

Extradimension models aim to give a solution to the so-called 'gauge hierarchy' problem of particle physics [67]. Higher order corrections of the Higgs boson include loops of massive particles. The added correction for a fermion loop is for instance

$$\Delta M_H^2 = \frac{\lambda_f^3}{4\pi} (\Lambda^2 + m_H^2) \quad . \quad (3.1)$$

If cutoff at a scale  $\Lambda$ , close to the Planck mass ( $M_{Pl}$ ) of about  $10^{19}$  GeV, and with  $m_H = v \approx 246$  GeV, a cancellation of the radiative correction for this fermion loop



**Figure 3.1:** The left picture shows a sketch of the ADD space with the SM 3+1 dimensional brane and the bulk, including EDs. The apparent 4-dim. space on 'our brane' is shown as a solid line. Right: in the ADD model, the SM particles are localized on a 4-dim. domain wall and gravity spreads in all  $4 + \delta$  dimensions [72].

requires a precision of  $(m_H/\Lambda)^2 \approx 10^{34}$ , the so-called 'fine tuning'. In the SM, this fine-tuning can not be explained by an underlying physical mechanism and is therefore called 'unnatural'. It can however be explained with the concept of extradimensions.

### The general idea of extra dimensions

Extra dimensions (ED) were first thought of as an approach to unify electromagnetism with Einstein's general relativity by Kaluza-Klein (KK) [68, 69]. The four-dimensional Minkowski space, three spatial dimensions plus one time dimension, would be supplemented by at least one additional spatial dimension. The weakness of gravity in our apparent 4-dimensional world can then be explained by its propagation through extradimension(s). This concept is in the following outlined with the example of the model for large EDs from N. Arkani-Hamed, S. Dimopoulos, and G. Dvali (ADD) [70]. Large EDs means in this context 'large' with respect to the weak scale. This model predicts  $\delta$ -extra compact EDs of radius 'R'. The SM physics are contained on a 3+1 SM brane, while gravitons are allowed to propagate in the 'bulk' [71], including also EDs. The concept is illustrated by the left sketch in Figure 3.1.

Gauss' law of gravity is extended by  $\delta$ -extra dimensions and the gravitational potential ( $V(r)$ ) is reformulated by expressing the Newton's constant by the fundamental  $(3 + 1 + \delta)$ -dimensional Planck mass ( $M_{\text{Pl}_{3+1+\delta}}$ ) [73]:

$$G = \frac{\hbar c}{M_{\text{Pl}_{3+1+\delta}}^2} .$$

The gravitational potential inside a compact extra dimension of radius 'R' can then be rewritten as [70]:

$$V(r) = -\frac{m}{M_{\text{Pl}_{3+1+\delta}}^{2+\delta} r^{\delta+1}} \quad (r \ll R) \quad (3.2)$$

Outside of the compact extradimension ( $r \gg R$ ), this equation is reduced to the classical Gauss' law of gravity since the gravitational flux cannot propagate through the EDs and

reduces to a constant multiplicative factor:

$$V(r) = -\frac{m}{M_{\text{Pl}_{3+1+\delta}}^{2+\delta}} \frac{1}{R^\delta} \frac{1}{r} \quad (r \gg R) \quad (3.3)$$

This solution results in an effective four-dimensional Planck mass of

$$M_{\text{Pl}}^2 = M_{\text{Pl}_{3+1+\delta}}^{2+\delta} R^\delta \quad (3.4)$$

The fundamental Planck mass  $M_{\text{Pl}_{3+1+\delta}}$  would then be small and with a gravitational force much stronger than what is observed in 4-dimensions. The apparent weakness would be a consequence of the propagation of gravity in  $\delta$ -extradimensions. If the fundamental Planck mass is chosen to be of the order of the electroweak scale, and  $2 \leq \delta \leq 7$ , the size of the EDs would allow a detection in the LHC experiments [70].

Kaluza-Klein excitations [68, 69], which are hypothetical particles carrying momentum in the ED(s) are then a consequence of this theory. Mathematically, they are described as a standing wave in the extra compactified dimension, with an invariant mass of

$$M_{\text{KK}} = \frac{\delta \hbar}{Rc} \quad . \quad (3.5)$$

Since we measure extradimensions in our 4-dimensional world, we could not measure the KK-particle momentum of the ED. In the detector, we would instead see a set of  $\delta$  possible mass values from excited KK-modes, the so-called Kaluza-Klein tower. If the number of extradimensions allows an observation of the KK-particles, they would be observed as an apparent continuous enhancement of particles with a mass in the TeV range. The separation of the different excitation modes is in the meV range and as such too small to be resolved with the LHC detectors.

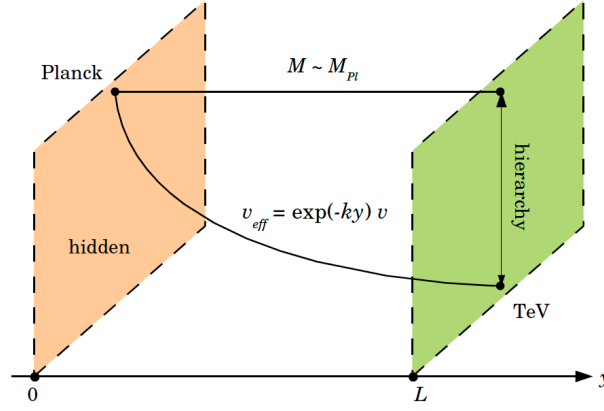
In the subsequent section, another model is detailed, which solves the hierarchy model with an extended extradimension.

### Randall-Sundrum model

The warped geometry of the Randall-Sundrum (RS-1) model [74] introduces a non-compact extra-dimension to the 4-dim. Minkowski space. Its metric is a solution to the Einstein equations. The extra dimension ( $y$ ) is 'warped', meaning that it is curled up to a circle with a finite radius ( $r_c$ ) and curvature parameter ( $k$ ). The 4-dim. universe is supposed to be flat and static. The warped geometry has therefore the following metric tensor:

$$ds^2 = e^{-2k|y|} \eta_{\mu\nu} dx^\mu dx^\nu + dy^2 \quad (3.6)$$

The geometry consists of the well-known Cartesian product of the 4-dim. Minkowski metric ( $\eta_{\mu\nu} dx^\mu dx^\nu$ ), only rescaled by an exponential function. At any given y-point



**Figure 3.2:** Sketch of the warped RS-ED geometry with the hidden Planck brane in orange and the TeV brane in green. In between the two is the 5-dim. 'bulk'. The exponential behavior of the Higgs vacuum expectation value is depicted [75].

of the ED, the metric is still flat with a different overall scaling. From the left sketch of Figure 3.1 it is visible that the opposite coordinate points on the circle need to be identified with each other, imposing the boundary conditions of  $y = 0$  and  $|y| = \pi r_c = L$ . The two boundary conditions determine the warp factor of Equation 3.6:

$$\frac{e^{-k|y(L)|}}{e^{-k|y(0)|}} = e^{-2kr_c} \quad (3.7)$$

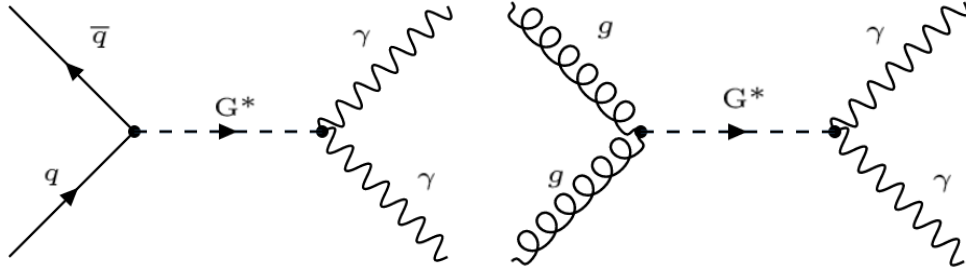
A value of  $kr_c \approx 35$  gives  $M_{Pl}/M_H \approx 10^{16}$  in this exponentially falling function and solves the discrepancy in hierarchy. The result is an Anti-de-Sitter (AdS) space between two branes at  $y = 0$ , which is called the Planck or Gravity brane, and  $|y| = L$ , the TeV or weak brane. A sketch of this geometry is given in Figure 3.2. The SM is confined on the TeV brane, similar to the right sketch of Figure 3.1.

The wave function of the massless graviton mode is then localized close to the Planck brane and is exponentially suppressed on the TeV brane, resulting in a weak interaction on this brane.

Evaluating this metric for the mass scale, one finds that there is only a small probability that the SM particles are on the second brane of  $|y| = L$ . The Higgs vacuum expectation value evaluates for instance to [74]:

$$v = e^{-kr_c\pi} v_0$$

and is depicted in Figure 3.2. This agrees with the intuitive understanding of the Planck scale and the scale of the Higgs boson: if the Higgs boson mass value is of the order of the Planck scale on the Planck brane, it is warped down to the weak scale on the first brane, giving us the measured physical Higgs mass. The described mass scaling of the Higgs boson can be applied to any matter particle, also KK-gravitons. The graviton



**Figure 3.3:** Feynman diagram for the s-channel of virtual graviton production through quark-antiquark annihilation (left) and gluon fusion (right), decaying into two photons.

is expected to only have  $1/M_{\text{Pl}}$  interactions at the TeV brane, since its wavefunction is peaked near the Planck brane. The wavefunctions of the KK-particles are however expected to peak near the TeV brane with a coupling strength of  $1/\text{TeV}$ , a  $\mathcal{O}(10^{16})$  stronger interaction strength compared to the graviton. The KK-excitation modes would appear as well separated spin-2 resonances in the TeV range and can be identified by measuring its mass and spin.

The masses ( $m_n$ ) of the KK-tower are given by the zero solutions ( $j_n$ ) of the Bessel function:

$$m_n = k \times e^{-kL} j_n \quad (3.8)$$

The decay width of the KK-particles would depend on the mass of the KK-particles ( $m_G$ ) and the number of its SM decay articles ( $n_{\text{SM}}$ ):

$$\Gamma_G \approx n_{\text{SM}} \frac{m_G^3}{(M_{\text{Pl}} e^{-2kr_c})^2} \quad (3.9)$$

The graviton production cross-section and its decay rates depend on the warp factor and the AdS curvature. In the RS-1 model, the KK-gravitons decay mainly to the dijet final state, with a branching fraction of about 0.5 for the  $gg$ -decay and 0.15 for the  $qq$ -decay. The dilepton final state, including muons, electrons and tau leptons, has a branching fraction of close to 0.1. The diphoton final state is with a branching fraction of 0.06 and its rather unambiguous event signature also an interesting search decay channel. If an excess is observed in this diphoton decay channel and is aimed to be explained by a RS-1 graviton signal, this excess would also need to be observed in the dijet and dilepton decay channel.

The RS model is the chosen benchmark model for the spin-2-diphoton resonance search of this dissertation. The production and decay s-channel Feynman diagram is depicted in Figure 3.3. The intrinsic width ( $\Gamma_G$ ) of the resonance with mass  $m_G$  is described by the dimensionless coupling parameter to the SM fields  $\tilde{k} = k/M_{\text{Pl}}$  [76] and was simulated for three benchmark values:  $\tilde{k} = 0.01, 0.1$  and  $0.2$ .

The previously described RS-1 model was further developed to a RS-2 model. In this model the 5th dimension is infinite, since the gravity brane is set at an infinite distance ( $L \rightarrow \infty$ ) and allows matter to propagate in the bulk [77]. During the recent excitement of the 750 GeV excess, Csáki and Randall interpreted the signal in terms of the Bulk RS model [78].

## 3.2 Additional neutral scalars in the extended Higgs sector

The existence of a heavy neutral scalar is motivated by many BSM models, among them SUSY, Little Higgs and Gauge Higgs unification [66, 79–83]. As a benchmark model for a heavy neutral scalar (spin-0), the two-Higgs-Doublet-Model (2HDM) was chosen [79, 80, 82–84]. The 2HDM is for instance motivated by the Minimal Supersymmetric Standard Model (MSSM) [85], a theory which gives among others a solution to the fine-tuning problem. This theory predicts one supersymmetric (SUSY) partner to each gauge boson and chiral fermion of the SM [8]. To generate the mass for each (SUSY) particle an additional second complex scalar Higgs field is defined. Usual constraints on the 2HDM are that the ratio  $\rho = m_W^2/m_Z^2 \cos^2 \theta_W$  needs to be close to one and that the Glashow-Weinberg criterion guarantees the absence of tree-level flavor-changing neutral current effects [86]. The two Higgs doublets can then be defined as:

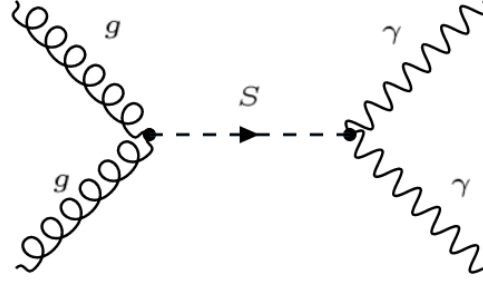
$$\phi_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} \phi_1^0 + ia_1^0 \\ \sqrt{2}\phi_1^- \end{pmatrix}, \quad \phi_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{2}\phi_2^+ \\ \phi_2^0 + ia_2^0 \end{pmatrix} \quad (3.10)$$

with the  $\phi_{1/2}^0$  and  $a_{1/2}^0$  being the CP-even and CP-odd neutral components and  $\phi_{1/2}^\pm$  being the complex charged component of the respective Higgs doublet. In this definition, the  $\phi_1$  has  $Y = -1$  and  $\phi_2$  has  $Y = 1$  [8]. Due to the spontaneous electroweak symmetry breaking, five physical Higgs boson states are created: the CP-even scalars, the light Higgs boson ( $h$ ) with mass  $m_h$  and the heavier Higgs boson ( $H$ ) with mass  $m_H$ , as well as the CP-odd pseudoscalar ( $A$ ) with mass  $m_A$  and one charged Higgs pair ( $H^\pm$ ) with mass  $m_{H^\pm}$  [83]. Besides the Higgs boson masses, this model has two more free parameters:

- the ratio of the two vacuum expectation values  $\frac{\langle \phi_2^0 \rangle}{\langle \phi_1^0 \rangle} = \frac{v_2}{v_1} = \tan(\beta)$ . This angle  $\beta$  diagonalizes both the CP-odd and charged Higgs sectors.
- the mixing angle  $\alpha$ , which diagonalizes the CP-even Higgs ( $2 \times 2$ ) squared matrix and is given in terms of the quartic couplings.

**Table 3.1:** Leading 2HDM decay topologies with unsuppressed production cross-sections near the alignment limit for neutral scalars with mass spectra  $m_H, m_A > 2m_h$ .

|                                                     |
|-----------------------------------------------------|
| 2HDM decay topology, enhanced in alignment limit:   |
| $H, A \rightarrow \gamma\gamma$                     |
| $H, A \rightarrow \tau\tau, \mu\mu$                 |
| $H, A \rightarrow tt$                               |
| $t \rightarrow H^\pm b$                             |
| 2HDM decay topology, suppressed in alignment limit: |
| $H \rightarrow VV$                                  |
| $A \rightarrow Zh$                                  |
| $H \rightarrow hh$                                  |



**Figure 3.4:** Feynman diagram of a s-channel scalar production through gluon fusion, decaying into two photons.

In the so-called alignment limit ( $\cos(\beta - \alpha) = 0$ ), the lighter CP-even Higgs boson 'h' would have couplings like the SM Higgs boson [79]. The four other Higgs boson masses can have a different mass scale than  $m_h$ , but should be of similar scale among each other:  $m_H \approx m_A \approx m_{H^\pm}$ . To be detectable at the LHC experiments, the masses would need to be at the TeV scale [87]: In the alignment limit, the associated production modes of the heavier neutral Higgs bosons (H,A) and decay modes to vector bosons are suppressed. A list of the affected decay modes can be found in Table 3.1. The branching fractions of other decays of H and A, which do not decouple, are consequently enhanced, among others the decay into the diphoton final state. At moderate values of  $\tan(\beta)$ , the neutral Higgs bosons are expected to be produced mainly via gluon-gluon fusion, mediated by loops containing heavy top and bottom quarks and the corresponding SUSY partners [8]. Other production mechanisms add only up to 10 % to the overall neutral Higgs boson production. For the search of high mass diphoton resonances of this dissertation, it is therefore assumed that the Higgs bosons are only produced by gluon-gluon fusion via the Feynman diagram shown in Figure 3.4 Since the search of this dissertation also looks for spin-2 resonances, the widths of the resonances was chosen to be similar. The

relative width ( $\Gamma_X/m_X$ ) of the spin-0 resonance corresponds to

$$\Gamma_X/m_X = \tilde{k}^2/1.4$$

and was simulated for values of  $\Gamma_X/m_X = 1.4 \times 10^{-4}$ ,  $1.4 \times 10^{-2}$  and  $5.6 \times 10^{-2}$ .

### 3.3 Previous searches for high mass diphoton resonances at collider experiments

The search for high mass diphoton resonances presented in part I of this dissertation is performed on a dataset, which was recorded at a center-of-mass energy of 13 TeV. The results are interpreted in terms of spin-0 and spin-2 resonances and is compared to the most recent results at 13 TeV of the ATLAS collaboration [13, 15].

These results at 13 TeV are preceded by several searches for high mass resonances, decaying in the diphoton final state. A chronological overview of the published results from the respective collaborations is given in Table 3.1. It lists the respective center-of-mass energy and integrated luminosity, the search range and the spin of the hypothetical signal of the published result.

The first searches for high mass diphoton resonances were performed at the Tevatron collider [88] with a center-of-mass energy of 1.96 TeV. The CDF [89] and D0 [90] experiments probed the highest diphoton masses for RS-graviton resonances with a width of  $k/M_{Pl} = 0.1$  up to 963 GeV and 1050 GeV at 95 % confidence level (C.L.), respectively. The exclusion limits at 95 % C.L for the narrow width hypothesis ( $k/M_{Pl} = 0.01$ ) are 459 GeV and 560 GeV, for the CDF and D0 collaboration. The more stringent exclusion limits of the D0 collaboration may be partly due to the inclusion of dielectron data. For the D0 analysis, the determination of the background shapes relied at least partly on MC simulations. The background normalization was determined by fitting the invariant diphoton mass spectrum in data to a superposition of the background components in a low mass control region  $60 < m_{\gamma\gamma} < 200$  GeV, where the RS-gravitons were previously excluded at a 95 % C.L. [91].

The CDF analysis used instead a functional form, determined with MC simulations, to describe the sum of background contributions in data. The leading-order graviton production cross-section was multiplied by mass-dependent K-factors in MC, which may have also contributed to the more conservative limits at high diphoton masses [89].

At the start of the LHC, the collider provided collisions with a center-of-mass energy of 7 TeV. Two searches for extradimensions in the high mass diphoton spectrum were performed by the ATLAS [92] and CMS collaboration [93], respectively. The higher

| Experiment | $\sqrt{s}$<br>(GeV) | $\mathcal{L}$<br>(fb <sup>-1</sup> ) | Mass range<br>(GeV) | Spin | Year | Ref. |
|------------|---------------------|--------------------------------------|---------------------|------|------|------|
| CDF        | 1.96                | 5.94                                 | 100-700             | 2    | 2010 | [89] |
| D0         | 1.96                | 5.94                                 | 220-1050            | 2    | 2010 | [90] |
| ATLAS      | 7                   | 4.9                                  | 142-3000            | 2    | 2013 | [92] |
| CMS        | 7                   | 2.2                                  | 200-2000            | 2    | 2012 | [93] |
| ATLAS      | 8                   | 20.3                                 | 65-650              | 0,2  | 2014 | [94] |
| CMS        | 8                   | 19.7                                 | 150-850             | 0,2  | 2014 | [95] |
| CMS        | 8                   | 19.5                                 | 300-3500            | 2    | 2014 | [96] |

**Table 3.2:** A list of previous searches of high mass diphoton resonances at collider experiments. The experiment, center-of-mass energy ( $\sqrt{s}$ ), integrated luminosity ( $\mathcal{L}$ ), mass range, spin, the year of the latest publication and the reference to the publication are listed.

collision energy and improved data-driven analysis techniques lead to exclusion limits at 95 % C.L. of up to 2.23 TeV and 1.84 TeV for the RS-graviton with a dimensionless coupling of  $k/M_{\text{Pl}} = 0.1$  for the ATLAS [92] and CMS [93] collaborations. For the narrow width hypothesis ( $k/M_{\text{Pl}} = 0.01$ ), an exclusion limit at 95 % C.L. of 1 TeV for the ATLAS and 0.86 TeV for the CMS collaboration could be set. To improve their sensitivity, the ATLAS collaboration combined their results with the search for high mass resonances decaying in the dilepton final state. With respect to the results from the Tevatron, the excluded diphoton production cross-section could be lowered by a factor 2-3, leading to more stringent limits for the RS-graviton of the order of 10 – 15 %. Both collaborations interpreted their results also in terms of a non-resonant diphoton production, the ADD model.

For the next increase in center-of-mass energy to 8 TeV, the CMS collaboration published two different searches for high mass diphoton resonances. The first analysis [96] searched for RS-gravitons in the high mass diphoton spectrum and extended the RS-graviton limit at 95 % C.L. to 1.34 TeV, 2.12 TeV and 2.62 TeV for  $k/M_{\text{Pl}} = 0.01, 0.05$  and  $0.1$ , respectively. The left side of Figure 3.5 shows the corresponding 95 % C.L. exclusion limit for RS-gravitons.

The second search performed by the CMS collaboration, concentrated on a search range of 150-850 GeV and extended the search to new resonances with natural widths of up to 10 % of the mass value [95]. The limits were interpreted in terms of RS-graviton resonances and a new heavy scalar, predicted among others by the 2HDM model. The right of Figure 3.5 shows the observed exclusion limit at 95 % C.L. on the cross-section times the branching ratio of a new resonance decaying into two photons as a function of the resonance mass hypothesis and width combining the four classes of events of the search.

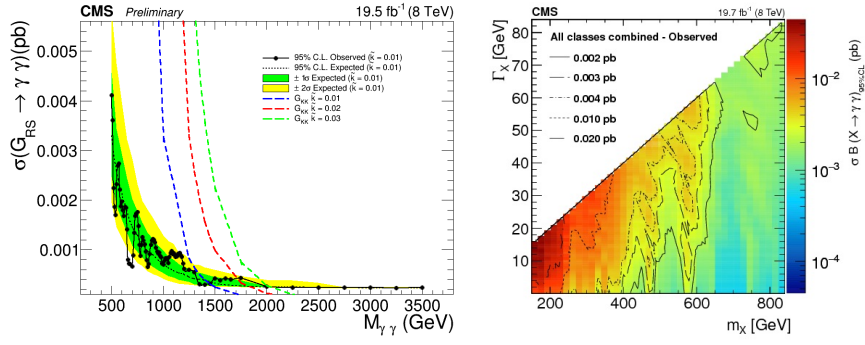
To improve the sensitivity of the search presented in this thesis, the results obtained at

13 TeV were combined statistically with the two searches at 8 TeV. At each  $m_X$ , the analysis with the most stringent expected 95 % C.L. on resonant diphoton production was taken for the final combination. For resonance masses below  $m_X = 850$  GeV, the event selection of Ref. [95] entered the combination, for masses above 850 GeV the event selection of Ref. [96] was taken. In the context of this combination, further details on these two searches are given in Section 14.1.

The ATLAS collaboration interpreted their results of a search for high mass diphoton resonances at 8 TeV in terms of a rather independent event topology, their results were as well interpreted for heavy scalar and RS-graviton resonances, decaying into two photons [94]. Analysis techniques of the measurement of the Higgs boson, decaying to the diphoton final state [44, 45] were adapted for the search of high mass diphoton resonances. In contrast to the search at CMS [95], the ATLAS collaboration extended their search range down to 65 GeV and fitted analytical descriptions of signal and background distributions to the diphoton invariant mass spectrum in data. The observed limit at 95 % C.L. for an additional scalar diphoton resonance ranged from 90 fb for  $m_X = 650$  GeV down to 1 fb for  $m_X = 600$  GeV [94].

The recent change in center-of-mass energy to 13 TeV, enhanced again the discovery potential for high mass resonances: to find a possible new resonance at 13 TeV, for instance produced via gluon-gluon fusion and with a mass of about 1 TeV, only about one sixth of the integrated luminosity at 8 TeV would be needed [97]. The first results for resonance searches with an integrated luminosity of  $3.3 \text{ fb}^{-1}$  were therefore expected to show signs of new physics, if they would have existed at this mass scale.

The results of the search for heavy scalar and RS-graviton resonances, decaying to the diphoton final state is the subject of the first part of this dissertation. The selection of the diphoton events is thereby independent of the final interpretation. A similar search from the ATLAS collaboration employed in contrast to that a slightly different event selection for the search of heavy scalars and RS-gravitons [13, 15]. The results of this search are compared to the ones of the CMS collaboration in part I of this dissertation.



**Figure 3.5:** Left: expected and observed 95 % CL<sub>s</sub> exclusion limit for RS-gravitons, decaying via  $G_{RS} \rightarrow \gamma\gamma$  as published in Ref. [96]. Right: observed exclusion limit at 95 % C.L. on the cross-section times the branching ratio of a new resonance decaying into two photons as a function of the resonance mass hypothesis and width combining the four classes of events as published in Ref. [95].



## 4

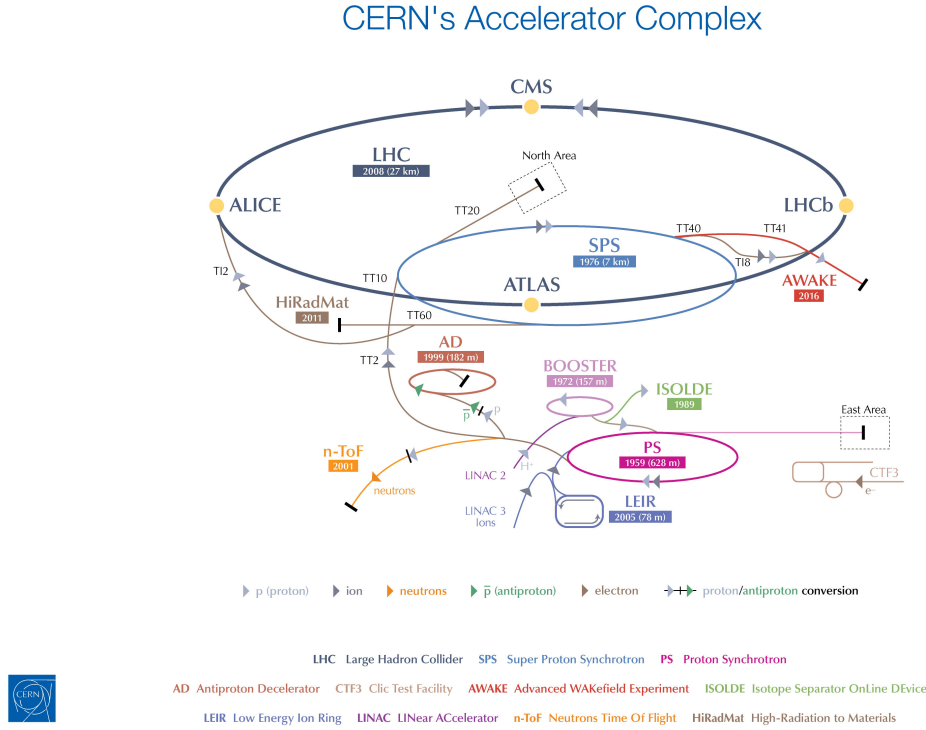
# The CMS detector, its electromagnetic calorimeter and the reconstruction of photons

## 4.1 The CMS detector at the LHC

The European Organization for Nuclear Research (CERN) is a particle physics research facility in Geneva, located at the boarder between Switzerland and France. It provides the infrastructure and the instruments for fundamental particle physics research. The central unit is the Large Hadron Collider (LHC) ring [9, 10, 98, 99], accelerating and colliding high energy protons and heavy ions. These collisions are used by several experiments located around the accelerator, probing the standard model of particle physics and searching for new physics beyond the SM. The LHC is located 100 m underground, inside a 26.659 km circumference tunnel, originally built for the Large Electron Positron collider (LEP) [100].

Since the analysis presented in this thesis searches for new particles being produced in proton-proton collisions, the pp-acceleration process is shortly outlined. A sketch of the accelerator chain complex is given in Figure 4.1. The protons are obtained by ionizing hydrogen and are subsequently accelerated to an energy of 50 MeV by the linear accelerator LINAC 2. The protons are subsequently further accelerated by the PROTON SYNCHROTRON BOOSTER (PSB) to 1.4 GeV and the PROTON SYNCHROTRON (PS) to 25 GeV. In the latter ring accelerator, the proton beam is split into bunches of  $1.2 \times 10^{11}$  protons with a time spacing of 25 ns among them. The protons subsequently enter the SUPER PROTON SYNCHROTRON (SPS) where they are accelerated to 450 GeV and injected into the LHC. The LHC is the largest particle accelerator of the world, providing protons with energies in the TeV regime.

At the start of the LHC, during the 'run-I' period, the energy per proton beam was 3.5 TeV, which was then increased to 4 TeV. After a few upgrades and repairs of the LHC, an energy of 6.5 TeV per proton beam could be achieved in 2015 for the



**Figure 4.1:** The LHC is the last ring (dark gray line) in a complex chain of particle accelerators. The smaller machines boost the particle energies and provide beams to a whole set of smaller experiments [101].

'run-II' period. The design beam energy for the LHC is 7 TeV, which will presumably be achieved in the upcoming years. The LHC accelerates two counter-circulating proton beams, each consisting of nominal 2736 proton bunches. Each proton beam is accelerated by 8 radiofrequency (RF) cavities with an alternating current of 400.8 MHz and an electromagnetic field of  $5.5 \text{ MV m}^{-1}$  [98]. They also reshape the proton bunches automatically in their longitudinal direction. The beams are kept in a circular orbit by 1232 superconducting dipole Niobium Titanium magnets with a magnetic field of 8.33 T. Quadrupoles and higher order magnets are used to focus and correct the two counter-circular beams at the interaction points.

#### 4.1.1 The performance of the LHC

A key parameter of an accelerator is quantified by the instantaneous luminosity ( $\mathcal{L}$ ), the total number of particle collisions per unit time in the given collision point. This instantaneous luminosity is dependent on several parameters [99]: the revolution frequency  $f_{\text{rev}}$ , the number of bunches per beam  $n_B$ , the number of protons per bunch  $N_p$  and the relativistic gamma factor  $\gamma_r$ . It is further parametrized by the normalized beam emittance  $\epsilon_n$ , quantifying the transverse beam profile, and  $\beta^*$ , the  $\beta$ -function at

**Table 4.1:** LHC parameters for run-II pp-collisions planned in the context of the Chamonix 2016 conference and measurements in July 2016, taken from [99, 102].

| Parameter                                                                            | Chamonix 16          | July 16               |
|--------------------------------------------------------------------------------------|----------------------|-----------------------|
| Energy per beam                                                                      | 6.5 TeV              |                       |
| Bunch spacing                                                                        | 25 ns                |                       |
| $f_{\text{rev}}$                                                                     | 11246 Hz             |                       |
| $\beta^*$ for CMS                                                                    | 0.4 m                |                       |
| Half crossing angle $ \eta_{\text{SC}} $ (assuming $\epsilon_n = 3.75 \mu\text{m}$ ) | 185 $\mu\text{rad}$  |                       |
| Relativistic $\gamma_r$                                                              | 3730-7461            |                       |
| Bunch length at the start of fill - $4\sigma$                                        | 1.25 ns              | 1.05 ns               |
| Number of bunches $n_b$                                                              | 2736                 | 2076                  |
| Maximal number of protons per bunch $N_p$                                            | $1.2 \times 10^{11}$ | $1.18 \times 10^{11}$ |
| Emittance into stable beams $\epsilon_n$                                             | 3.5 $\mu\text{m}$    | 2.6 $\mu\text{m}$     |

the interaction point as well as the geometry factor 'F', describing the crossing angle between the colliding beam and the transverse Root Mean Squared (RMS) beam size:

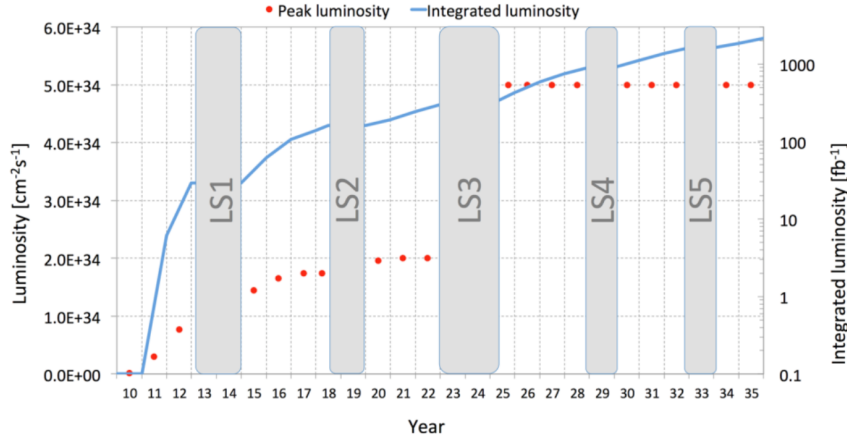
$$\mathcal{L} = f_{\text{rev}} n_b \frac{N_p^2 \gamma_r}{4\pi \epsilon_n \beta^*} F \quad (4.1)$$

The instantaneous luminosity is measured in  $\text{cm}^{-2} \text{s}^{-1}$ . The parameter values of the LHC for run-II are listed in Table 4.1. The left column quotes the planned parameters during the Chamonix 2016 conference, the right column denotes the measured values in July 2016. The measured values agree with or even exceed the expected performance.

This luminosity is provided for experiments, which record the particle collisions. From the detector point of view, a proton-proton run is subdivided in so-called 'lumi-sections', denoting the run period where the instantaneous luminosity stays approximately unchanged. It is defined as  $2^{18}$  proton orbits in the LHC, which corresponds to a fixed time period of approximately 23.3 s. The integrated luminosity ( $\mathcal{L}$ ) is defined as the integrated instantaneous luminosity over time:

$$\mathcal{L} := \int \mathcal{L} dt \quad (4.2)$$

The current run schedule of the LHC is given in Figure 4.2. The search for high-mass diphoton resonances, which is subject of Part I of this dissertation, is designed for the run-II period, which finishes in 2019. The LHC or 'phase-I' program is expected to end in 2024, followed by an upgrade to the High-Luminosity LHC (HL-LHC) and the 'phase-II' program. For this phase-II program several detector parts will be upgraded, which is subject of Part II of this thesis.



**Figure 4.2:** Luminosity schedule of the LHC and High-Luminosity LHC from 2010 until 2035. The long-shutdowns are marked as gray areas [17].

The purpose of the LHC is to provide a high pp-collision rate ( $R$ ) in order to collect a large amount of interesting particle physics processes. A high collision rate depends linearly on the instantaneous luminosity:

$$R_{\text{process}} = \sigma_{\text{process}} \times \mathcal{L} \quad (4.3)$$

or total number of events for any given physical process by

$$N_{\text{process}} = \sigma_{\text{process}} \times \mathcal{L} \quad (4.4)$$

The LHC provides proton and heavy ion collisions to four major experiments, marked in Figure 4.1:

- ALICE (A Large Ion Collider Experiment) [103], focusing on heavy-ion physics.
- ATLAS (A Toroidal LHC ApparatuS) [104], a general-purpose detector.
- CMS (Compact Muon Solenoid) [11], the general-purpose detector on which all results of this thesis are based on. Its main components are outlined in Chapter 4.3.
- LHCb (LHC beauty) [105], focusing on heavy-flavor physics.

Next to these experiments, three smaller experiments are placed around the LHC: LHCf [106], MoEDAL [107, 108], and TOTEM [109].

## 4.2 Pile-up description in proton-proton collision

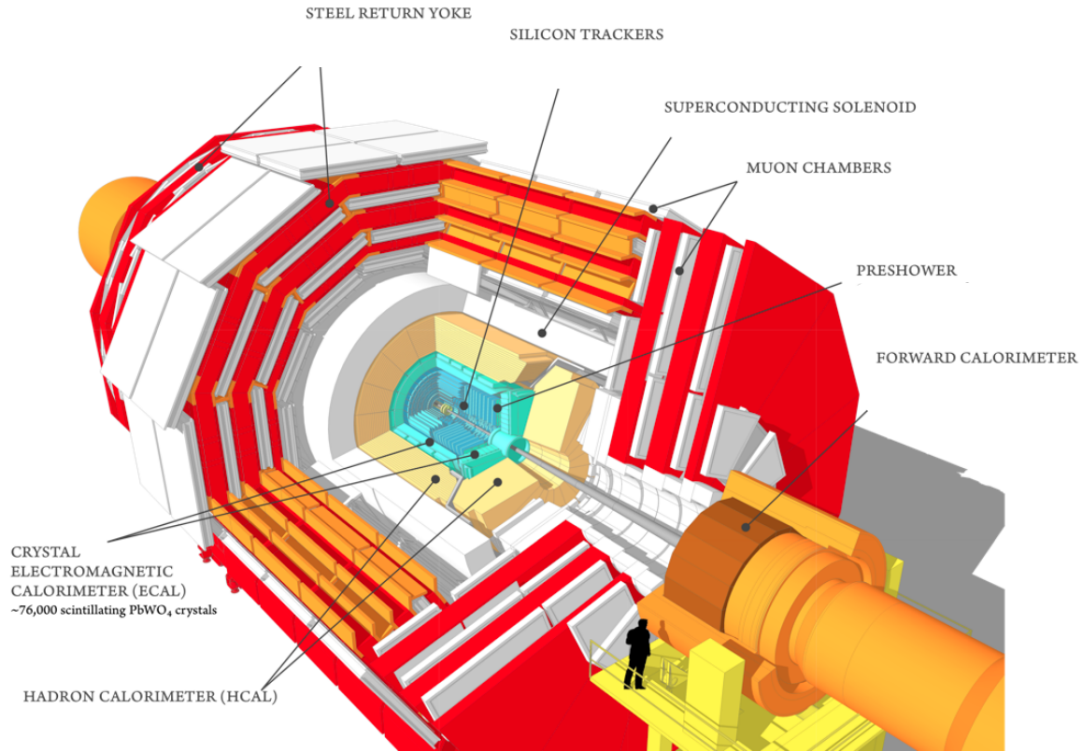
The general-purpose experiments ATLAS and CMS need a high event rate to probe the standard model of particle physics and search for new physics beyond the SM. This is accomplished by increasing the bunch intensity, since the number of bunches can not be easily raised. The underlying physics of pp-collisions is detailed in Section 2. For a collision in the CMS detector, two proton bunches cross each other at the center of the detector and several protons collide simultaneously. The number of pp-interactions per bunch-crossing is thereby Poisson distributed. Most of these interactions produce low-energy QCD processes with low-momentum jets. With increasing luminosity, these events 'pile-up' and complicate the trigger as well as the offline identification of particles. The pile-up events create further hits in the tracking system, leading to mismeasured or misidentified tracks. They deposit additional energy in the calorimeter, which complicates the identification of electrons or photons. Photons for instance are isolated objects with little activity around them. With higher in-time pile-up, more energy from the pile-up events is recorded around them and they are less distinguishable from jets. The calorimeter readout, which time-window is longer than 25 ns, also suffers from the out-of-time (OOT) pile-up, which describes the residuals from interactions at previous or following bunch crossings.

## 4.3 The Compact Muon Solenoid experiment

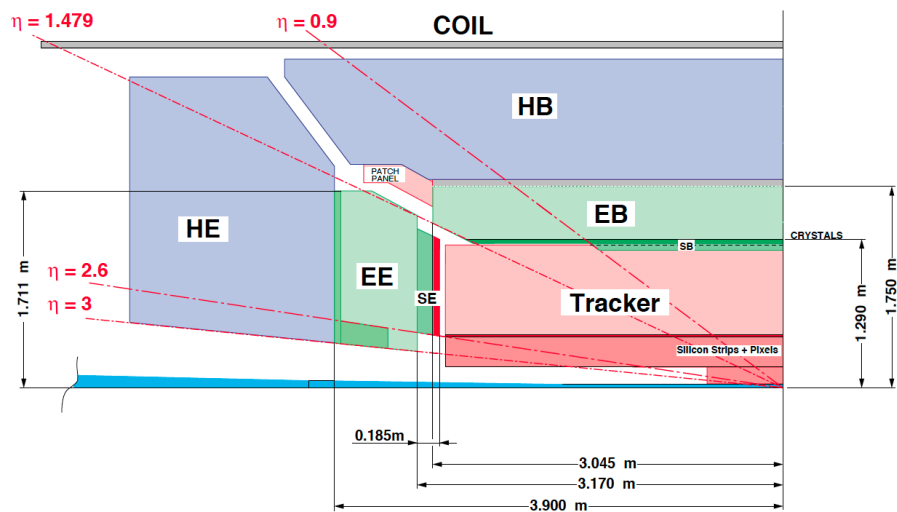
The CMS experiment is a general purpose detector for particle physics. The detector includes several subsystems in an onion-like structure, symmetrically centered around the interaction point. The 22 m long and 15 m wide detector is depicted in Figure 4.3.

It consists of a central, 'barrel', part and two forward regions, the 'endcaps', which detect particles at small deflection angles. The central piece of the detector is the superconducting solenoid with a magnetic field of 3.8 T. The tracking and calorimeter systems are contained within the solenoid as outlined in Figure 4.4. This design benefits the particle reconstruction as it minimizes the probability for a charged particle to generate a shower before reaching the calorimeters. Most of the detector is placed inside a steel skeleton which serves also as the return yoke for the magnetic field of 1.8 T. The muon detection system is placed inside this return yoke. The CMS detector has a weight of about 12,500 tonnes, mainly due to the steel skeleton and the solenoid.

The origin of the right-handed coordinate system of CMS is the central collision point, with the z-axis oriented in the anticlockwise-beam direction. The x-axis is oriented towards the center of the LHC accelerator ring, the y-axis points upwards. The azimuthal



**Figure 4.3:** Sketch of the Compact Muon Solenoid experiment [110].



**Figure 4.4:** Sketch of one quarter of the tracking detector and calorimeter system in CMS with their respective dimensions in the y-z plane [111].

angle ( $\phi$ ) is depicted on the right side of Figure 4.4, lies in the x-y plane and is measured from the x-axis. A slice of the CMS detector in this x-y plane is shown in Figure 4.5. The polar angle ( $\theta$ ) is directed upwards from the z-axis. With the polar angle, the pseudorapidity ( $\eta$ ) can be defined:

$$\eta = -\ln(\tan(\theta/2)) \quad (4.5)$$

The longitudinal momentum of the colliding partons is not precisely known. Detected particles within the detector are therefore often just described by their transverse momentum ( $p_T$ ) or transverse energy ( $E_T$ ).

A detailed description of the CMS detector can be found in Ref. [11]. The following paragraph shortly outlines the main detector parts. Special attention is given to the electromagnetic calorimeter in Section 4.4, since it is the central subdetector for the results of Part I and II of this thesis.

### Inner tracking system

The tracking detector surrounds the beampipe with a distance of the innermost layer of about 4 cm from the interaction point (IP). It has a length of 5.8 m, a diameter of 2.6 m, and covers a range of  $|\eta| < 2.5$  with an area of over 200 m<sup>2</sup> active silicon sensors. It is designed to measure the trajectories of particles as highlighted in Figure 4.5. As such, it has to provide a high spatial resolution and a fast signal readout while withstanding a harsh radiation environment of about 10<sup>6</sup> particles/(cm<sup>2</sup> s) (at a distance of 8 cm from the IP).

The innermost tracking system, the silicon pixel detector, is made of 66 million pixels with a size of  $100 \times 150 \mu\text{m}^2$ , enabling the reconstruction of primary and secondary vertices. The silicon pixel detector is followed by a silicon strip detector with coarser granularity. The track recognition is performed by about 15.200 highly sensitive modules containing 10 million detector strips. The tracking system is surrounded by the calorimeter system. The tracking detector has a radiation length ( $X_0$ ) of 0.4 at  $\eta = 0$ , which increases for higher  $\eta$  to approximately  $1.8 X_0$  at  $|\eta| = 1.4$  as visible from Figure 4.4. The tracking system is surrounded by the ECAL, which is described in detail in Section 4.4.

### Hadron calorimeter

The hadronic calorimeter measures the energy of hadrons by stopping them within its hermetic volume and reading out the deposited energy. Its dimensions, given in Figure 4.4, are constrained by the ECAL ( $R = 1.77$  m) and the surrounding magnet coil ( $R = 2.95$  m). The chosen design is the one of a sampling calorimeter with brass absorbers and scintillating tiles for the energy measurement. The readout is performed via

optical fibers by hybrid photodiodes.

It has a thickness equivalent to 11.8 nuclear interaction lengths. A small hadron outer calorimeter is placed behind the solenoid to capture very high energetic hadrons. The granularity is  $\Delta\eta \times \Delta\phi = 0.087 \times 0.087$ . The forward region extends to  $|\eta| = 3$  with a granularity of  $\Delta\eta \times \Delta\phi = 0.17 \times 0.17$ . Beyond that, a radiation hard, Cherenkov-based calorimeter (HF) for very forward directed particles is located at a distance of 11.2 m in  $z$  from the IP, covering a range of up to  $|\eta| = 5.2$ .

### **Muon detectors**

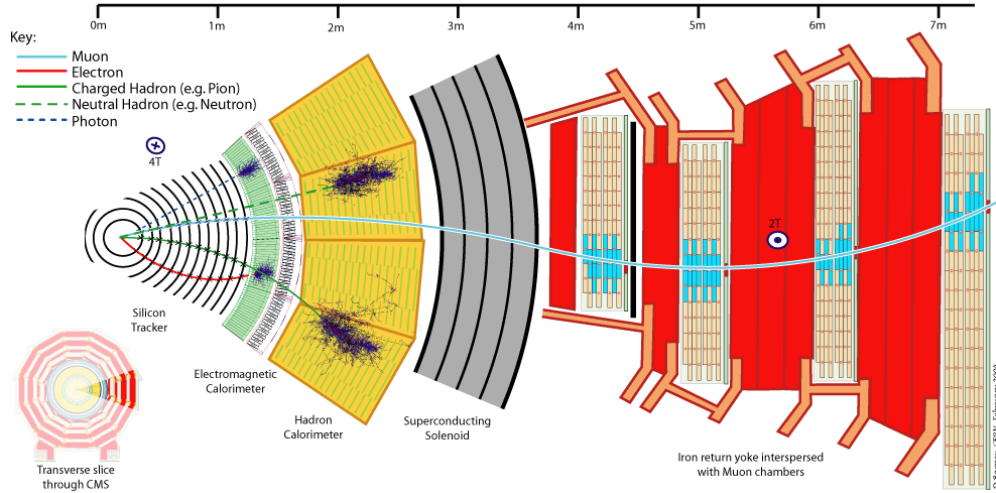
The outermost part of the detector is the muon detection system, identifying muons and providing a precise measurement of their momentum. In the barrel part of the detector, the muons are measured in drift tubes ( $|\eta| < 1.2$ ). In the endcaps region the muons are detected by cathode strip chambers, especially designed for a less uniform magnetic field and higher particle rates. Resistive plate chamber detectors are a crucial part of the trigger system for muon candidates and extend up to a pseudorapidity of 2.1. Since the detector parts are mounted within the return yoke of the magnetic field, its orientation and therefore the direction of the muon momentum is inverted with respect to the trajectory inside the solenoid as sketched Figure 4.5.

### **Trigger system**

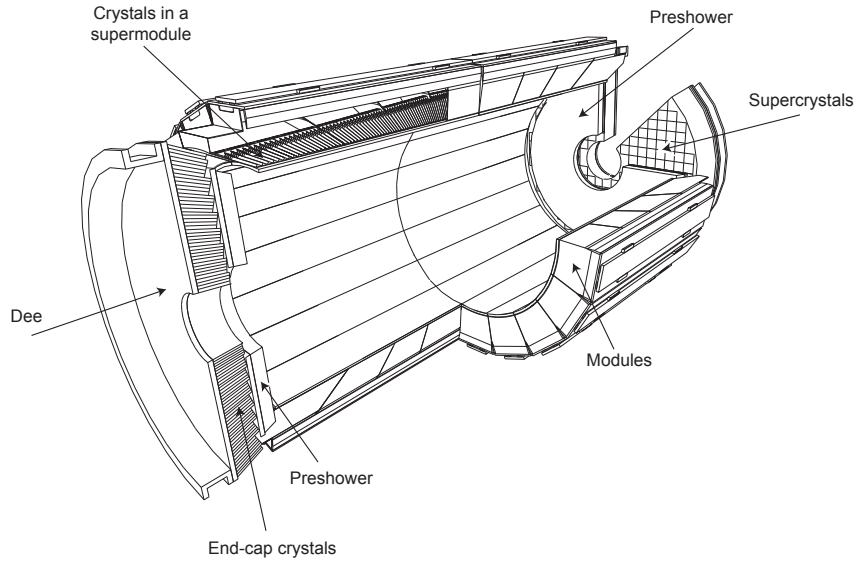
The collision rate of 40 MHz with a high-pile-up environment together with a limited storage space for the recorded events require a highly efficient trigger system. The trigger hierarchy is divided in a level-1 (L1) trigger system with an event rate of 100 kHz and the high-level trigger system (HLT) with 1 kHz. The L1-trigger relies on the decision of dedicated electronics, which record signals above a certain threshold. The events passing the L1-trigger are then forwarded to the HLT trigger. The HLT decision is determined by dedicated software algorithms, running on a computer farm. The decision process is more elaborate and is based on a first full reconstruction of the particles by including the tracking information and identifying calorimeter deposits.

## **4.4 The CMS electromagnetic calorimeter**

The electromagnetic calorimeter surrounds the tracking system and is depicted in Figure 4.6. The energy of electrons and photons ( $e/\gamma$ ) is measured in a calorimeter by stopping the particles within the material and measuring the thereby deposited energy. The ECAL of CMS is an hermetic and homogeneous calorimeter, consisting of 75,848 scintillating lead tungstate ( $\text{PbWO}_4$ ) crystals. The physics goals of CMS require a compact and highly granular ECAL, which is realized by these high density



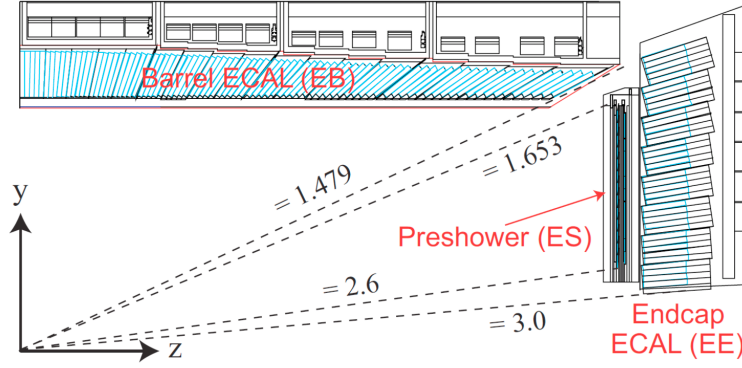
**Figure 4.5:** A slice in the x-y plane of CMS detector as depicted in the left corner of the illustration. The detection of typical particles in the individual detector layers is outlined [112].



**Figure 4.6:** Layout of the electromagnetic calorimeter [113].

( $\rho = 0.28 \text{ g/cm}^3$ ) crystals with a small Molière radius ( $R_M = 2.2 \text{ cm}$ ).

One goal of the ECAL design is to provide an excellent intrinsic photon energy resolution for the  $H \rightarrow \gamma\gamma$  search. An energy resolution at the level of 0.5 % for photons above 100 GeV is also important for the search presented in this thesis. The electromagnetic calorimeter consists of a barrel part (EB), two endcap parts (EE) and a preshower (ES). The exact dimensions of all subdetectors are written in Figure 4.4 and 4.7.



**Figure 4.7:** ECAL layout in y-z plane [113].

#### 4.4.1 The barrel electromagnetic calorimeter

The barrel part of ECAL extends to  $|\eta| < 1.479$ . It consists of 61,200 crystals with a length of 230 mm, equivalent to  $25.8 X_0$ . The crystal cross-section of  $0.0174 \times 0.0174$  in  $\eta$ - $\phi$  direction translates to a surface area of  $22 \times 22 \text{ mm}^2$  at the front face and  $26 \times 26 \text{ mm}^2$  at the rear face. The ECAL barrel was built with a quasi-projective geometry, with a tilted crystal axis of  $3^\circ$  in  $\phi$  and  $\eta$  with respect to the nominal interaction vertex to avoid particles passing undetected through the gaps between the crystals. The barrel crystals are grouped in  $5 \times 5$  matrices, 40-50 of these matrices are then placed inside one module. The module is held by an aluminum grid and mounted at the rear of the EB. Four modules with 1700 crystals each form a so-called supermodule (SM). The full EB consists of 36 SM.

When an electron or photon hits the  $\text{PbWO}_4$  crystals, it interacts with the material and deposits most of its energy within the crystals. Through the interaction with the particles of the induced electromagnetic shower, the atoms of  $\text{PbWO}_4$  get excited. The scintillation light emitted during the de-excitation is read out by high-efficiency avalanche photodiodes (APD). APDs are suitable photodetectors as they provide a high signal gain, which is required because of the low light yield (LY) of  $\text{PbWO}_4$  (see Table 19.1). A solid state device had to be used since the magnetic field is perpendicular to the crystal axis in the EB, which makes magnetic-field sensitive phototubes unusable. A stable temperature of  $18 \pm 0.05^\circ\text{C}$  for the EB is necessary as both, the gain of the APDs as well as the LY of the  $\text{PbWO}_4$  crystals, are highly temperature dependent.

#### 4.4.2 The endcap electromagnetic calorimeter

The endcap electromagnetic calorimeter covers the range of  $1.479 < |\eta| < 3$  in the two forward regions of the detector. Each endcap side consists of two 'dees' as shown in Figure 4.6, containing 3,662 crystals each. A set of  $5 \times 5$  crystals form a super crystal,

held by a carbon fiber alveolar structure. The crystals, mounted in a rectangular x-y grid, are focused beyond the interaction point, resulting in off-pointing angles of  $2-8^\circ$ , such that the electrons or photons do not pass through the gaps between the crystals. Each crystal has a length of 220 mm, corresponding to  $24.7 X_0$ , which is shorter compared to the EB crystal due to the additional  $3 X_0$  of ES. The truncated pyramid shaped crystals have a front face cross-section of  $28.62 \times 28.62 \text{ mm}^2$  and a rear face cross-section of  $30 \times 30 \text{ mm}^2$ . The crystals are read out by vacuum photo-triodes (VPT). APDs could not be used because of the high radiation levels. The use of phototubes is possible due to a quasi-parallel position to the magnetic field and the gain loss of VPTs in this radiation environment is acceptable. VPTs have a lower gain and lower quantum efficiency compared to APDs, but due to the larger rear face area of the crystals, the LY is still comparable.

#### 4.4.3 The preshower detector

The preshower detector is a small sampling detector in front of the endcap calorimeter with a range of  $1.65 < |\eta| < 2.61$ . Its primary purpose is to improve the  $\pi^0$ - $\gamma$  separation as the small angle between the two emerging photons of the  $\pi^0$ -decay in the EE can not be easily distinguished by EE crystals with a width of 28.62 mm. The preshower was only realized for EE, since the average energy of neutral pions is in this part higher than for the EB. The separation of the decay photons is therefore more difficult and is aimed to be improved by the tracking information of the preshower. The  $3 X_0$  long detector consists of two lead absorbers, with  $2 X_0$  and  $1 X_0$  length respectively, interleaved with two silicon strip detectors. The two silicon strip detectors are orthogonal to each other to improve the track reconstruction. The strip pitch provides a granularity of 1.9 mm, resulting in a resolution of  $300 \mu\text{m}$  for a 50 GeV photon. The preshower detector has to be operated at  $-10^\circ\text{C}$  to limit radiation damage. An electromagnetic particle of 20 GeV deposits roughly 5 % of its energy in ES. The fraction of its deposited energy decreases for higher energies.

#### 4.4.4 Lead tungstate crystals

Lead tungstate is a dense and radiation hard material. A list of the physical properties of lead tungstate can be found in the second part of this dissertation, where it is compared to other heavy inorganic scintillators (Table 19.1). In addition to the above mentioned properties,  $\text{PbWO}_4$  provides a fast response to electrons or photons, which is crucial for a bunch spacing of 25 ns. About 80 % of the light is emitted within 25 ns after excitation. The emitted light has a broad wavelength maximum of about 420 nm. The major

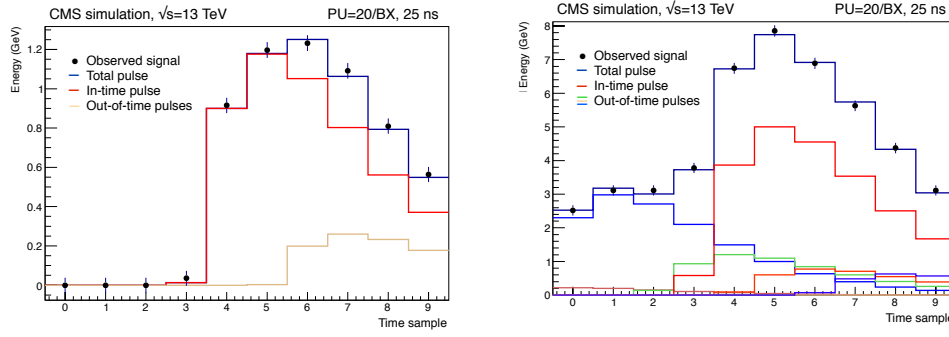
disadvantage of  $\text{PbWO}_4$  is its low light yield (LY) of 6-10 photoelectrons/MeV [114, 115], which impacts the timing resolution as well as the energy resolution. The LY varies due to different growing and doping mechanisms. The  $\text{PbWO}_4$  crystals were produced by two independent companies: the Bogoroditsk Techno-Chemical Plant (BTCP) in Russia and the Shanghai Institute of Ceramics (SIC) in China. The latter provided a 50 % higher LY and its crystals were therefore used for the high- $|\eta|$  part of the EE. The light yield also depends on the temperature (2.1 %/°C at 18°C), which requires a temperature stabilization within 0.05 °C to provide a constant intrinsic energy resolution of 0.5 % [116].

#### 4.4.4.1 The irradiation induced damage in lead tungstate crystals

The peak luminosity of about  $1.5 \times 10^{34} \text{ cm}^{-2} \text{ s}^{-1}$  (October 2016) results in a harsh radiation environment for ECAL. Fast hadrons, mainly pions, interact with the ECAL crystals and produce secondary hadrons. They build up a flux of low energy neutrons, mostly with energies below 10 MeV. The electromagnetic showers inside the crystals result also in a significant dose to the material. The dose rate is predicted to be  $0.17 - 0.25 \text{ Gy h}^{-1}$  at the shower maximum for the EB and  $5 \text{ Gy h}^{-1}$  at  $|\eta| = 2.5$  [117]. There are two different types of radiation damage:

- hadron-induced damage, which is the reason for the upgrades discussed in the second part of this dissertation. In this context, it is detailed in Section 16.2.2. Its impact on the energy resolution is expected to be below the design limits up to  $500 \text{ fb}^{-1}$  [118].
- recoverable radiation damage from ionizing electromagnetic radiation. This radiation damage does not affect the scintillation mechanism or the uniformity of the readout and recovers spontaneously at room temperature.

The recoverable radiation damage leads to a response change of the crystals. When the  $\text{PbWO}_4$  crystals are exposed to ionizing radiation, intrinsic point structure defects may act as traps for electrons or holes. These charged defects have different discrete energy levels with corresponding optical transitions and can therefore absorb the scintillation light of a certain wavelength. Due to the characteristic absorption bands, these defects are called 'color centers'. They are a result of the growing conditions of the crystal [119–123].



**Figure 4.8:** Two examples of fitted pulses for simulated events with 20 average pile-up interactions and 25 ns bunch spacing, for a signal in the barrel (a) and in the endcaps (b). Dots represent the 10 digitized samples, the red distributions (other light colors) represent the fitted in-time (out-of time) pulses with positive amplitude. The dark blue histograms represent the sum of all the fitted contributions [124].

#### 4.4.5 Reconstruction of the signal pulse shape

The scintillation light, emitted by  $\text{PbWO}_4$ , is measured by the photodetectors and read out as an analog signal by front-end electronics. The signal is pre-amplified, shaped and processed by a multi-gain amplifier. To enlarge the dynamic range between approximately 50 MeV and 3 TeV [111], the signal can be amplified with three parallel amplification stages: 1, 6 and 12. For very high energy photons, the ECAL readout electronic system saturates. The limit of their dynamic range is reached when the energy deposit in a single crystal has a value of about 1.7(2.8) TeV in the barrel (endcaps). The highest, non-saturated signal among the three amplifications is then digitized by a 12-bit ADC operating at 40 MHz. It reads out a set of ten consecutive digitized samplings and the signal amplitude is reconstructed based on them.

In run-II, the local energy reconstruction is performed by using the so-called 'multi-fit' method, which allows to reduce the impact of OOT pile-up [125]. In-time and OOT pile-up energy deposits have a considerable impact on the signal pulse reconstruction. As visible in Figure 4.8, the signal pulse shape is altered by these low amplitude pulses. The multi-fit method estimates the in-time signal amplitude and up to nine out-of-time amplitudes for each signal pulse by a  $\chi^2$ -minimization via the non-negative-least-squares technique to the ten digitized samples [125]. Two examples of a fitted pulse shape for a simulated event are shown in Figure 4.8 for the EB and the EE category, respectively. With this, an effective suppression of contributions from OOT energy deposits to the hit energy is achieved.

It was found out recently that the multi-fit algorithm does not take into account a non-linearity of the electronic readout system, which appears near the gain saturation. The reconstructed amplitude at a gain switch, especially from gain 12 to gain 6 and gain 1, is

therefore too low. This has an impact on the photon energy reconstruction for the high mass diphoton resonance search and is discussed in Chapter 6.

#### 4.4.6 Energy reconstruction in the ECAL

The deposited energy of electrons and photons is spread over several ECAL crystals. Around 94 % of the incident energy of an unconverted photon with an energy of  $\mathcal{O}(10 \text{ GeV})$  is deposited in a  $3 \times 3$  crystal matrix and 97 % in a  $5 \times 5$  crystal matrix [126]. The energy depositions in several ECAL crystals are first logically grouped under the hypothesis that they represent an electromagnetic shower. For run-II, the clustering is mainly performed by an 'island' algorithm [127, 128]. Groups of these clusters are then summarized by dynamic clustering algorithms [113] to a 'supercluster' (SC) under the hypothesis that they originate from the same electromagnetic particle produced in the collision. These clustering algorithms need to take into account the following effects: the tracking detector material in front of the ECAL leads to a conversion of the photons and causes bremsstrahlung from the electrons. The conversion probability ranges from 20 % for  $\eta = 0$  to 65 % at  $|\eta| = 1.5$ . It slightly decreases for the forward region, where the amount of tracker material upstream to the ECAL decreases compared to  $|\eta| = 1.5$  [129].

Electrons lose 33 – 86 % of their incident energy due to interaction with the tracking material. The radiated energy is spread along the azimuthal angle ( $\phi$ ) due to the bending of electron trajectories in the magnetic field. The energy spread in  $|\eta|$ -direction is negligible for  $p_T \geq 5 \text{ GeV}$ . This leads to an  $E_T$  dependent shower profile in  $\Delta\eta$  and  $\Delta\phi$  and needs to be recovered by the dynamic clustering algorithms. The newly developed supercluster 'Mustache' algorithm, named after its characteristic shape in the  $\eta$ - $\phi$  plane, takes the combined effect of conversion and energies spread in  $\phi$  into account. It allows energy sharing among different clusters, providing a finer spatial granularity, and improves the electromagnetic shower containment and rejection of pile-up particles.

The reconstruction of the electron or photon energy depends on the following variables:

- the signal amplitude of the  $i$ -th crystal  $A_i$ .
- the time dependent correction to the crystal response  $S_i(t)$ , which is mostly due to changes in the crystal transparency.
- the relative geometry calibration constant  $C_i$ , which accounts for differences in the crystal light yields, the energy leakage from the lateral faces of the crystal, and the individual photodetector responses.

- the scale factor  $G$ , which converts the digital scale to the energy scale, which is denoted in GeV.
- for the energy reconstruction in the endcaps, the measured energy in the preshower ( $E_{ES}$ ) needs to be added.
- the correction term  $F_{e,\gamma}$ , which takes into account material effects, the  $\eta - \phi$  dependent geometry and the slightly different shower development for electrons and photons.

The electron or photon energy ( $E_{e,\gamma}$ ) is then expressed as the sum over all clustered crystals (i) [113]:

$$E_{e,\gamma} = F_{e,\gamma} \times \left( G \times \sum_i (C_i \times S_i(t) \times A_i + E_{ES}) \right) \quad (4.6)$$

The excellent energy reconstruction relies on precision calibration and stable timing measurement. A detailed explanation of the applied calibrations methods can be found in Ref. [113, 125, 130]. A few important methods are shortly outlined in the following, focusing on the correction of the loss in crystal transparency and the relative calibration of the crystals.

The loss in crystal transparency due to ionizing radiation is monitored by a dedicated laser system. It injects light of a wavelength which is close to the peak scintillation light spectrum of  $PbWO_4$  in each EB crystal to derive corrections during run time with a transparency precision down to 0.1 % [131]. The system stability is further followed by additional laser systems and for EE also by LEDs. Figure 4.9 shows the evolution of the ECAL response to the laser light for six pseudorapidity regions, normalized to the measurements at the start of 2011. The radiation damage recovers spontaneously at room temperature as visible from the figure. The measurement of the transparency loss shows that it is stable with a constant dose rate. For this situation, the rate of annihilation and creation of color centers balance each other. The loss in transparency can then be translated to the change in response for the scintillation light.

The corrections can be validated with the following copious physics processes:

- the monitoring of the stability of the reconstructed invariant mass of  $\pi^0 \rightarrow \gamma\gamma$ .
- the usage of the ratio 'E/p', which measures the energy (E) of isolated electrons from  $W \rightarrow e\nu$  decays in the ECAL and their momentum (p) in the tracker. The stability of this ratio was better than 0.1 % in EB and 0.4 % in EE in 2012 [125].
- the invariant mass from  $Z \rightarrow e^+e^-$  decays.

To intercalibrate the light yield and the response of the photodetectors among the crystals, the  $\phi$ -symmetry of the energy deposition for a fixed pseudorapidity value in minimum bias events can be used. These events are required to have passed a minimum bias trigger in order to obtain an event sample which is minimal biased with respect to the different event topologies originating from pp-collisions. The  $\phi$ -symmetry method reaches a statistical precision of better than 0.2 % (0.4 %) in EB (EE) [125]. The accuracy is however limited to a few percent by the systematic uncertainties in the distribution due to the material upstream of ECAL. Since these systematic uncertainties do not vary with time, the  $\phi$ -symmetry can also be used to determine time dependencies in the intercalibration values. Another method for the intercalibration is the invariant mass reconstruction of  $\pi^0/\eta \rightarrow \gamma\gamma$  decays, which are measured in  $3 \times 3$  crystal matrices, centered around the crystal with the highest energy deposit. This gives a reliable estimate of the intercalibration value of each crystal.

Isolated and non-showering electrons from the  $Z \rightarrow e^+e^-$  decays are used to intercalibrate different ECAL regions in rings of pseudorapidity. The obtained  $\eta$ -scale is compared to simulation and the energy scale  $G$  from Equation 4.6 can be derived for EB and EE, respectively.

For run-II, the intercalibration constants are also derived by employing invariant mass constraints on dielectron events. This is aimed at improving the accuracy for the endcap region, for pseudorapidity values still covered by the tracker ( $|\eta| = 2.5$ ) as well as beyond this point in pseudorapidity, where the identification of the two electrons solely relies on calorimetric information.

The combined intercalibration residual miscalibration was below 0.5% for  $|\eta| < 0.7$  and lower than 1 % for  $|\eta| < 1.5$  after  $2.6 \text{ fb}^{-1}$  in 2016 [124, 132]. At this point, the intercalibration values derived from the decay processes  $W \rightarrow e\nu$  and  $Z \rightarrow e^+e^-$  were still dominated by statistical uncertainties.

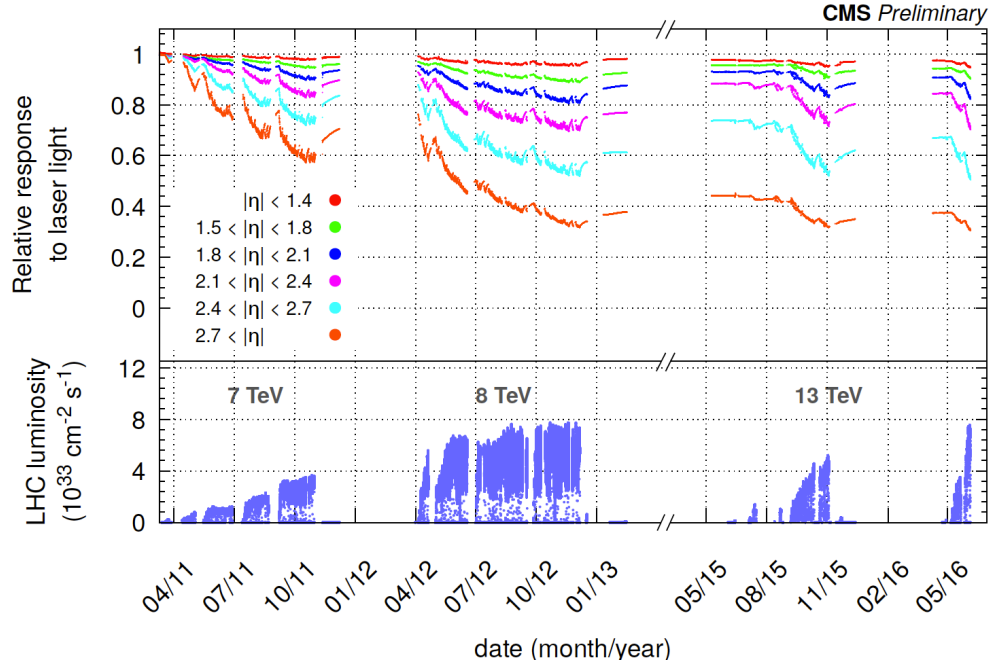
#### 4.4.7 The ECAL energy resolution

The intrinsic energy resolution of the ECAL was measured in dedicated test beams, employing electron beams with momenta from 20 GeV up to 250 GeV [133]. The energy was reconstructed by summing the energy deposits in a  $3 \times 3$  crystal matrix and was measured to be (in GeV):

$$\frac{\sigma(E)}{E} = \frac{2.8 \%}{\sqrt{E}} \oplus \frac{12 \%}{E} \oplus 0.3 \% \quad (4.7)$$

consisting of three contributions:

- the first term describes fluctuations in the photostatistics.

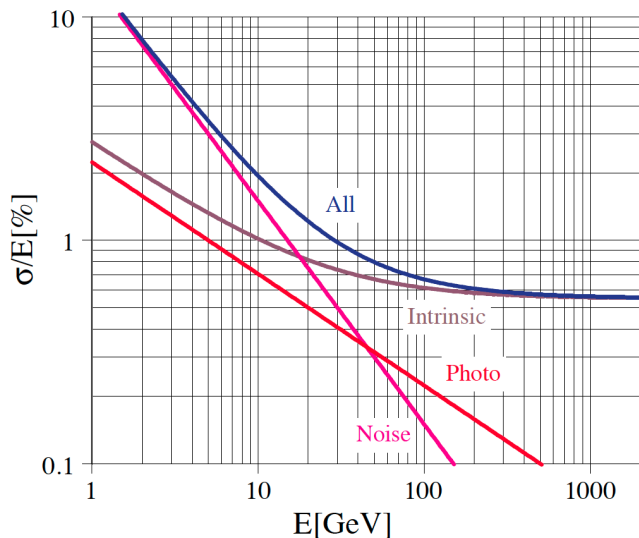


**Figure 4.9:** Relative response to laser light (440 nm in 2011 and 447 nm from 2012 onwards) injected in the ECAL crystals, measured by the ECAL laser monitoring system, averaged over all crystals in bins of pseudorapidity, for the 2011, 2012, 2015 and 2016 data taking periods, with magnetic field at 3.8 T. The response change observed in the ECAL channels is up to 6 % in the barrel and it reaches up to 30 % at  $|\eta| \approx 2.5$ , the limit of the tracking detector acceptance. The response change is up to 70 % in the region closest to the beam pipe. The recovery of the crystal response during the Long-Shutdown-1 period is visible, where the response was not fully recovered, particularly in the region closest to the beam pipe. These measurements are used to correct the physics data. It includes measurements taken up to June 2016. The bottom figure shows the instantaneous LHC luminosity delivered during this time period [124].

- the second term describes the noise from electronics and digitization.
- the third term is the constant term, summarizing the non-uniformity of the light collection, intercalibration uncertainties and rear energy leakage.

This energy resolution from test beams is better than what is observed in-situ in CMS, since the test beam facility is a rather isolated environment and no material was placed in front of the  $3 \times 3$  crystal matrix.

The low light yield of  $\text{PbWO}_4$  is impacting the first two terms of the energy resolution since the photostatistics are less precisely measured and the electronic noise has a higher relative impact. A GEANT4 simulation of the individual contributions to the energy resolution versus the incident energy is depicted in Figure 4.10 [111]. The electron energy resolution from  $Z \rightarrow e^+e^-$  events at 13 TeV evaluates to 1 – 3 % in the EB and 2.5 – 4.5 % in the EE [134]. The differences in the measured and simulated photon



**Figure 4.10:** The energy resolution of the  $\text{PbWO}_4$  calorimeter with its three components: the photostatistics ('Photo'), the electronic noise ('Noise') and the intrinsic constant ('Intrinsic') [17].

energy resolution of the search for high mass diphoton resonances are determined in Chapter 6.

## 4.5 Photon reconstruction in CMS

The aim of this section is to describe the reconstruction of the photons, used in the search for new physics in the diphoton final state. The identification and selection of the ultimately used high transverse momentum photon objects is discussed in the context of the analysis, in particular in Section 5.7.

The Mustache clustering algorithm, described in Section 4.4.5, reconstructs the energy of an electron or photon based on its energy deposits in the ECAL [126, 129]. It does not make any assumptions if the reconstructed energy belongs to a photon or electron. This enables the use of the copious physics process  $Z \rightarrow e^+e^-$  to further study photon triggers, the photon energy scale and resolution.

To distinguish (converted) photons from electrons, the main handle is a precise electron track reconstruction. This is performed with a Gaussian-sum filter (Gsf) algorithm [135]. Two algorithms aim at avoiding a misidentification of electrons as photons: the 'conversion-safe electron veto' and the 'pixel-seed veto'. Both reject photon candidates if a well-enough reconstructed track is found [129]. Photons which convert in the tracking system leave a measurable track such that the conversion vertex can be reconstructed. To separate converted photons from electrons, the 'conversion-safe electron veto' requires that a charged-particle track, pointing to a photon super cluster in the ECAL and without a

matched conversion vertex, must not have a hit in the inner layer of the pixel detector. The misidentification of electrons as photons can also be prohibited by the 'pixel-seed veto', which has a lower efficiency, but provides a higher purity of selected prompt photons than the conversion-safe electron veto. It forbids the photon candidates to have two hits in the pixel detector, suggesting a charged-particle trajectory to an ECAL supercluster [129].

Another important photon identification variable is the  $R_9$  variable, which gives the ratio of the energy reconstructed in the  $3 \times 3$  crystals centered on the crystal with the most energy in the supercluster and the raw energy of the whole supercluster. Unconverted photons have mostly very high  $R_9$  values, whereas converted photons and misidentified photons tend to have a broader  $R_9$  distribution. First results of photon and electron distributions can be found in Ref. [136] for the first dataset at 13 TeV and Ref. [137] for first results of the 2016 data-taking period.

The most important source of background originates from boosted neutral mesons produced in jets. If these neutral mesons carry a high transverse momentum and a large fraction of the overall jet momentum, they decay to collimated two photon pairs with a rather low jet activity around them. These collimated photon pairs are reconstructed as single photons, since the minimum separation of two photons from a  $\pi^0$  decay with  $p_T = 15$  GeV is about the same as the transverse crystal size in EB [129]. These jet fragments can be misidentified as a single prompt photon, originating from the interaction point, and are called a 'fake' photon.

The shape of the reconstructed shower in  $|\eta|$ -direction can be used to discriminate fake and prompt photons as the shape of the fake photons tends to be broader. This is partly due to the slightly separated decay photons (still reconstructed as single prompt photons) from the neutral mesons and the higher conversion probability of these photons upstream to the ECAL.

With a magnetic field, the shower shape in  $\phi$ -direction is however too similar for fake and prompt photons due to the bended (conversion)  $e^\pm$  tracks as to be used as a discriminating variable.

Another discriminating variable is the activity in a  $\eta - \phi$  cone around the photon candidate, since fake photons tend to be less isolated than prompt photons due to the surrounding jet. The discrimination power of the above mentioned variables is studied in Chapter 9 in the context of the estimation of the individual diphoton background components.

The particles in the isolation cone around the photon candidates are reconstructed with the 'particle flow algorithm' [127, 128]. Its general particle reconstruction relies on a global event description of the detector, including all tracking, calorimeter and muon

detector information. The success of this approach is among others possible due to the excellent track reconstruction purity and efficiency ( $> 90\%$ ) and the precise energy resolution of the ECAL, which can resolve the energy deposits of neighboring particles. It reconstructs the four-momenta of all particles in the event and identifies the particles as charged or neutral hadrons, photons, electrons or muons. The final list and information of particles in an event, determined by this particle flow algorithm, resembles that provided by an event generator.

## PART I

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### *Search for resonant production of high-mass photon pairs in proton-proton collisions*

*Daß ich erkenne, was die Welt im Innersten zusammenhält.*

Goethe, *Faust I*

This part of the dissertation presents the search for resonant production of high mass photon pairs in pp-collisions with the CMS experiment at the LHC collider. The search is motivated by a possible resonant production of spin-0 or spin-2 particles, decaying into two photons. These resonances would be signs of physics beyond the standard model, for instance an extended Higgs sector or extradimensions as detailed in Chapter 3. In December 2015, the CMS and ATLAS collaborations presented their first results for this search at  $\sqrt{s} = 13$  TeV [12, 13]. The ATLAS collaboration published their results, studying a mass range of 200 GeV – 2 TeV (500 GeV – 5 TeV) for spin-0 (spin-2) hypotheses with an integrated luminosity of  $3.2 \text{ fb}^{-1}$  in Ref. [13]. The CMS collaboration presented their results, analyzing a mass range of 500 GeV – 4.5 TeV with an integrated luminosity of  $3.3 \text{ fb}^{-1}$  in Ref. [12]. For this dataset, both collaborations observed a modest excess of events compared to the background-only hypothesis compatible with the production of a resonance with a mass of 750 GeV. Over 550 papers interpreted this excess in terms of new physics [14]. The analyses of a larger dataset by both collaborations, presented at the ICHEP16 conference in August 2016, could not confirm this excess [1, 15].

This chapter outlines the results of this search from the CMS collaboration for the first dataset of  $3.3 \text{ fb}^{-1}$  and the later dataset of  $16.2 \text{ fb}^{-1}$ , documented in Ref. [12] and Ref. [1], respectively. The discussions, text and illustrations which can be found in those references are closely followed here. The first sections concentrate on the data-driven analysis strategy, followed by a detailed description of the background model and the background determination, which were focus of my work. It is important to note that for a dataset of  $0.6 \text{ fb}^{-1}$  the magnetic field of  $B = 3.8 \text{ T}$  was not available due to problems with the cryogenic system of CMS. This required a dedicated event selection and corrections to the photon energy for this part of the dataset and is detailed in the respective chapters. This part of the dissertation closes with a statistical analysis of the results and its statistical combination with previous analyses of the CMS collaboration at 8 TeV.

# 5

## CHAPTER

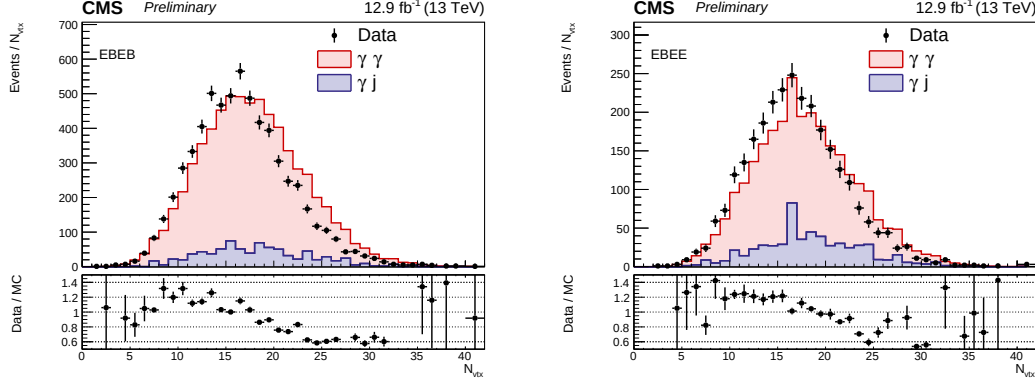
# Event simulation and selection

In this chapter, the analyzed data samples, the event simulation and subsequent event selection for the search of high mass diphoton resonances at 13 TeV is discussed.

In the first Section 5.1, the analyzed dataset and the high pile-up environment in pp-collisions is described. All analysis steps need to be verified with a Monte-Carlo prediction, requiring a precise knowledge of the underlying QCD processes and signal models. The subsequent Section 5.3 therefore focuses on the description of the event simulation. Section 5.4 discusses the filtering of the desired diphoton events among all other recorded events with dedicated triggers. The identification of the primary vertex of a diphoton event is detailed in Section 5.5. This chapter concludes with the identification and selection of high momentum photon candidates in Section 5.6 and 5.7, which requires dedicated studies to ensure a high selection efficiency of these candidates over the full momentum range. It is important to note that for part of the data-taking the magnetic field of  $B = 3.8\text{ T}$  was not available due to problems with the cryogenic system of CMS. This required a dedicated event selection and corrections to the photon energy.

## 5.1 Analyzed data samples

The data sample of this analysis consists of pp-collision events collected by the CMS experiment at the LHC accelerator at a center-of-mass energy of 13 TeV. The first search, presented at the Moriond 2016 conference in April 2016 and published in Ref. [12], analyzed a dataset with an integrated luminosity of  $3.3\text{ fb}^{-1}$ , which was recorded throughout 2015. A total of  $0.6\text{ fb}^{-1}$  was recorded with a magnetic field configuration of  $B = 0\text{ T}$  due to problems with the cryogenic system of CMS. The second analysis, presented at the ICHEP 2016 conference in August 2016 was performed on a dataset of  $16.2\text{ fb}^{-1}$ , combining the above dataset of  $3.3\text{ fb}^{-1}$  with a dataset of  $12.9\text{ fb}^{-1}$ , recorded in 2016. These results were combined statistically with those obtained in similar



**Figure 5.1:** Number of vertices distribution for EBEB (left) and EBEE (right) after pile-up reweighting with events selected by the analysis trigger for  $12.9 \text{ fb}^{-1}$ . The MC prediction is scaled by a factor of 1.4.

searches performed by the CMS collaboration at 8 TeV and with an integrated luminosity of  $19.7 \text{ fb}^{-1}$ . These analyses are documented in Ref. [95] and Ref. [96], respectively.

## 5.2 Pile-up description in proton-proton collisions

The pile-up in pp-collisions is explained in Section 4.2. This section aims at comparing the pile-up, observed at 13 TeV, with the MC prediction. The instantaneous luminosity in data is measured by the Pixel Luminosity Telescope for each luminosity section [138]. The instantaneous luminosity distribution is then converted to the number of interactions per bunch crossing (pile-up) by the 'minimum bias cross-section' of  $\sigma = 63 \text{ mb}$ . For the first dataset of  $3.3 \text{ fb}^{-1}$ , the average pile-up in data was found to be 11.4 with a RMS of 2.1. Due to the higher instantaneous luminosity, the average pile-up increased to approximately 18 with a RMS of about 4 for the dataset of  $12.9 \text{ fb}^{-1}$ . In simulation, the underlying event distribution was simulated by minimum-bias PYTHIA 8.2 MC samples. The same bunch spacing of 25 ns and an out-of time pile-up in a time window of 12 bunch crossings was taken into account. The pile-up distribution built on these simulated events had an average of 20 interactions per bunch crossing. The MC pile-up distribution was reweighted to match the corresponding distribution in data. The comparison between data and MC after the application of pile-up reweighting for  $12.9 \text{ fb}^{-1}$  can be seen in Figure 5.1.

## 5.3 Event simulation

All simulated samples are produced with Monte-Carlo (MC) methods. First, the simulation of the diphoton resonance signal samples is described. Secondly, the simulation of underlying standard model processes for diphoton events is detailed, with a focus on the higher-order corrections to the  $\gamma\gamma$ -background predictions.

### 5.3.1 Diphoton resonance signal Monte-Carlo samples

The resonant production of two photons was simulated by the PYTHIA 8.2 [139] event generator, using NNPDF 2.3 [140] parton distribution functions. PYTHIA 8.2 includes  $2 \rightarrow 2$  tree-level matrix element calculations. It is able to compute initial and final state radiation, fragmentation, hadronization and underlying event processes.

A diphoton resonance would need to have a spin of zero or an integer spin of equal or greater than two as detailed in Chapter 3. Thus, signal samples for spin-0 and spin-2 hypotheses were produced at leading order in perturbative QCD for a mass range of  $0.5 < m_X < 4.5$  TeV. For the RS-graviton model, which is the chosen benchmark model for the spin-2 resonance, the intrinsic width ( $\Gamma_X$ ) of the resonance with mass  $m_X$  is determined by the dimensionless coupling parameter  $\tilde{k}$ . Three benchmark values were simulated ( $\tilde{k} = 0.01, 0.1$  and  $0.2$ ) to match all widths of possible RS-gravitons. The relative width ( $\Gamma_X/m_X$ ) of the spin-0 resonance was chosen to have the same three benchmark values, which correspond to

$$\Gamma_X/m_X = \tilde{k}^2/1.4 = 1.4 \times 10^{-4}, 1.4 \times 10^{-2} \text{ and } 5.6 \times 10^{-2} \quad .$$

The RS-gravitons were predicted to be produced via approximately 90% gluon-gluon fusion and 10% quark-antiquark annihilation. For scalar resonances, the only production mechanism considered is gluon-gluon fusion as explained in Section 3.2. The complete set of full signal samples, which are signal samples folded with the detector response, is listed in Table 5.1. These full simulation samples were produced for the three width hypotheses and for different points in mass. The finest mass grid was produced under the narrow width hypothesis:

- 5 GeV bins for  $740 \text{ GeV} < m_X < 770 \text{ GeV}$ .
- 250 GeV bins for  $1000 \text{ GeV} < m_X < 4000 \text{ GeV}$ .
- otherwise 500 GeV bins for  $500 \text{ GeV} < m_X < 4500 \text{ GeV}$ .

At generator level, which means without a simulated detector response, a finer scan of mass points with 125 GeV spacing was used and further coupling strengths of  $\tilde{k} = 0.01, 0.05, 0.07, 0.1, 0.15, 0.2, 0.25, 0.3$  were studied.

### 5.3.2 Simulation of standard model processes for diphoton events

The SM background can be divided in irreducible and reducible components. The main SM background process of this search originates from the direct production of two photons, which is described in Chapter 2.3. It contributes as an irreducible background to the analysis and was simulated at leading-order by the SHERPA 2.1 (Simulation of High-Energy Reactions of PArticles) event generator [60], using the CT10NLO PDF set [141]. SHERPA 2.1 includes tree-level multi-leg matrix element calculations. The emission of up to three extra partons from initial or final state legs was included in the calculation. The hadronization is modeled by the cluster algorithm.

A reducible background can theoretically be completely eliminated as it originates from misidentified, so called 'fake' objects. The reducible background in this search arises from  $\gamma + \text{jets}$  ( $\gamma j$ ) as well as multi-jet final states, where the jet fragments are misidentified as photons. A 'fake' photon is mostly created by boosted neutral mesons produced in jets, mainly neutral pions or  $\eta$  mesons, which lead to a similar detector response as a true prompt photon. For the reducible background with one misidentified jet, the event generator MADGRAPH5\_aMC@NLO 2.2 [142] was used, employing the NNPDF 3.0 [51] PDF set. MADGRAPH5\_aMC@NLO 2.2 includes tree-level multi-leg predictions at the matrix element level at leading order. It has to be interfaced with another simulation program to compute parton showering and hadronization. For this purpose PYTHIA 8.2 (tune CUETP8M1 [143]) was used, employing the Lund string model for the hadronization steps. The multi-jet final states were produced by PYTHIA 8.2 (tune CUETP8M1) with the PDF set NNPDF 2.3. In this sample, the electromagnetic jet fragment component was enriched to simulate photon-like jets with higher efficiency. It is important to note that the final sample contained too few events with very high weights as to be used for the final analysis (see Chapter 9).

Besides these background MC samples, an event sample for the Drell-Yan production of two electrons were used to analyze the efficiency of the photon identification criteria. The sample was produced using the POWHEG generator [144, 145, 145, 146]. All datasets are listed with their corresponding cross-section in Table 5.2. The detector response was simulated with the GEANT4 package [147].

| Dataset                                                   |
|-----------------------------------------------------------|
| /RSGravToGG_kMpl-001_M-XXX_TuneCUEP8M1_13TeV-pythia8/     |
| /RSGravToGG_kMpl-01_M-XXX_TuneCUEP8M1_13TeV-pythia8/      |
| /RSGravToGG_kMpl-02_M-XXX_TuneCUEP8M1_13TeV-pythia8/      |
| /GluGluSpin0ToGG_W-0p014_M-XXX_TuneCUEP8M1_13TeV-pythia8/ |
| /GluGluSpin0ToGG_W-1p4_M-XXX_TuneCUEP8M1_13TeV-pythia8/   |
| /GluGluSpin0ToGG_W-5p6_M-XXX_TuneCUEP8M1_13TeV-pythia8/   |

**Table 5.1:** Generated signal datasets with a mass between 500 GeV and 7000 GeV.

| Dataset                                                           | Cross section<br>[pb] |
|-------------------------------------------------------------------|-----------------------|
| /GGJets_M-60To200_Pt-50_13TeV-sherpa/                             | 5.971                 |
| /GGJets_M-500To1000_Pt-50_13TeV-sherpa/                           | 1.510e-01             |
| /GGJets_M-1000To2000_Pt-50_13TeV-sherpa/                          | 1.181e-02             |
| /GGJets_M-2000To4000_Pt-50_13TeV-sherpa/                          | 3.690e-04             |
| /GGJets_M-4000To6000_Pt-50_13TeV-sherpa/                          | 2.451e-06             |
| /GGJets_M-6000To8000_Pt-50_13TeV-sherpa/                          | 1.753e-08             |
| /GGJets_M-8000To13000_Pt-50_13TeV-sherpa/                         | 7.053e-11             |
| /GJets_DR-0p4_HT-40To100_TuneCUETP8M1_13TeV-madgraphMLM-pythia8/  | 18420.0               |
| /GJets_DR-0p4_HT-100To200_TuneCUETP8M1_13TeV-madgraphMLM-pythia8/ | 4881.0                |
| /GJets_DR-0p4_HT-200To400_TuneCUETP8M1_13TeV-madgraphMLM-pythia8/ | 1092.0                |
| /GJets_DR-0p4_HT-400To600_TuneCUETP8M1_13TeV-madgraphMLM-pythia8/ | 126.3                 |
| /GJets_DR-0p4_HT-600ToInf_TuneCUETP8M1_13TeV-madgraphMLM-pythia8/ | 44.75                 |
| /QCD_Pt-20to30_EMEnriched_TuneCUETP8M1_13TeV_pythia8/             | 557600000             |
| /QCD_Pt-30to50_EMEnriched_TuneCUETP8M1_13TeV_pythia8/             | 6.876e+06             |
| /QCD_Pt-50to80_EMEnriched_TuneCUETP8M1_13TeV_pythia8/             | 2.180e+06             |
| /QCD_Pt-80to120_EMEnriched_TuneCUETP8M1_13TeV_pythia8/            | 4.140e+05             |
| /QCD_Pt-120to170_EMEnriched_TuneCUETP8M1_13TeV_pythia8/           | 7.517e+04             |
| /QCD_Pt-170to300_EMEnriched_TuneCUETP8M1_13TeV_pythia8/           | 1.899e+04             |
| /QCD_Pt-300toInf_EMEnriched_TuneCUETP8M1_13TeV_pythia8/           | 1.249e+03             |
| /DYToEE_NNPDF30_13TeV-powheg-pythia8/                             | 2008                  |

**Table 5.2:** Monte-Carlo datasets with their cross-sections.

### 5.3.3 Higher order corrections to $\gamma\gamma$ -background prediction

The irreducible diphoton background was simulated with SHERPA 2.1. For most of the analysis, higher order corrections could be neglected. However, in Chapter 9.5, a data-driven determination of the  $\gamma\gamma$ -component was performed and subsequently compared to its prediction. For that reason, a theoretical calculation of the SM diphoton production to NNLO was needed. The  $2\gamma$ NNLO parton-level MC program [62] was used to calculate separately the Born, NLO and NNLO contributions (see Chapter 2.3 for further details). The three contributions were added together and the ratio of the  $2\gamma$ NNLO prediction to the SHERPA 2.1 calculation at event generator level, the so-called 'k-factor', was calculated as a function of the diphoton invariant mass ( $m_{\gamma\gamma}$ ). The final SHERPA 2.1 prediction, folded with the detector response, was then reweighted by this k-factor. Due to the different event kinematics, one k-factor is calculated for each event category. The two event categories are specified in Chapter 5.6 and summarized as follows:

- **EBEB:** both photons were detected centrally (ECAL barrel with  $|\eta_{SC}| < 1.44$ ).
- **EBEE:** one photon was detected centrally, the other one in the endcaps of the detector ( $1.56 < |\eta_{SC}| < 2.50$ ).

For both event generators, the photon had to satisfy the following selection criteria:

- an isolation cut of 5 GeV in a cone with radius

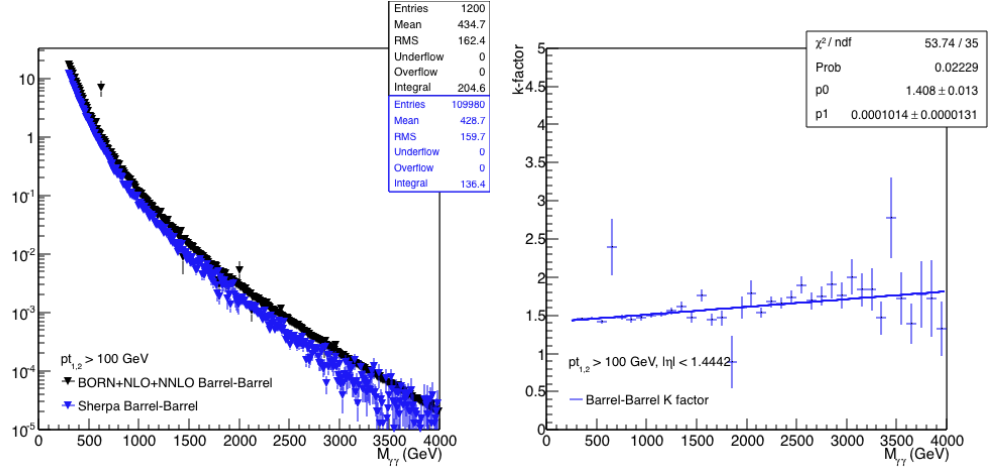
$$\Delta R = \sqrt{(\eta_\gamma - \eta_{\text{cand}})^2 + (\phi_\gamma - \phi_{\text{cand}})^2} < 0.4$$

to suppress photons, which are radiated from jets.

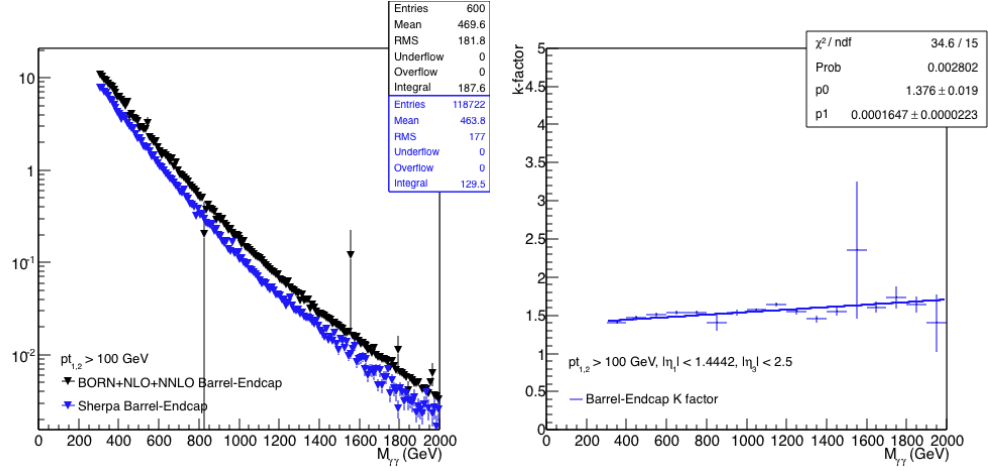
- a minimum transverse momentum of  $p_T > 100$  GeV.

The invariant mass distributions and the k-factor as a function of  $m_{\gamma\gamma}$  are reported in Figure 5.2 and Figure 5.3 for EBEB and EBEE, respectively. More results can be found in Ref. [148]. The distributions contain a few outliers with large uncertainties, which originate from numerical problems in the integration of the NNLO program. The presence of these pathological bins does not affect the final result.

Table 5.3 shows the total cross-section for each of the three diphoton production processes (Born, NLO and NNLO). The left (right) column lists the resulting cross-section, when the renormalization and factorization scales in the  $2\gamma$ NNLO calculation were varied by a factor 0.5 (2), respectively. This variation was used to calculate the uncertainty on the k-factor.



**Figure 5.2:** Left: invariant mass distributions  $m_{\gamma\gamma}$  obtained from 2 $\gamma$ NNLO compared to SHERPA 2.1 prediction for the barrel-barrel category. Right: k-factor as a function of  $m_{\gamma\gamma}$  of the diphoton pair (EBEB) [148].



**Figure 5.3:** Left: invariant mass distributions  $m_{\gamma\gamma}$  obtained from 2 $\gamma$ NNLO compared to SHERPA 2.1 prediction for barrel-endcap events. Right: k-factor as a function of  $m_{\gamma\gamma}$  of the diphoton pair (EBEE) [148].

**Table 5.3:** Total cross-sections of the prompt diphoton processes, obtained varying the renormalization and factorization scales.

| $\mu_R, \mu_F$              | 0.5,0.5 | 1,1   | 2,2   |
|-----------------------------|---------|-------|-------|
| $\sigma_{\text{BORN}}$ (fb) | 93.44   | 92.29 | 90.63 |
| $\sigma_{\text{NLO}}$ (fb)  | 69.82   | 61.07 | 55.11 |
| $\sigma_{\text{NNLO}}$ (fb) | —       | 51.26 | —     |

## 5.4 Event trigger

This section details the extraction of high mass diphoton events by the trigger system of CMS, which is outlined in Chapter 4.3. The events of this analysis are triggered in a first stage by the following 'level-1' (L1) triggers, which are connected via 'OR':

- **SingleEG30,32,34,36,38**, which triggers on single electron or photon objects with  $p_T = 30 - 38$  GeV. These triggers were sometimes prescaled, which means that only a fraction of the triggered events was recorded.
- **SingleEG40**, which triggers on single electron or photon objects with  $p_T > 40$  GeV. This trigger was unprescaled for the full dataset.
- **SingleJet170,180,200**, triggering on single jet objects with  $p_T > 170, 180, 200$  GeV.
- **SingleTau100,120**, triggering on single  $\tau$ -objects with  $p_T > 100, 120$  GeV.
- **DoubleEG\_22\_12,22\_15,23\_10,24\_17,25\_12**, which triggers on dielectron or diphoton objects with  $p_{T,1} > 22, 22, 23, 24, 25$  GeV and  $p_{T,2} > 12, 15, 10, 17, 12$  GeV, respectively.
- **HTT300,320** or **ETM70,80,90,95,105,110,115,120**, which are the seeds for the **HLT\_ECALHT800** trigger. This HLT-trigger was added to recover possible inefficiencies for high transverse momenta as explained below.

The most important L1-trigger for this analysis is the **SingleEG40** as it filters photon and electron ( $e/\gamma$ ) candidates with a momentum close to the one used in this analysis. Its efficiency was studied with a Tag-and-Probe method, employing a dielectron ( $Z \rightarrow e^+e^-$ ) control sample with an invariant mass between 70 GeV and 110 GeV.

A Tag-and-Probe method takes a well-known di-object resonance (here  $Z \rightarrow e^+e^-$ ) and measures the selection efficiency of a certain object as a function of an object variable. It applies a tight selection to one of the two legs (the 'tag'). The second 'probe' leg only needs to fulfill loose requirements and is assumed to be unbiased with respect to the variable being studied. The selection efficiency of these probes as a function of a variable (e.g.  $p_T$ ) can then be evaluated.

The  $Z \rightarrow e^+e^-$  sample can be used to study photons, since the ECAL detector response to photon and electron objects is identical. The requirement for both 'photon' candidates, being the decay products of the  $Z \rightarrow e^+e^-$  events, was to have two pixel clusters, respectively. They were further required to have passed the high- $p_T$  photon ID (see Chapter 5.7) with an inverted electron veto. The transverse momentum of the leading

(subleading) photon candidate was required to be above 40 (25) GeV.

For the trigger efficiency studies both photon candidates were required to match with a L1  $e/\gamma$ -trigger object with  $E_T > 26$  GeV to be unbiased from the L1 trigger selection. The leading photon candidate ('tag') was further required to match with the `SingleEle35_WPLoose_Gsf` HLT trigger object and to exceed a transverse momentum of 40 GeV. The matching efficiency of the subleading photon to an  $e/\gamma$  L1-trigger candidate with a transverse energy above 40 GeV was then studied as a function of  $p_T$ . The result is depicted in Figure 5.4.

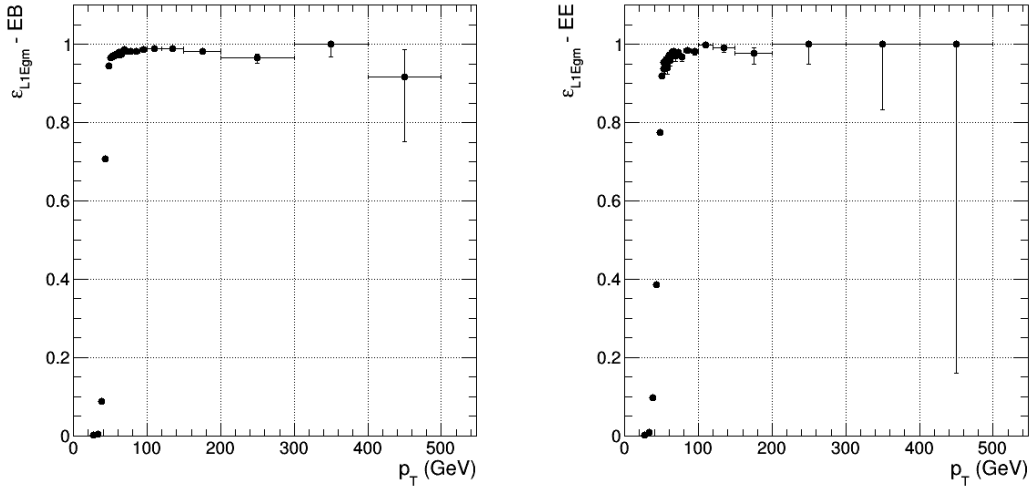
The efficiency was found to be above 97 % for photon candidates with a transverse momentum of  $75 \text{ GeV} < p_T < 400 \text{ GeV}$  in the barrel part of the ECAL. The overall L1 efficiency was therefore higher than  $1 - (1 - \epsilon_{\text{SingleEG40}})^2 \approx 99 \%$  under the assumption that there are no correlated sources of inefficiency between the two legs.

In the ECAL endcaps, fewer high transverse momentum photon candidates were observed, which increased the statistical uncertainty for the  $p_T$  bins above 300 GeV. The efficiency was found to be above 97 % for photon candidates with a transverse momentum of  $75 < p_T < 300 \text{ GeV}$ . For higher transverse momenta no conclusive efficiency could be derived.

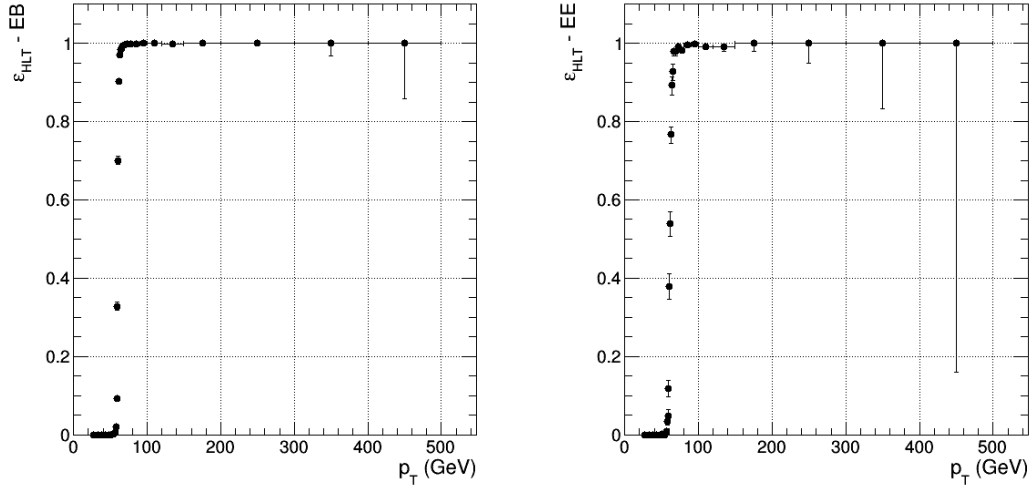
Accidentally, all `SingleEG` and `DoubleEG` triggered candidates had a tight 'H/E' online-cut applied for part of the dataset. The H/E variable characterizes the hadronic leakage of the shower, the ratio between the energy collected by the HCAL towers behind an ECAL supercluster and the energy of the supercluster itself [129]. `SingleEG` or `DoubleEG` candidates, which deposited more than 3.125 % (6.25 %) of their energy in the hadronic calorimeter in EB (EE) were rejected because of this online-cut. This cut was not relaxed with increasing transverse momentum of the  $e/\gamma$  objects, which might have lead to an unwanted rejection of high transverse momentum photon candidates, since their energy is more likely to also spread into the hadronic calorimeter. On top of the `SingleEG` and `DoubleEG` L1-triggers, the `SingleJet` and `SingleTau` triggers were therefore added as seeds. These L1-triggers do not have a H/E online-cut as they trigger for jet or  $\tau$ -objects and can therefore recover possible inefficiencies originating from the H/E online-cut.

The L1-triggers are followed by 'high level triggers' (HLT) as described in Chapter 4.3. The main trigger path of this analysis is the `HLT_DoublePhoton_60` trigger, which is seeded by an OR of the above mentioned L1-triggers, except for the `HTT300`, `320` L1-triggers. It was developed to select two high transverse momentum photon candidates in data. To pass this trigger, the transverse momentum of the two photon candidates is required to be above 60 GeV and their H/E ratio has to be below 0.15.

The efficiency of the `HLT_DoublePhoton_60` was studied using the above described  $Z \rightarrow e^+e^-$  control sample. The matching efficiency with the analysis trigger of the subleading photon candidate was studied as a function of its transverse momentum. The



**Figure 5.4:** Efficiency for the subleading photon candidate to match an  $e/\gamma$  L1 trigger object with transverse energy above 40 GeV for  $12.9 \text{ fb}^{-1}$ . The left and right figures refer to photon candidates in the barrel and endcaps regions, respectively [149].



**Figure 5.5:** Efficiency for the HLT\_DoublePhoton\_60 trigger to fire in dielectron events where SingleEle\_35\_WPLoose\_Gsf has fired as a function of the subleading photon  $p_T$  for  $\mathcal{L} = 12.9 \text{ fb}^{-1}$ . The left and right figures refer to photon candidates in the barrel and endcaps regions respectively [149].

result is depicted in Figure 5.5. The trigger was fully efficient for  $p_T > 75 \text{ GeV}$  for both categories, the barrel and endcaps regions of the detector.

The HLT\_ECALHT800 trigger only accepts very high momentum  $e/\gamma$  candidates ( $\sum E_T > 800 \text{ GeV}$ ) pass and was included as OR to the analysis trigger (HLT\_DoublePhoton\_60) to recover possible inefficiencies induced by the above mentioned H/E online-cut. Further details can be found in Ref. [149].

## 5.5 Diphoton vertex identification

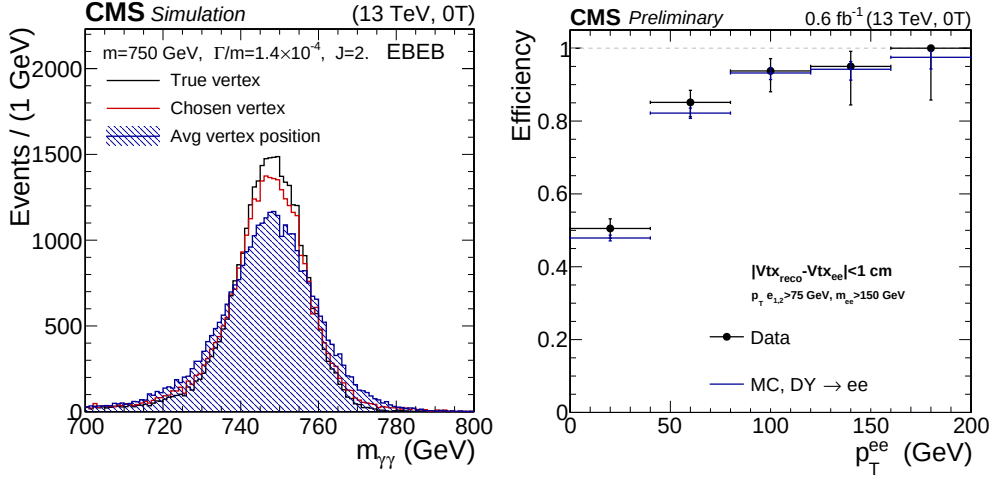
The invariant mass of a diphoton candidate depends on the energy ( $E_{1/2}$ ) of the two photons and the opening angle ( $\alpha_{\gamma\gamma}$ ) between them.

$$m_{\gamma\gamma} = \sqrt{2E_1E_2(1 - \cos(\alpha_{\gamma\gamma}))}$$

The resolution of  $m_{\gamma\gamma}$  is therefore determined by the precision of the photon energy resolution (see Chapter 6) and the resolution of the opening angle. The latter depends on the correct identification of the diphoton vertex. It has a subdominant impact as long as the difference between the selected reconstructed vertex and the true vertex is smaller than 1 cm:  $|Vtx_{\text{reco}} - Vtx_{\text{true}}| < 1 \text{ cm}$ .

Since photons are neutral particles and unconverted photons do not leave a track in the detector, the identification of the diphoton production vertex relies on the recoiling tracks. For most of the analyzed data, recorded at  $B = 3.8 \text{ T}$ , a boosted decision tree (BDT) was used for the vertex identification. It exploits the  $p_T$  variables associated to the recoil of the hard-interaction and its correlation with the diphoton system. This BDT was developed for the search of the Higgs boson decaying into two photons [150] and validated for high mass diphoton candidates. Employing these algorithms, the interaction vertex is correctly assigned for about 90 % of the signal events [1].

For the part of the dataset where the magnetic field is at 0 T, the vertex had to be identified differently as most variables of the BDT depend on the  $p_T$  of the tracks and therefore on the full magnitude of the magnetic field [151]. Also the standard vertex algorithm in CMS, which identifies the vertex with the highest sum of  $p_T^2$  of the tracks as the primary vertex, could therefore not be used. The missing information about the track  $p_T$  was replaced by the counting of the tracks and the vertex with the highest track multiplicity was chosen. The left histogram in Figure 5.6 reports the mass resolution for a hypothetical resonance at  $m_X = 750 \text{ GeV}$  under different vertex finding algorithms. Compared to the average vertex position, which averages the measurement of the collision point by the tracking system over one lumi-section, the chosen vertex algorithm improves the resolution by approximately 20%. The vertex identification efficiency, satisfying  $|Vtx_{\text{reco}} - Vtx_{\text{true}}| < 1 \text{ cm}$ , was studied with a  $Z \rightarrow e^+e^-$  sample. The result is depicted versus its transverse momentum in the right panel of Figure 5.6. The comparison of data with the MC prediction shows good agreement within their uncertainties. The probability for the correct vertex assignment is approximately 60 %.



**Figure 5.6:** Left: expected reconstructed invariant mass distribution for a narrow diphoton resonance at a mass of  $m_{\gamma\gamma} = 750$  GeV at  $B = 0$  T for different primary vertex choices, when both photons are centrally detected (EBEB). Right: matching efficiency within 1 cm with respect to the vertex extrapolated from electrons tracks, using the track counting algorithm evaluated on double electron data (black) and MC (blue) samples [2].

## 5.6 Kinematic preselection and event categorization

The photon reconstruction is described in the last part of Section 4.4 and Section 4.5. If more than one diphoton pair passed the selection, which was the case in approximately 1 % of all events, the pair with the highest scalar sum of transverse momentum was chosen. Then, the two photons needed to satisfy the following kinematic selection:

- The transverse momentum of each candidate had to be above 75 GeV.
- The absolute value of the pseudorapidity of the supercluster ( $|\eta_{SC}|$ ) of both candidates had to be below  $|\eta_{SC}| < 2.5$  and not between  $1.444 < |\eta_{SC}| < 1.566$ , due to the geometric acceptance of the ECAL.
- At least one of the photon candidates had to be detected at  $|\eta_{SC}| < 1.444$ .
- To avoid a distortion of the background shape due to the transverse momentum cut, the minimum invariant mass of the diphoton pair had to be 230 GeV, when both photons were centrally detected ( $|\eta_{SC}| < 1.444$ ). If one photon candidate was detected in the endcap region ( $|\eta_{SC}| > 1.566$ ), the minimum invariant mass had to be 320 GeV.

The events were split into two categories:

- barrel-barrel (EBEB): both candidates are centrally ( $|\eta_{\text{SC}}| < 1.444$ ) detected.
- barrel-endcap (EBEE): one candidate is in the endcaps  $1.566 < |\eta_{\text{SC}}| < 2.500$ , the other one at  $|\eta_{\text{SC}}| < 1.444$ .

The endcap-endcap category was not included in the analysis as the kinematic acceptance of a signal for this region reached only a few percent and the reducible SM background would have been considerably higher than for the above categories. More details about the signal acceptance are given in Chapter 12.

The 2015 dataset was divided in two further categories due to the two different configurations of the magnetic field ( $B = 3.8 \text{ T}$  and  $B = 0 \text{ T}$ ).

After the kinematic preselection, the diphoton pair had to further satisfy the selection criteria of the high- $p_{\text{T}}$  photon ID .

## 5.7 Selection criteria

The two photon candidates of the diphoton system needed to satisfy a dedicated set of selection criteria. These criteria were optimized for photons with high transverse momentum and based on the following variables:

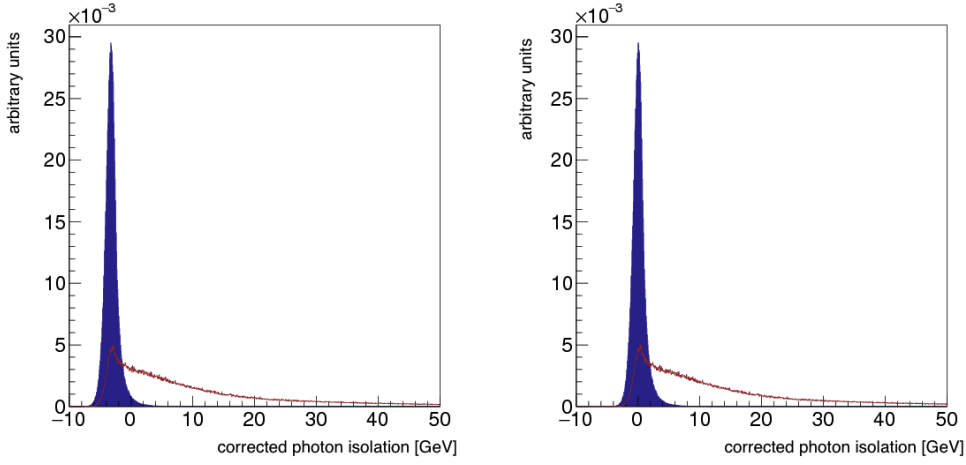
- $\text{Iso}_{\text{Ch}}$ : the scalar sum of the transverse momenta of the particle flow charged hadron candidates, which are assigned to the chosen primary vertex. The candidates need to be within a radius of  $\Delta R < 0.3$  from the photon in the  $\eta - \phi$  plane, which is defined as:

$$\Delta R = \sqrt{(\eta_{\gamma} - \eta_{\text{cand}})^2 + (\phi_{\gamma} - \phi_{\text{cand}})^2} \quad .$$

- $\text{Iso}_{\gamma}$ : the scalar sum of the transverse energies of the particle flow photon candidates for which  $\Delta R < 0.3$ .

If a particle flow candidate inside the above isolation cones was sharing part of its energy with the supercluster of a selected photon candidate of the diphoton pair, it was excluded from all isolation sums. Other studied variables for the high- $p_{\text{T}}$  photon ID are:

- H/E as detailed in Section 5.4.



**Figure 5.7:** Left: distribution of photon isolation variable  $\text{Iso}_\gamma$  corrected for the pile-up and  $p_T$  dependence. Right: distribution of the corrected photon isolation variable, shifted by the  $\alpha$ -term ( $\bar{\text{Iso}}_\gamma$ ). The blue solid (red empty) histogram shows the prompt (fake) photons of the  $\gamma j$ -sample in the barrel region.

- $\sigma_{i\eta i\eta}$ : the weighted spatial second order moment of the photon candidate in the  $\eta$ -direction, computed as

$$\sigma_{i\eta i\eta} = \sqrt{\frac{\sum_{i \in 5 \times 5} (\eta_i - \bar{\eta})^2 w_i}{\sum_{i \in 5 \times 5} w_i}}, \quad w_i = \max(0, 4.7 + \log(E_i/E_{5 \times 5})).$$

- the 'conversion-safe electron veto', detailed in Section 4.5.

This list of identification criteria and the following paragraph refers to data-taking conditions with a magnetic field of  $B = 3.8$  T. The thresholds of the chosen selection variables were taken such that the diphoton selection efficiency stayed flat as a function of its invariant mass. To achieve a stable selection efficiency, the event pile-up and  $p_T$  dependence of the photon candidates needed to be studied. A dependence on these quantities was found for the  $\text{Iso}_\gamma$  variable and corrections were applied. The corrections included the 'effective area'  $A$  for the event pile-up density ( $\rho$ ), the scale factor ( $\kappa$ ) for  $p_T$  and a shift ( $\alpha$ ) of the numerical value of  $\text{Iso}_\gamma$  in the form of:

$$\bar{\text{Iso}}_\gamma = \alpha + \text{Iso}_\gamma - \rho \cdot A - \kappa \cdot p_T$$

The values of  $A$  and  $\kappa$  were taken such that the 95 % quantile of the  $\text{Iso}_\gamma$  variable for the signal distribution stayed flat as a function of  $\rho$  and  $p_T$ . The left distribution of Figure 5.7 shows the  $\text{Iso}_\gamma$  variable, corrected for its pile-up and  $p_T$  dependence. Since the slope of the 95 % quantile of this distribution is steeper than the one of its median, the corrections tend to over-subtract energy in the bulk of the distribution. The median of the  $\text{Iso}_\gamma$  distribution on the left of Figure 5.7 is therefore negative. Intuitively though,

| Region                             | $\alpha$ (GeV) | A    | $\kappa$ (1/GeV)     |
|------------------------------------|----------------|------|----------------------|
| $ \eta_{\text{SC}}  < 0.9$         | 2.5            | 0.17 | $4.5 \times 10^{-3}$ |
| $0.9 <  \eta_{\text{SC}}  < 1.444$ | 2.5            | 0.14 | $4.5 \times 10^{-3}$ |
| $1.566 <  \eta_{\text{SC}}  < 2.0$ | 2.5            | 0.11 | $3 \times 10^{-3}$   |
| $2.0 <  \eta_{\text{SC}}  < 2.2$   | 2.5            | 0.14 | $3 \times 10^{-3}$   |
| $2.2 <  \eta_{\text{SC}}  < 2.5$   | 2.5            | 0.22 | $3 \times 10^{-3}$   |

**Table 5.4:** Corrections factors for the  $\text{Iso}_\gamma$  variable.

| Photon category                                          | $\text{Iso}_{\text{Ch}}$ (GeV) | $\text{Iso}_\gamma$ (GeV) | H/E                | $\sigma_{i\eta i\eta}$ |
|----------------------------------------------------------|--------------------------------|---------------------------|--------------------|------------------------|
| $ \eta_{\text{SC}}  < 1.444$ non-sat.                    | 5                              | 2.75                      | $5 \times 10^{-2}$ | 0.0105                 |
| $ \eta_{\text{SC}}  < 1.444$ sat.                        | 5                              | 2.75                      | $5 \times 10^{-2}$ | 0.0112                 |
| $ \eta_{\text{SC}}  > 1.566$ non-sat.                    | 5                              | 2.0                       | $5 \times 10^{-2}$ | 0.028                  |
| $ \eta_{\text{SC}}  > 1.566$ sat.                        | 5                              | 2.0                       | $5 \times 10^{-2}$ | 0.030                  |
| conversion-safe electron veto applied for all categories |                                |                           |                    |                        |

**Table 5.5:** Photon identification criteria used in the analysis for  $B = 3.8$  T [149].

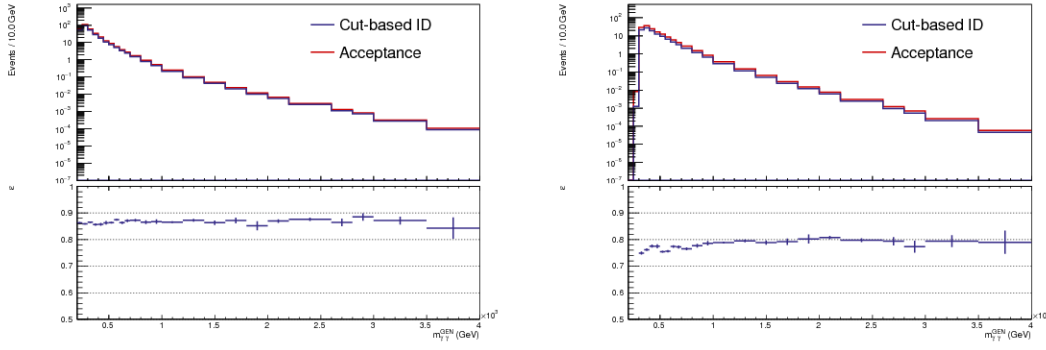
the  $\text{Iso}_\gamma$  distribution should be centered around zero. The  $\alpha$ -term was therefore added to shift the mean of the corrected distribution back to a value of approximately zero as shown on the right of Figure 5.7.

The values for  $\alpha$ , A and  $\kappa$  were derived for different pseudorapidity regions as listed in Table 5.4. The coefficients were individually calculated for both datasets and are consistent within 5 – 10 % such that the thresholds of the dataset of  $2.7 \text{ fb}^{-1}$  were also applied to the dataset of  $12.9 \text{ fb}^{-1}$ . The final set of identification criteria is listed in Table 5.5.

For very high energy photons, the ECAL readout electronics could have saturated. The limit of their dynamic range is reached when the energy deposit in a single crystal has a value of about 1.7(2.8) TeV in the barrel (endcaps). The criteria for this situation were studied and listed in Table 5.5. No saturated photons were found in the dataset of  $16.2 \text{ fb}^{-1}$ . With this high- $p_T$  photon ID, the per-photon-efficiency at generator level for  $B = 3.8$  T was tuned to 90 % (85 %) for EBEB (EBEE), respectively. The resulting diphoton identification efficiency is shown in Figure 5.8 for both categories. It was found to be above 85 % (80 %) for EBEB (EBEE) and stayed flat as a function of the diphoton invariant mass.

### 5.7.1 Selection criteria at $B=0$ T

Since the photon identification relies on track momentum variables, the high- $p_T$  photon ID at  $B = 0$  T required a dedicated study, which is detailed in Ref. [151]. Due to the missing magnetic field, the photon energy is less spread and collinear in the direction of



**Figure 5.8:** Distribution of the MC events passing the high- $p_T$  photon ID criteria (blue) and the MC events passing the preselection (red) as a function of the diphoton invariant mass. Lower insert: diphoton identification efficiency as a function of the diphoton invariant mass at event generator level, evaluated on the  $\gamma\gamma$  background. The efficiency is computed with respect to the diphoton candidates passing the preselection detailed in 5.6 and with two photons isolated at generator level. Events in the EBEB (EBEE) category are reported on the left (right) [149].

the photon. Most photons had therefore very high  $R_9$  values and a cut of  $R_9 > 0.8$  was applied. Moreover, the energy shower in ECAL was expected to be symmetric in  $\eta$ - and  $\phi$ -direction. The weighted spatial second order moment of the photon candidate in the  $\phi$ -direction could therefore be added to the set of identification criteria. Its definition is analogous to the one of  $\sigma_{i\eta i\eta}$  and is computed as

$$\sigma_{i\phi i\phi} = \sqrt{\frac{\sum_{i \in 5 \times 5} (\phi_i - \bar{\phi})^2 w_i}{\sum_{i \in 5 \times 5} w_i}}, \quad w_i = \max(0, 4.7 + \log(E_i/E_{5 \times 5})).$$

On top of the above detailed preselection for  $B = 3.8$  T, the H/E ratio was required to be below 0.15 due to the trigger requirements, which imposed this threshold on the photons. The set of identification variables was further enriched by the following variables:

- $N_{\text{TRK}}$ : the number of tracks in a cone of  $\Delta R = 0.3$  around the photon candidates. This variable replaced the  $\text{Iso}_{\text{Ch}}$  variable, which is based on the momenta information of the charged particles.
- $N_{\text{missing hits}}$ : number of missing hits of the GsfTrack (see Chapter 4.5) associated to the photon supercluster, applied only if there was an associated GsfTrack. It is a subset the above defined 'conversion-safe electron veto', which also relies on track momentum information.

The selection criteria were optimized using fake and prompt photons from a  $\gamma + \text{jets}$  MC sample. The photon candidate was required to have matched the event generator level

| Photon category              | R <sub>9</sub> | H/E      | Iso <sub>γ</sub> (GeV) | N <sub>TRK</sub> | $\sigma_{i\eta i\eta}$ | $\sigma_{i\phi i\phi}$ |
|------------------------------|----------------|----------|------------------------|------------------|------------------------|------------------------|
| $ \eta_{\text{SC}}  < 1.444$ | $> 0.8$        | $< 0.15$ | $< 3.6$                | $< 4$            | $< 0.0106$             | $< 0.0106$             |
| $ \eta_{\text{SC}}  > 1.566$ | $> 0.8$        | $< 0.15$ | $< 3$                  | $< 4$            | $< 0.028$              | $< 0.028$              |

**Table 5.6:** Photon identification criteria used in the analysis for  $B = 0$  T [149].

information and to have subsequently passed the preselection. Again, the 95 % quantile was used to study the selection efficiency.

After the preselection, the discrimination power of the H/E and R<sub>9</sub> variables were found to be negligible for the final selection and were not included in the set of selection criteria. The power of the electron rejection by the N<sub>missing hits</sub> variable was studied with a  $DY \rightarrow ee$  sample. The rejection efficiency was found to be above 95 % while keeping a photon selection efficiency of above 90 % for EB (above 80 % for EE). Compared to the conversion-safe electron veto at 3.8 T, this requirement is less efficient as additional information on the quality of the electron track fit is missing. This results in a lower per-photon-efficiency of 85 % (70 %) for EB (EE) at  $B = 0$  T. The final list of selection criteria is reported in Table 5.6.





## Energy scale and resolution corrections

The photon energy resolution ( $\sigma_{E_{1/2}}$ ) is crucial for a precise knowledge of the diphoton mass resolution ( $\sigma_{m_{\gamma\gamma}}$ ). Under the assumption that the resolution of the opening angle between the two photons is negligible (see Section 5.5), the mass resolution is determined by:

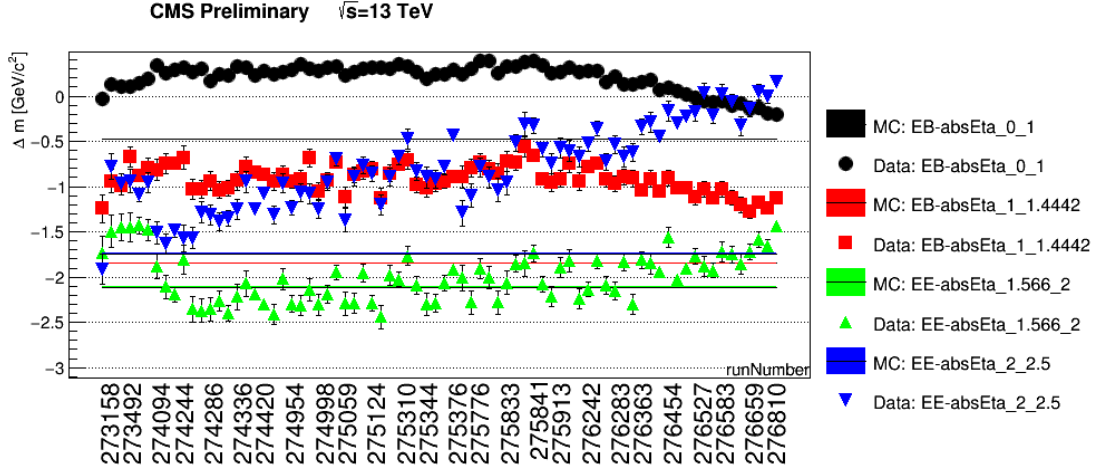
$$\frac{\sigma_{m_{\gamma\gamma}}}{m_{\gamma\gamma}} = \frac{1}{2} \sqrt{\frac{\sigma_{E_1}^2}{E_1^2} + \frac{\sigma_{E_2}^2}{E_2^2}} .$$

The general reconstruction of the photon object and its energy assignment is described in Section 4.4 and 4.5.

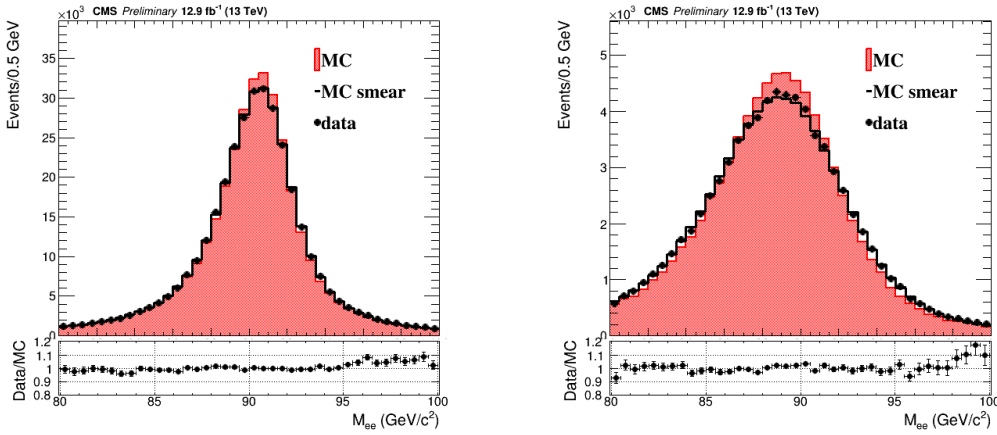
This supercluster based energy assignment might need some adjustments for the photons entering this analysis: one reason could be the longitudinal non-containment of the photon energy in ECAL, which increases with the momentum of the photon candidates. It is predicted to lead to an energy scale shift of 0.5 % for energies up to about 500 GeV and stays below 1 % for energies up to 1.5 TeV according to Ref.[152].

Since the energy determination depends primarily on ECAL, electrons from  $Z \rightarrow e^+e^-$  decays can also alternatively be used for the photon energy correction. The disagreement between the observed and predicted energy of these electrons is assessed by its energy scale and energy resolution, employing a method which was developed for Ref. [153].

The corrections are derived in two steps: at first, the energy scale is corrected by adjusting the scale in data to match the MC prediction. Data and MC samples is fitted by a Breit-Wigner function convoluted with a crystal ball (CB) function [154], describing the theoretical signal line shape of the Z-boson and the detector response, respectively. The parameters of the Breit-Wigner function for the Z boson are taken from the Particle Data Group (PDG) [8]:  $m_Z = 91.1876 \text{ GeV}$  and  $\Gamma_Z = 2.4952 \text{ GeV}$ . By fitting the distribution in data and MC separately, the energy scale offset can be extracted. The mean of the CB function ( $\Delta m$ ) is shown in Figure 6.1 as a function of the run numbers during data-taking. Different systematic behaviors of  $\Delta m$  as a function of time and the pseudorapidity can be observed. As a result, run dependent energy corrections were



**Figure 6.1:**  $Z \rightarrow e^+e^-$  lineshape peak values in several run ranges for four  $|\eta_{SC}|$  categories: two categories in EB, two categories in EE. MC value is displayed as a continuous line [149].



**Figure 6.2:** Observed and predicted  $Z \rightarrow e^+e^-$  distribution before and after the energy scale and energy resolution corrections. For this illustration both corrections are applied to the MC distribution. Left: both electrons in EB with  $|\eta_{SC}| < 1$  and  $R_9 > 0.94$ . Right: both electrons in EE with  $|\eta_{SC}| < 2$  and  $R_9 < 0.94$  [149].

necessary to correct for the energy scale variations during data-taking. The energy scale correction ( $\Delta P$ ) is defined as the relative shift in mass between data and MC prediction:

$$\Delta P = \frac{\Delta m_{\text{data}} - \Delta m_{\text{MC}}}{m_Z}.$$

After correcting the energy scale in data by  $\Delta P$ , a stable behavior of  $\Delta m$  over time within 0.1 GeV was observed.

In a second step, the residual difference between the observed and predicted electron energy was assessed by a maximum likelihood fit to the smeared MC prediction and data: the probability density function (PDF) of the super cluster energy  $E_{MC}$  was modified

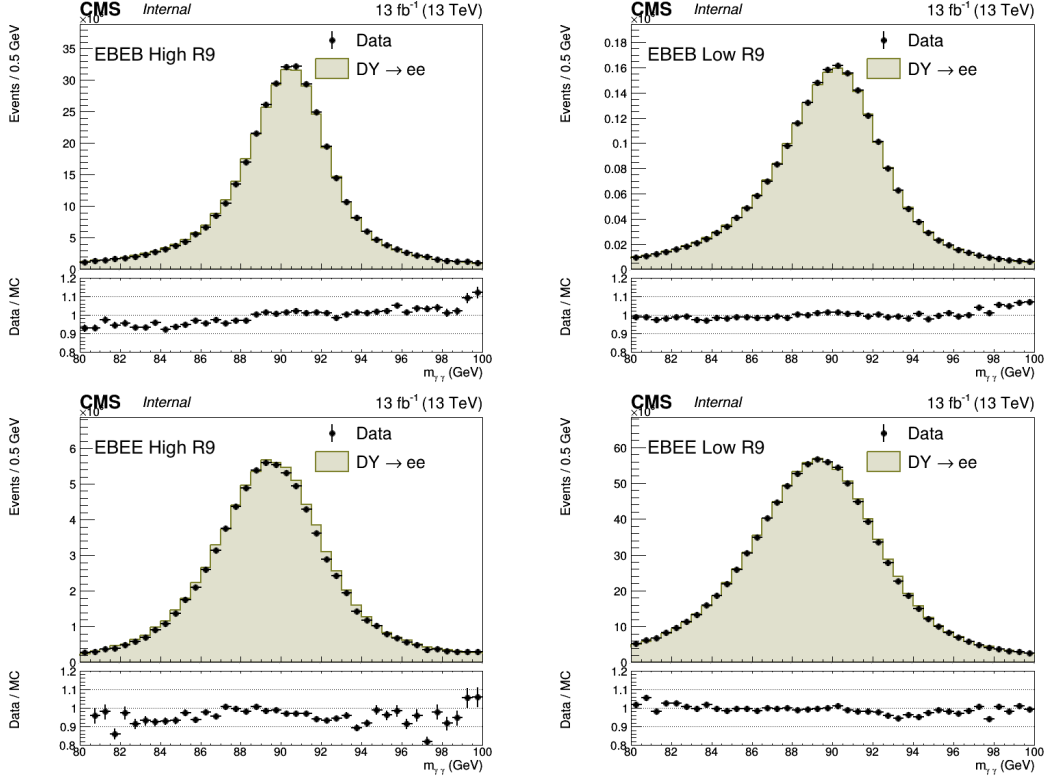
by a multiplicative Gaussian distribution, centered at  $1 + \Delta P$  and with resolution  $\Delta C$ . The resolution  $\Delta C$  denotes the additional constant term of the energy resolution which is added to the MC prediction:

$$E_{MC} \rightarrow E_{MC} \times \text{Gauss}(1 + \Delta P, \Delta C)$$

The final values for  $\Delta P$  and  $\Delta C$  are determined by maximizing the likelihood between the data and MC distributions. These corrections were derived in eight categories in pseudorapidity of the crystals  $|\eta_{SC}|$  and the  $R_9$  variable ( $4|\eta_{SC}| \times 2R_9$ ). Figure 6.2 shows the level of agreement between the observed and predicted  $Z \rightarrow e^+e^-$  distributions before and after the energy corrections were applied for two different categories. Residual differences of the MC prediction to the data can be explained by missing identification efficiency corrections which are discussed in the subsequent Section 7. The energy scale varied between 0.2 % and 1.2 % for  $|\eta_{SC}| < 2$  and was up to 2 % or  $2 < |\eta_{SC}| < 2.5$ . An additional smearing was applied to MC of 0.8 – 1.5 % for  $|\eta_{SC}| < 1.4442$  and 2 – 2.5 % for  $1.566 < |\eta_{SC}| < 2.5$ . The comparison between the predicted and observed dielectron invariant mass, applying the high- $p_T$  photon ID selection and all energy corrections, is reported in Figure 6.3.

In a final step, the stability of the energy scale for higher energies of the photon candidates had to be verified. For that reason, dielectron final states of Z bosons with very high transverse momentum were studied. This approach tested a transverse energy range of up to 150 (100) GeV in the EB (EE) region. The linearity of the energy response was studied by employing the dielectron invariant mass as a function of the scalar sum ( $H_T$ ) of the squared transverse energies of the two electrons:  $H_T = E_{T1}^2 + E_{T2}^2$ . The MC PDF was fitted to the corresponding distribution in data and a scale factor was extracted. For electrons detected in the barrel part of the detector, the energy scale corrections were observed to be stable within 0.4 %. Electrons detected in the endcap region of the detector were found to provide a stability of better than 0.8 %. More information can be found in Ref. [149]. A final 1 % uncertainty on the energy scale stability was assigned.

After the publication of the results on the  $16.2 \text{ fb}^{-1}$  dataset, inaccuracies in the signal reconstruction induced by the ‘gain switch’ of the ECAL electronics system were discovered. To enlarge the dynamic range of the ECAL electronics, the signal of an ECAL crystal can be amplified with three different gains: 1, 6 and 12 as detailed in Chapter 4.4.5. For high energies of electromagnetic particles, no amplification of the signal is necessary (gain 1). It is known that the electronics exhibit a non-linearity near this gain saturation. This was however overlooked in the design of the newly developed ‘multi-fit’ method for the signal reconstruction, which main aspects are also outlined in Chapter 4.4.5. It is however not trivial to define a general ‘per-photon’ correction, as the energy scale and resolution correction are defined per crystal. The deposited energy



**Figure 6.3:** Comparison between the predicted and observed invariant mass distribution of electron pairs obtained after the application of energy scale and resolution corrections. Distributions are shown for events where both electrons are reconstructed in the barrel, with at least one having  $R_9 > 0.94$  (top left) and at least one having  $R_9 < 0.94$  (top right), as well as where one electron is reconstructed in barrel and the other in the endcap with at least one having  $R_9 > 0.94$  (bottom left) and at least one having  $R_9 < 0.94$  (bottom right). The simulation predictions are scaled to match the number of events observed in data [149].

of a photon in a crystal is strongly dependent on the point of impact of the photon and also the intercalibration constants of the crystals play a role in the final correction. This has an impact on the energy scale and resolution on the diphoton events and will be discussed in the relevant sections.

## 6.1 Energy corrections at $B=0$ T

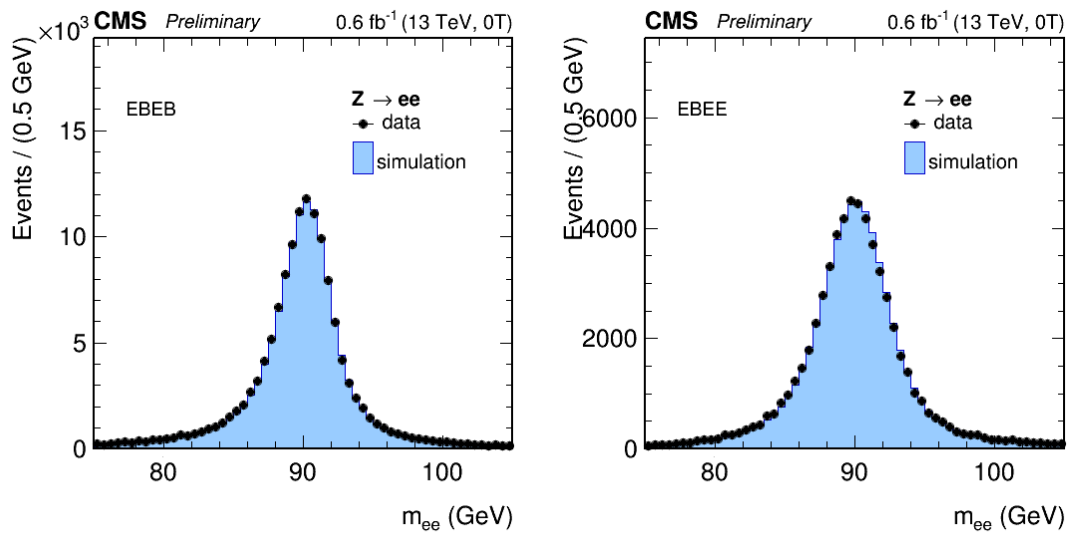
The extraction of the data-driven energy correction factors for the dataset at 0 T is similar to the method used at  $B = 3.8$  T and is detailed in Ref. [151]. The  $Z \rightarrow e^+e^-$  dataset had to pass a dedicated electron identification. The chosen selection is the 'high  $p_T$ ' photon ID of Chapter 5.7.1 with an inverted electron veto at  $B=0$  T and loose  $E_T$  cuts ( $E_T > 20$  GeV). Additionally, a match within 0.01 in  $|\eta_{SC}|$  and  $\phi$  between the electron GsfTrack and the ECAL supercluster was required. The correction factors were derived

in 4  $|\eta_{\text{SC}}|$  categories. Since the electrons at 0 T have high  $R_9$  values as explained in Chapter 5.7.1, the events were not further separated in  $R_9$  categories. The energy scale corrections were of the order of 1 %. The applied Gaussian smearing was similar as for  $B = 3.8$  T. The full list of the energy scale and the energy resolution corrections is given in Table 6.1. The comparison between the predicted and observed dielectron invariant mass after all energy corrections applied is depicted in Figure 6.4. It is visible that the  $Z \rightarrow e^+e^-$  resolution is narrower than at  $B = 3.8$  T. The intrinsic energy resolution without a magnetic field is much better, since the radiated energy is not spread in  $\phi$ . It is however important to note that for the photons entering the final event selection, the energy resolution at  $B = 0$  T is not optimized, since the applied photon energy regression was trained at  $B = 3.8$  T.

The stability of these corrections was verified as a function of the transverse energy of the electrons up to  $E_T < 150$  GeV ( $E_T < 100$  GeV) in EB (EE). Again, a 1 % uncertainty was assigned to account for further extrapolation in addition to a 1 % uncertainty on the knowledge of the relative energy scale in the analysis.

| Category                    | $\Delta P$ [%] | Stat. Err [%] | $\Delta C$ [%] | Stat. Err [%] |
|-----------------------------|----------------|---------------|----------------|---------------|
| EB $ \eta_{\text{SC}}  < 1$ | -1.449         | 0.009         | 0.862          | 0.030         |
| EB $ \eta_{\text{SC}}  > 1$ | -0.990         | 0.021         | 1.364          | 0.061         |
| EE $ \eta_{\text{SC}}  < 2$ | 0.688          | 0.025         | 2.205          | 0.057         |
| EE $ \eta_{\text{SC}}  > 2$ | 0.992          | 0.026         | 2.397          | 0.049         |

**Table 6.1:** Data energy scale corrections and MC energy smearing factors for 0 T obtained with  $Z \rightarrow e^+e^-$  events in four  $|\eta_{\text{SC}}|$  categories [151].



**Figure 6.4:** Comparison between the predicted and observed invariant mass distribution of electron pairs obtained after the application of energy scale and resolution corrections. Pairs of photon candidates satisfying the analysis identification criteria and compatible with electrons tracks are selected. Distributions are shown for events where both electrons are reconstructed in the barrel (left) and events where one electron is in an endcap (right) of the  $B = 0$  T dataset. The simulation predictions are scaled to match the number of events observed in data [2].

## 7

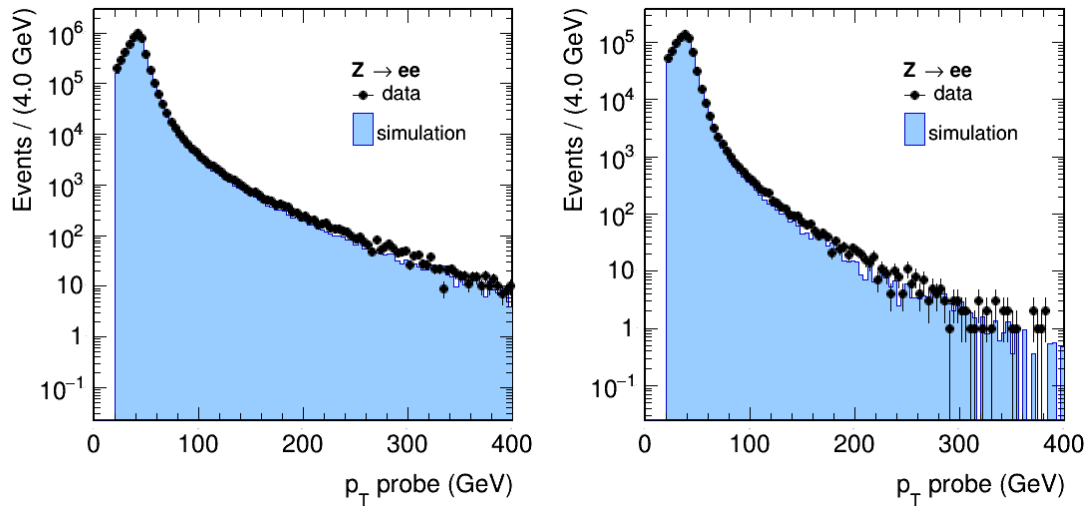
## CHAPTER

**Efficiency measurement**

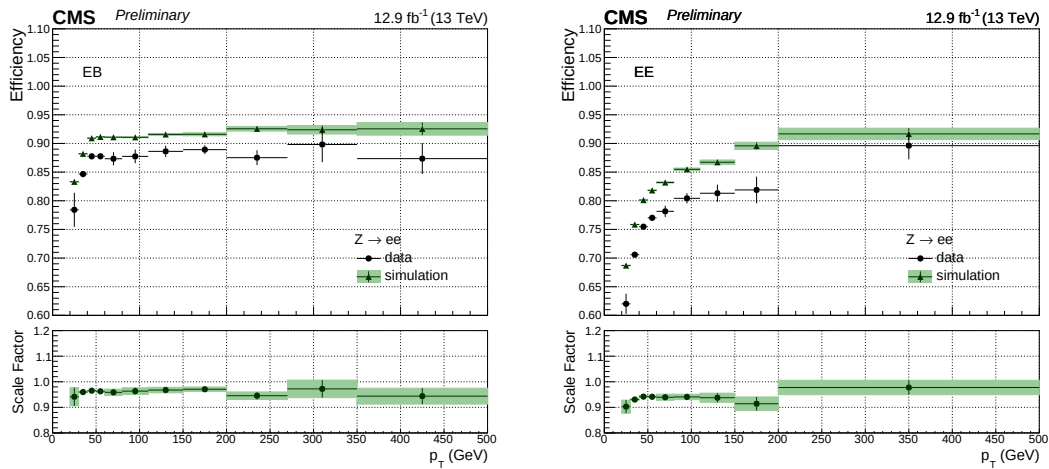
Before the selected dataset can be analyzed, the efficiency and therefore reliability of this selection needs to be verified with the MC prediction. The selection efficiency in data was measured by a Tag-and-Probe technique using a  $Z \rightarrow e^+e^-$  data sample. The Tag-and-Probe technique itself is described in Chapter 5.4. The events were required to pass the HLT\_Ele27\_eta2p1\_WPLoose\_Gsf trigger. The tag electron ( $p_T > 30$  GeV) passed the ‘tight’ working point of the electron selection and a designed preselection to mimic the online working point. These working points provide high purity electrons with a selection efficiency of about 70 %. Since the trigger requires the candidates to be within  $|\eta_{SC}| < 2.1$ , the tag electron had to further pass this  $|\eta_{SC}|$  cut. The probe electron was also restricted to  $|\eta_{SC}| < 2.1$  as the focus of this search is a centrally produced resonance. To obtain a rather pure  $Z \rightarrow e^+e^-$  sample, the invariant mass of the Tag-and-Probe system was further required to be within 70 GeV and 110 GeV. The electrons had to further match the HLT candidates in data. For the MC sample, a match with the MC truth information was required to select prompt electrons.

The  $p_T$  distribution of the probe photon ( $p_T > 20$  GeV), passing the inverted electron veto, is depicted in Figure 7.1. It was then required to pass the full high- $p_T$  photon ID selection, which is detailed in Chapter 5.7. The selection efficiency was studied as a function of  $p_T$  and for each event category. The binning in  $p_T$  was chosen such that the statistical uncertainty in each bin was within a few percent. The data events were fitted simultaneously for passing and failing probes with a signal plus background model. The signal was modeled by the Z lineshape as obtained from a QCD NLO (POWHEG) generator convoluted with a Gaussian, the background with an exponential function. As the choice of the fit model is one of the dominating systematics, different models were studied to assess it [149]. A simple cut-and-count method could be applied for the MC dataset as the MC truth information of the electrons was available.

For the 2015 dataset with  $\mathcal{L} = 2.7 \text{ fb}^{-1}$ , the resulting scale factor was compatible with 1 for all bins. In the 2016 dataset, the selection efficiency in data was generally lower than for MC. The results are reported in Figure 7.2. The scale factor was determined by fitting these curves with a constant factor for  $p_T > 50$  GeV. The efficiency per  $p_T$



**Figure 7.1:** Predicted and observed transverse momentum in logarithmic scale of the probes. The MC yield was rescaled to data. Probes in the barrel (endcaps) are shown on the left (right) [149].



**Figure 7.2:** Photon identification efficiency for all selection requirements except the electron rejection, measured in barrel (left) and endcaps (right) using the Tag-and-Probe method for both data and simulated events. The lower panel shows the ratio between the efficiencies in data and simulation [2].

| Region                           | Scale factor        |
|----------------------------------|---------------------|
| $ \eta_{\text{SC}}  < 1.5$       | $0.9627 \pm 0.0002$ |
| $1.5 <  \eta_{\text{SC}}  < 2.1$ | $0.9352 \pm 0.0007$ |

**Table 7.1:** Result of constant fits as a function of  $p_T$  to the data to MC scale factors [149].

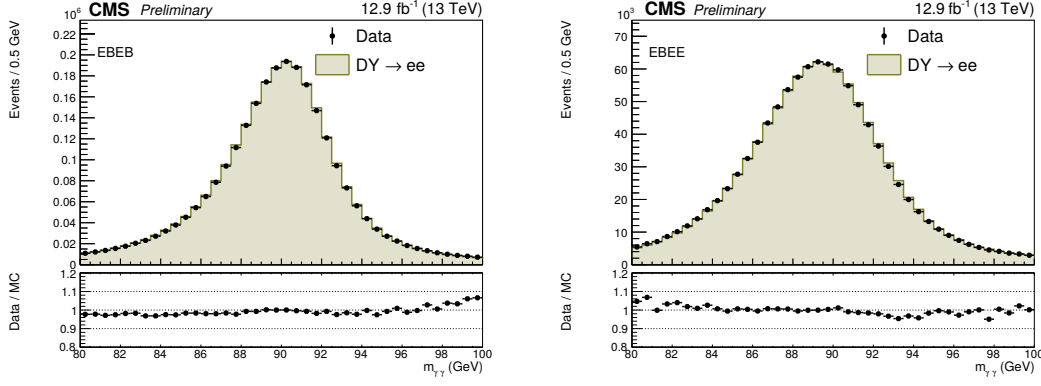
|                      | Data   |        | Simulation |        | Ratio  |        |
|----------------------|--------|--------|------------|--------|--------|--------|
|                      | Eff.   | Stat.  | Eff.       | Stat.  | Eff.   | Unc.   |
| Barrel; $R_9 > 0.85$ | 0.9932 | 0.0005 | 0.9972     | 0.0008 | 0.9960 | 0.0010 |
| Barrel; $R_9 < 0.85$ | 0.9750 | 0.0018 | 0.9824     | 0.0041 | 0.9924 | 0.0045 |
| Endcap; $R_9 > 0.90$ | 0.9851 | 0.0013 | 0.9852     | 0.0025 | 0.9999 | 0.0029 |
| Endcap; $R_9 < 0.90$ | 0.9525 | 0.0071 | 0.9658     | 0.0113 | 0.9862 | 0.0137 |

**Table 7.2:** Efficiency of the conversion-safe electron veto [155]. The data to simulation ratio is also shown with its uncertainty [149].

bin and category is listed in Table A.1 of the appendix. The final scale factor for each event category is listed in Table 7.1. The efficiency of the conversion-safe electron veto was taken from Ref. [150]. For this study, a high purity photon ( $Z \rightarrow \mu^+ \mu^- \gamma$ ) sample was used and a scale factor close to 1 was found for all categories. The results from Ref. [150] are reported in Table 7.2. A final comparison of observed and predicted  $Z \rightarrow e^+ e^-$  events is performed to validate the applied energy corrections of Chapter 6 and the efficiency scale factors. Data and MC distributions agree within 1 % as reported in Figure 7.3.

## 7.1 Efficiency measurement at 0 T

The measurement of the selection efficiency at  $B = 0$  T is similar to the one performed at 3.8 T with the exception of the electron rejection. The Tag-and-Probe method followed the same specifications as above, only the requirement of the probe electron was loosened: its identification was solely relying on its associated supercluster and had to pass a  $p_T$  cut of  $p_T > 25$  GeV. The signal was modeled in the same way as for the  $B = 3.8$  T dataset, but this time convoluted with a double sided crystal ball function. The background model had again an exponential shape. The systematic uncertainty from the fit shape was assumed to be the same as for  $B = 3.8$  T, because the purity of the selection and the shapes of signal and background were found to be similar. The selection efficiency is depicted in Figure 7.4, the individual efficiencies with their statistical uncertainties are listed in Table A.2 in the appendix. The observed and predicted



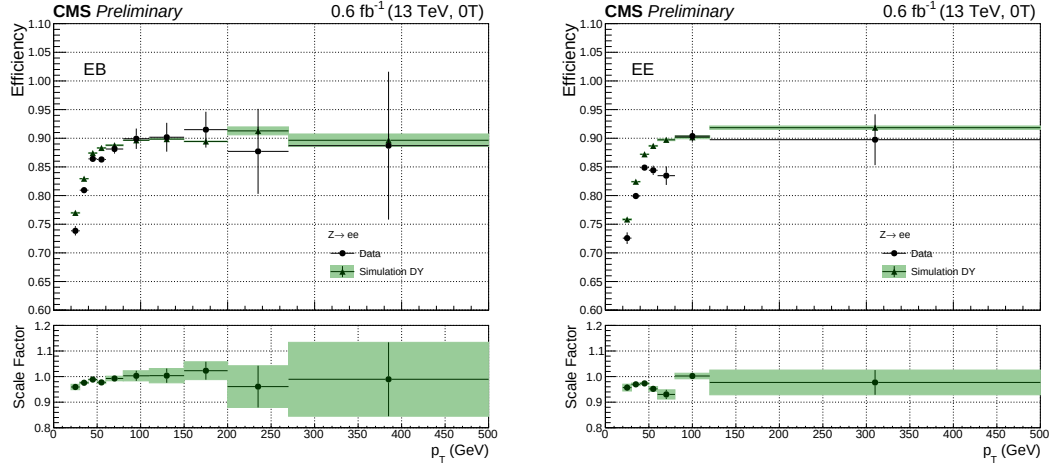
**Figure 7.3:** Comparison between the predicted and observed invariant mass distribution of electron pairs obtained after the application of energy scale, resolution and identification efficiency corrections. Distributions are shown for events where both electrons are reconstructed in the barrel (left) and events where one electron is in an endcap (right) [2].

efficiency agreed within  $< 3\%$ , the resulting scale factor is reported in Table 7.3.

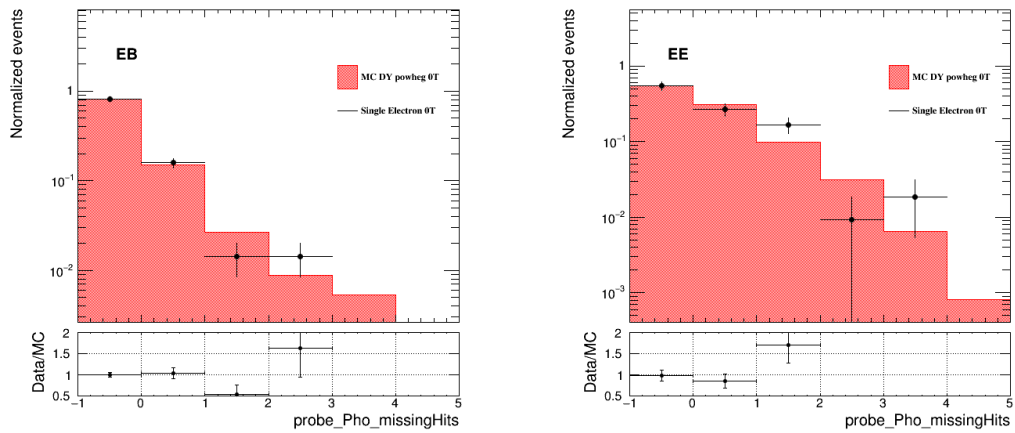
The electron rejection was studied with  $Z \rightarrow e^+e^-\gamma$  instead of  $Z \rightarrow \mu^+\mu^-\gamma$  events, since the reconstruction of the muon track momentum was not feasible due to the missing magnetic field. The two electrons had to satisfy the HLT\_Ele27\_eta2p1\_WPLoose\_Gsf trigger and passed the 'high pt' photon ID at  $B = 0$  T with inverted electron veto. They had to have a  $p_T$  above 30 GeV (20 GeV) for EB (EE) respectively. In order to select a photon which was radiated from the electrons, the photon needed to have a  $p_T$  of greater than 10 GeV, a  $\Delta R$  with each of the electron candidates of  $0.2 < \Delta R < 0.8$  and  $m_{ee\gamma} + m_{ee} < 180$  GeV. The electron rejection efficiency was then evaluated by the observed and predicted ratio of the first bin of the  $N_{\text{missing hits}}$  distribution of Figure 7.5. It was found to be close to one for both EB and EE, respectively.

| Region                    | Scale factor      |
|---------------------------|-------------------|
| $ \eta_{SC}  < 1.5$       | $0.982 \pm 0.004$ |
| $1.5 <  \eta_{SC}  < 2.5$ | $0.967 \pm 0.006$ |

**Table 7.3:** Data to MC scale factors for 0 T.



**Figure 7.4:** Photon identification efficiency for all selection requirements except the electron rejection, measured in barrel (left) and endcaps (right) using the tag-and-probe method for both data and simulated events. The lower panel shows the ratio between the efficiencies in data and simulation [2].



**Figure 7.5:** Data/MC comparison for the number of missing hits in barrel (left) and endcap (right) [151].



## 8

## CHAPTER

**Diphoton mass spectrum**

In the following, the number of events with diphoton candidates satisfying the full list of selection criteria and their  $m_{\gamma\gamma}$  spectra are presented. Table 8.1 and Table 8.2 compares the number of events in data and MC for the EBEB and EBEE event categories, respectively. The number of events are shown normalized to a luminosity of  $1 \text{ fb}^{-1}$ . The predicted and observed number of events may be compared for the part of the 2015 dataset with  $B = 3.8 \text{ T}$  ( $\mathcal{L} = 2.7 \text{ fb}^{-1}$ ) as well as the 2016 dataset with  $12.9 \text{ fb}^{-1}$ . The SM background processes were simulated to leading-order and were therefore scaled by a k-factor of 1.4 to account for higher order effects as detailed in Section 5.3.3.

The diphoton invariant mass spectra for both event categories of the 2016 dataset with  $12.9 \text{ fb}^{-1}$  are depicted in Figure 8.1. The mass spectra of the 2015 dataset are shown in Figure 8.2 and Figure 8.3 for the magnetic field configurations of  $B = 3.8 \text{ T}$  and  $B = 0 \text{ T}$ , respectively. All distributions were parametrized using the functional form

$$g(m_{\gamma\gamma}) = m_{\gamma\gamma}^{a+b \log(m_{\gamma\gamma})} \quad .$$

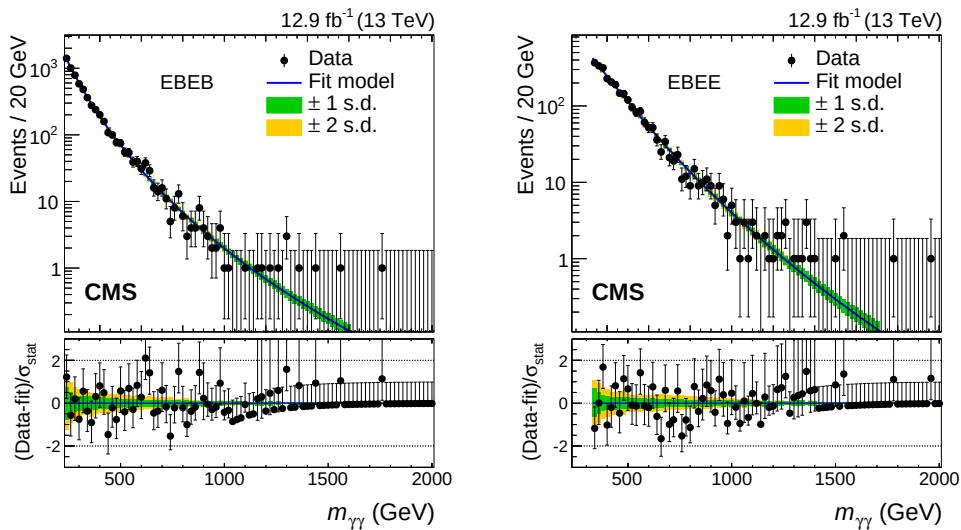
More details are given in Chapter 11.

|                | $m_{\gamma\gamma} > 230 \text{ GeV}$ |                 |      | $m_{\gamma\gamma} > 500 \text{ GeV}$ |                 |      |
|----------------|--------------------------------------|-----------------|------|--------------------------------------|-----------------|------|
|                | 2015, B = 0 T                        | 2015, B = 3.8 T | 2016 | 2015, B = 0 T                        | 2015, B = 3.8 T | 2016 |
| $\gamma\gamma$ | -                                    | 389             | 460  | -                                    | 34              | 35   |
| $\gamma j$     | -                                    | 124             | 57   | -                                    | 6               | 2.8  |
| Total          | -                                    | 513             | 517  | -                                    | 40              | 38   |
| Data           | 463                                  | 458             | 487  | 22                                   | 36              | 36   |

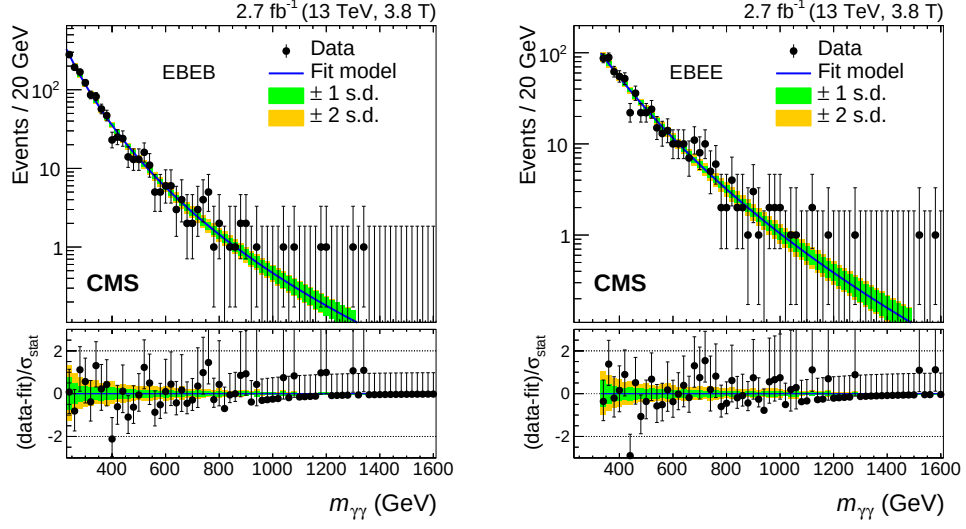
**Table 8.1:** Number of events selected in data and predicted from MC in the EBEB category. A scale factor of 1.4 is applied to the MC predictions. Numbers refer to a luminosity of  $1 \text{ fb}^{-1}$ .

|                | $m_{\gamma\gamma} > 320 \text{ GeV}$ |                 |      | $m_{\gamma\gamma} > 500 \text{ GeV}$ |                 |      |
|----------------|--------------------------------------|-----------------|------|--------------------------------------|-----------------|------|
|                | 2015, B = 0 T                        | 2015, B = 3.8 T | 2016 | 2015, B = 0 T                        | 2015, B = 3.8 T | 2016 |
| $\gamma\gamma$ | -                                    | 152             | 168  | -                                    | 47              | 47   |
| $\gamma j$     | -                                    | 82              | 44   | -                                    | 23              | 11   |
| Total          | -                                    | 234             | 212  | -                                    | 70              | 58   |
| Data           | 197                                  | 230             | 216  | 62                                   | 68              | 62   |

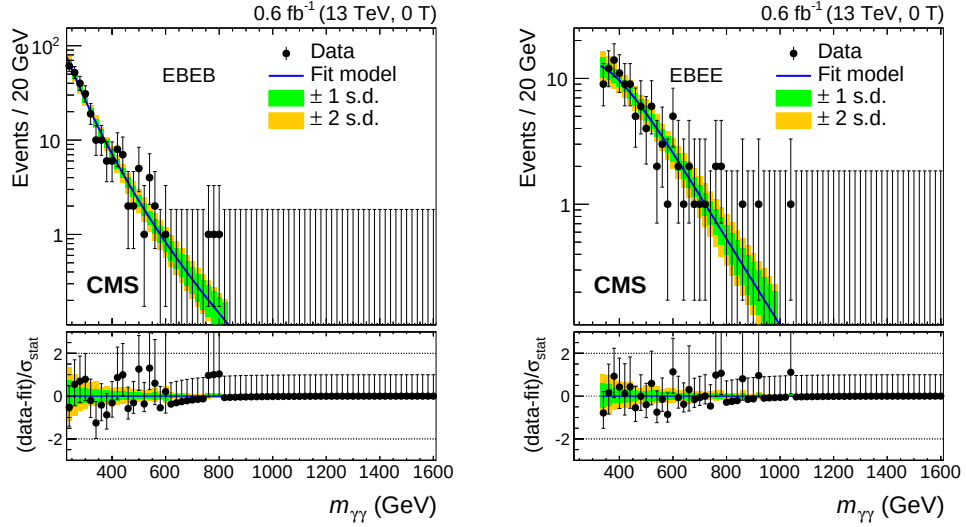
**Table 8.2:** Number of events selected in data and predicted from MC in the EBEE category. A scale factor of 1.4 is applied to the MC predictions. Numbers refer to a luminosity of  $1 \text{ fb}^{-1}$ .



**Figure 8.1:** Observed invariant mass spectrum  $m_{\gamma\gamma}$  in the EBEB (EBEE) category on the left (right) figure for  $12.9 \text{ fb}^{-1}$ . The result of the parametric fit is superimposed to the points, together with bands representing the statistical uncertainties on the knowledge of the background shape [1].



**Figure 8.2:** Observed invariant mass spectrum  $m_{\gamma\gamma}$  in the EBEB (EBEE) category on the left (right) figure for  $2.7 \text{ fb}^{-1}$  with a magnetic field configuration of  $B = 3.8 \text{ T}$ . The result of the parametric fit is superimposed to the points, together with bands representing the statistical uncertainties on the knowledge of the background shape [1].



**Figure 8.3:** Observed invariant mass spectrum  $m_{\gamma\gamma}$  in the EBEB (EBEE) category on the left (right) figure for  $0.6 \text{ fb}^{-1}$  with a magnetic field configuration of  $B = 0 \text{ T}$ . The result of the parametric fit is superimposed to the points, together with bands representing the statistical uncertainties on the knowledge of the background shape [1].



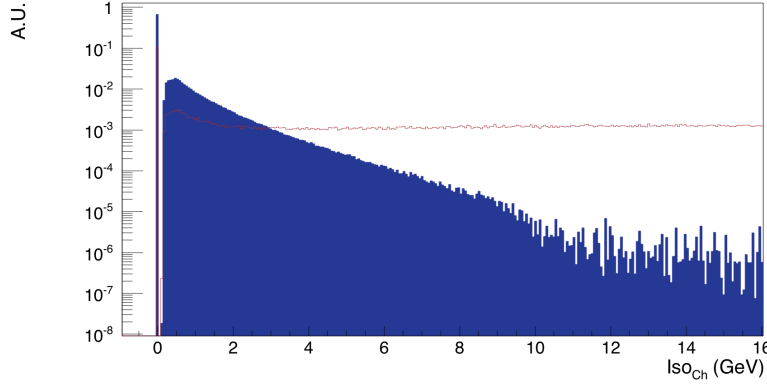


## Background composition determination in data

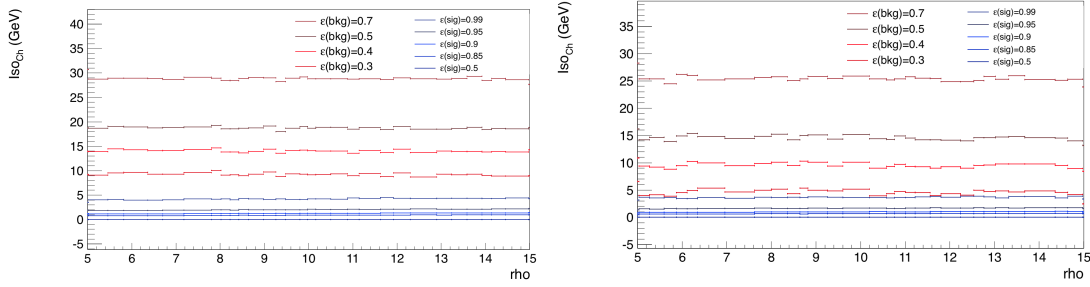
A thorough understanding of the diphoton standard model background increases the reliability of the overall background model. The individual background components were therefore determined as a function of the diphoton mass. The background can be divided into two parts: the irreducible and reducible components.

The irreducible background consists of two prompt photons ( $\gamma\gamma$ ). The reducible background of this analysis contains events where at least one photon candidate is a jet ( $j$ ). Since this jet is misidentified as a photon, it is referred to as a 'fake photon'. These fake photons are jets for which the hadronization process results in neutral mesons with high  $p_T$ , decaying to two photons. The corresponding background fractions are denoted as  $f_{\gamma j}$ , where only one photon candidate is a prompt photon, and  $f_{jj}$ , where both photon candidates are misidentified jets. From MC simulation, for instance Figure 5.8, it is known that the reducible background should be about 10 % for the EBEB category and a bit higher (about 15 %) for the EBEE category.

A discriminating variable had to be found to distinguish the prompt and fake photon candidates. Among the variables for the event selection, the  $\sigma_{i\eta i\eta}$ , the  $\text{Iso}_{\text{Ch}}$  and the  $\text{Iso}_{\gamma}$  variables show the most distinct shapes for prompt and fake photon candidates. The  $\text{Iso}_{\text{Ch}}$  variable is an ECAL specific variable and defined as the scalar sum of the transverse momenta of the charged PF hadron candidates assigned to the chosen primary vertex in a cone of  $\Delta R < 0.3$ . As discussed in Section 5.7, the photons of this analysis have to pass a threshold of  $\text{Iso}_{\text{Ch}} < 5 \text{ GeV}$  to enter the signal region. The  $\text{Iso}_{\text{Ch}}$ -distribution of the MC truth dataset of prompt and fake photons is shown in Figure 9.1. The MC truth dataset contains the 'true' prompt or fake photons. For that, the prompt photons need to match the generator level information of a true photon and they are required to have an isolation at generator level of below 10 GeV. For fake photons, at least one of these two requirements is not met. The  $\text{Iso}_{\text{Ch}}$ -distribution of prompt photons has a sharp maximum around zero and decreases to the permille level for  $\text{Iso}_{\text{Ch}} = 5 \text{ GeV}$ . This means that most of the prompt photons are well isolated, with only little energy



**Figure 9.1:**  $\text{Iso}_{\text{Ch}}$ -distribution for prompt (blue) and fake (red) single photons in MC for the EB category.



**Figure 9.2:**  $\text{Iso}_{\text{Ch}}$ -distribution vs the pile-up density  $\rho$  of the MC dataset for single prompt (blue) and fake (red/brown) photons in EB (left) and EE (right).

deposits from charged particles around them. The distribution of fake photons has on the contrary a broader spectrum. It shows a less sharp maximum around zero, and is, after a first decrease for  $\text{Iso}_{\text{Ch}}$  values of up to 1 GeV, nearly constant up to energies of 15 GeV. This comparison shows that the charged particle flow isolation is a suitable discriminating template variable.

An advantage of the  $\text{Iso}_{\text{Ch}}$  variable is that it is also approximately pile-up independent and does not need to be corrected for underlying event properties. Figure 9.2 depicts the  $\text{Iso}_{\text{Ch}}$ -distribution versus the median pile-up density ( $\rho$ ) [156]. The median pile-up density is the median of the transverse energy density per unit area in the event. For each  $\rho$  bin, the  $\text{Iso}_{\text{Ch}}$ -distribution is integrated up to a certain percentage, denoted by the respective quantiles. The resulting  $\text{Iso}_{\text{Ch}}$  value is the marked  $\text{Iso}_{\text{Ch}}$  value of each quantile. For uncorrelated variables, the quantiles should be flat as a function of  $\rho$ , which can be recognized for the EB category (left) and the EE category (right).

A comparison of the  $\text{Iso}_{\text{Ch}}$  to the photon isolation distribution of prompt and fake photons in MC showed that the  $\text{Iso}_{\text{Ch}}$  variable had the higher discrimination power and was less dependent on  $p_{\text{T}}$  and pile-up, to the extent that no corrections of the distribution for the event selection were necessary with respect to these parameters.

The shower shape variable  $\sigma_{i\eta i\eta}$  is the weighted spatial second order moment of a particle and quantifies the energy deposits in a  $5 \times 5$  crystal matrix around the most energetic crystal. It has a broader shape for a fake photon compared to a prompt one. The shape is broader, the more neutral mesons the jet contains. Above a certain  $\sigma_{i\eta i\eta}$  value, the collection should therefore consist mostly of misidentified jets. In principle,  $\sigma_{i\eta i\eta}$  could also have been the chosen template variable, but was instead used for the following sideband definition. This definition of the sideband implies that the  $\text{Iso}_{\text{Ch}}$  variable and the  $\sigma_{i\eta i\eta}$  variable need to be uncorrelated, which is discussed later in this chapter.

The diphoton events of this study passed the high- $p_T$  photon ID requirements of Chapter 5.7, with the exception of the  $\text{Iso}_{\text{Ch}}$  requirement which was relaxed to 15 GeV to obtain a good description of the fake photon candidate distribution.

To estimate the fraction  $\hat{f}$  of each of the  $\gamma\gamma$ -,  $\gamma j$ - and  $jj$ -background components, a binned likelihood fit of  $\text{Iso}_{\text{Ch}}$  was performed for several bins in the invariant diphoton mass spectrum in data. For each background component, a two-dimensional template  $T^{i,j}(\text{Iso}_{\text{Ch}1}, \text{Iso}_{\text{Ch}2})$  was built with one dimension per photon candidate.

The construction of these  $\text{Iso}_{\text{Ch}}$ -templates is discussed in Section 9.1. The template was divided into three bins as otherwise the statistical uncertainty of the bins with  $\text{Iso}_{\text{Ch}} > 0.1$  GeV, would have been too large for the subsequent fit. The binning of the template variable is chosen such that the first bin had the range of 0.0 – 0.1 GeV, containing all well isolated photon candidates. The second range (0.1 – 5 GeV) reflects the cut on the signal region at 5 GeV and the last bin (5 – 15 GeV) contains mostly fake photon candidates. Comparing this binning to the  $\text{Iso}_{\text{Ch}}$ -distribution for prompt and fake photons in Figure 9.1, it is visible that the second bin does not have a high discrimination power as the shapes between 0.1 – 5 GeV are similar for prompt and fake photons.

The events are again divided in EBEB and EBEE categories as for the rest of the analysis. The likelihood depends on the unconstrained three background fractions  $\hat{f}_{\gamma\gamma}$ ,  $\hat{f}_{\gamma j}$ ,  $\hat{f}_{jj}$  and was defined as follows:

$$L(\text{data}|\hat{f}_{\gamma\gamma}, \hat{f}_{\gamma j}, \hat{f}_{jj}) = \prod_{i=1}^{\text{Nbins}} (\hat{f}_{\gamma\gamma} \cdot T^{\gamma\gamma}(\text{Iso}_{\text{Ch } i,1}, \text{Iso}_{\text{Ch } i,2}) + \hat{f}_{\gamma j} \cdot T^{\gamma j}(\text{Iso}_{\text{Ch } i,1}, \text{Iso}_{\text{Ch } i,2}) + \hat{f}_{jj} \cdot T^{jj}(\text{Iso}_{\text{Ch } i,1}, \text{Iso}_{\text{Ch } i,2}))^{n_i} \quad (9.1)$$

Figure 8.2 depicts the  $m_{\gamma\gamma}$  spectra for both categories at  $B = 3.8$  T. These  $m_{\gamma\gamma}$  spectra were divided in several bins, which were chosen in such a way to approximately equalize the number of events in each bin:

- 9 bins in EBEB (GeV): [230, 253, 282, 332, 409, 500, 600, 800, 1000, 1600]
- 7 bins in EBEE (GeV): [320, 356, 444, 500, 600, 800, 1000, 1600]

No events were found above 1.6 TeV, such that no overflow had to be taken into account. The likelihood fit was performed for each of these  $m_{\gamma\gamma}$  bins. The associated statistical and systematic uncertainties are detailed later, in particular in Section 9.3. The results of the binned likelihood fit gave the fractions of the individual background components for the extended  $\text{Iso}_{\text{Ch}}$  range of up to 15 GeV and are discussed in Chapter 9.2. These estimates are extrapolated back to the range of  $\text{Iso}_{\text{Ch}} < 5$  GeV to obtain the individual background components for the used diphoton candidates of this search.

## 9.1 Charged particle flow isolation templates

The two-dimensional  $\text{Iso}_{\text{Ch}}$ -templates are built from data and compared to Monte Carlo simulations. To verify that the  $\gamma\gamma$ -templates, the  $\gamma j$ - and  $jj$ -templates are indeed representing prompt and fake photons, their construction had to be compared to MC simulations: The building of the templates had to be reproduced with the MC dataset and compared to the MC truth information. An agreement of the results from the MC truth dataset with the  $\text{Iso}_{\text{Ch}}$  MC template is necessary for the application of the data-driven approach. It is however not the only requirement on the method to be considered reliable. All three  $\text{Iso}_{\text{Ch}}$ -templates had to be sufficiently populated, such that the statistical uncertainty was at a level to not distort the fit. For that, the  $\gamma j$ - and  $jj$ -templates were enriched by an 'event-mixing' method to have a higher amount of fake photons, especially for high  $m_{\gamma\gamma}$  values. The construction of the templates is based on a similar approach, which was employed in Ref. [157] for a measurement of the SM diphoton production.

### 9.1.1 Prompt-prompt photon template with the random cone method

The  $\gamma\gamma$ -template is built with the 'random cone' technique. A prompt photon is a well-isolated object, with only little deposited energy around it. The energy deposition is often expressed as 'activity', which is just the sum of all transverse momenta of particles entering the isolation cone around the photon. In fact, the only activity in the isolation cone of the photon should be due to pile-up. Additionally, the ECAL electronics might add noise to the readout signal.

At a fixed  $\eta$ -coordinate, the energy deposits from pile-up events are symmetric in the azimuthal angle [129]. The random cone technique therefore fixes the  $\eta$ -coordinate of the photon, and finds a new isolation cone at a random angle in  $\phi$ . With this approach, the random cone is supposed to contain the same number of particles in its cone as the isolation cone of the photon. The azimuthal angle is allowed to have any value between 0.8 and  $(2\pi - 0.8)$  radians with respect to the original  $\phi_\gamma$  value to prohibit the isolation

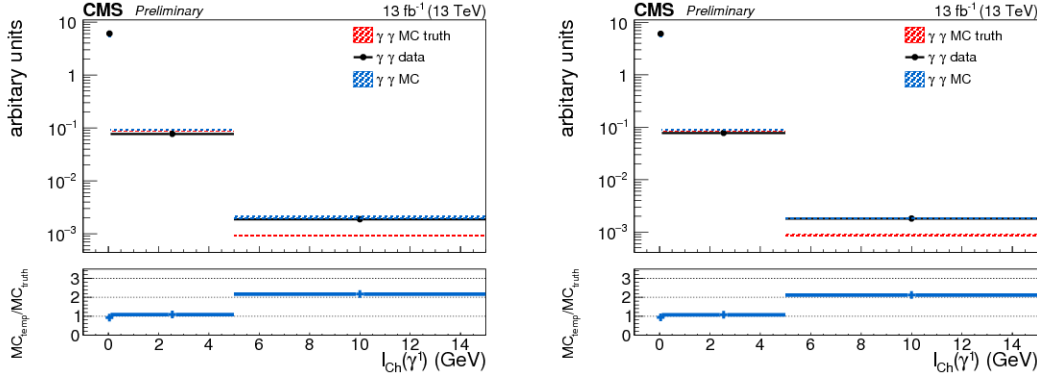
cones with a size of  $\Delta R < 0.4$  to overlap with each other.

It is important to reject random cones which contain decay products from other processes. The random cone is rejected if a jet with  $p_{t,jet} > 30$  GeV or a photon with  $p_{t,\gamma} > 10$  GeV is found inside the cone. This random cone technique is applied up to nine times on each  $\gamma\gamma$ -diphoton event in data to decrease the statistical uncertainty on the  $\gamma\gamma$ -Iso<sub>Ch</sub>-template.

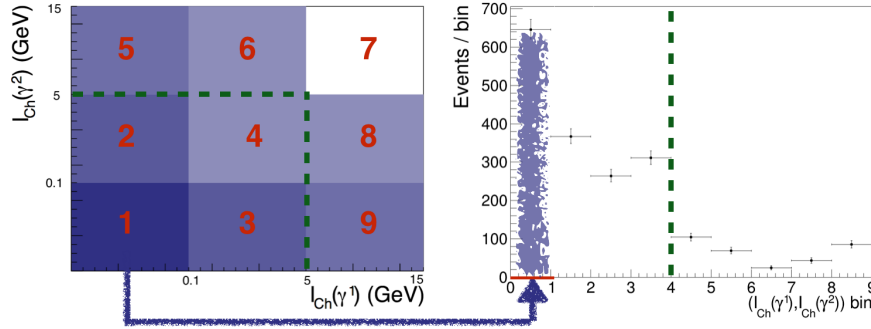
The Iso<sub>Ch</sub>-distribution of the diphoton events can be depicted in a two-dimensional histogram. For a first comparison of the observed and predicted Iso<sub>Ch</sub>-distribution of the first axis of the Iso<sub>Ch</sub>-distribution is looked at. Figure 9.3 shows the comparison of the  $\gamma\gamma$ -component in MC truth to the charged particle flow isolation of the random cones from the MC dataset for  $12.9 \text{ fb}^{-1}$ . The charged particle flow isolation distribution was normalized to its area, each bin and its uncertainty were divided by the bin width to compare the different number of entries for the individual bins.

The random cone has by definition the same distribution for leading and subleading photon. The first axis of the Iso<sub>Ch</sub> variable is therefore populated by the Iso<sub>Ch</sub> value of randomly chosen leading and subleading photons and is illustrated in the left panel of Figure 9.3. For the barrel-endcaps category, the random cone isolation of the barrel photon candidate is assigned to the first axis (right panel in Figure 9.3), the random cone isolation of the endcaps photon candidate to the second axis.

A necessary requirement for the random cone technique is that the distribution of the true prompt diphoton template from MC truth agree with the random cone template from the MC dataset. For barrel-barrel and barrel-endcaps, the first two bins show an agreement within  $1 \sigma$  for both legs as visible from the ratio on the bottom of both figures. A slight offset in the first bin of about 5 % will be included as a systematic uncertainty of the method. The third bin of the prompt photon template has in all cases much less entries as this is the bin of the extended Iso<sub>Ch</sub>-range and therefore barely populated by prompt photons. Since the  $\gamma\gamma$ -component in this bin is nearly zero, the disagreement of MC truth and the  $\gamma\gamma$ -template from the MC dataset on the final two-dimensional fit is negligible as demonstrated later. A closer look at the templates also shows that the purely statistical uncertainty on the MC templates and the MC truth is in some bins not of the same size. The reason for the variations in the uncertainty bars was tracked down to a corresponding variation in the weight of the MC events used to produce the figure. The final state topologies in MC simulations are not produced to the same amount as they are predicted by their individual cross-sections. Instead, every event has a weight assigned to it, which denotes its fraction to the total cross-section. For fake photons, some of these final state topologies are not simulated in great number and have instead a large weight assigned to them. When scaled to the integrated luminosity in data, the bulk of the events have fractional weights, while a small tail have weights of the order of unity.



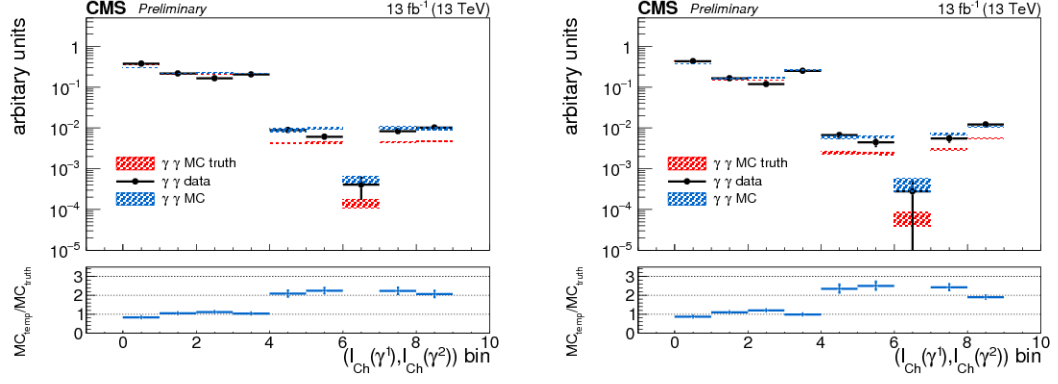
**Figure 9.3:** Projection of charged particle flow isolation of the first leg for  $\gamma\gamma$ -templates in EBEB (left) and EBEE (right) for the full  $m_{\gamma\gamma}$  range.



**Figure 9.4:** Sketch how the bin content of the two-dimensional charged particle flow isolation histogram is unrolled on a one-dimensional histogram. The procedure is highlighted for the first bin.

It is useful to visualize the two-dimensional templates in a one-dimensional histogram. A sketch of the method is visualized in Figure 9.4. The bin content of each bin of the two-dimensional histogram is normalized to its area and projected on a one-dimensional axis. An equal width for all bins was chosen to facilitate the comparison between MC truth, MC templates and templates in data. The first four bins correspond to the signal region of the analysis with  $\text{Iso}_{\text{Ch}} < 5$  GeV, the other five bins contain at least one photon with  $5 \text{ GeV} < \text{Iso}_{\text{Ch}} < 15$  GeV.

The result for the  $\gamma\gamma$ -template is shown in Figure 9.5, for the EBEB and EBEE event category, respectively. For the signal region, an agreement within  $1\sigma$  can be observed with an offset of about 15% for the first bin. The extended  $\text{Iso}_{\text{Ch}}$ -region, especially bins 6-8, is less populated and a larger disagreement between MC truth prediction and MC templates is observed. Since this range is used to estimate the fake contribution in the final two-dimensional fit, the disagreement has a negligible influence.



**Figure 9.5:** one-dimensional projection of two-dimensional charged particle flow isolation for  $\gamma\gamma$ -templates in EBEB (left) and EBEE (right) for the full  $m_{\gamma\gamma}$  range.

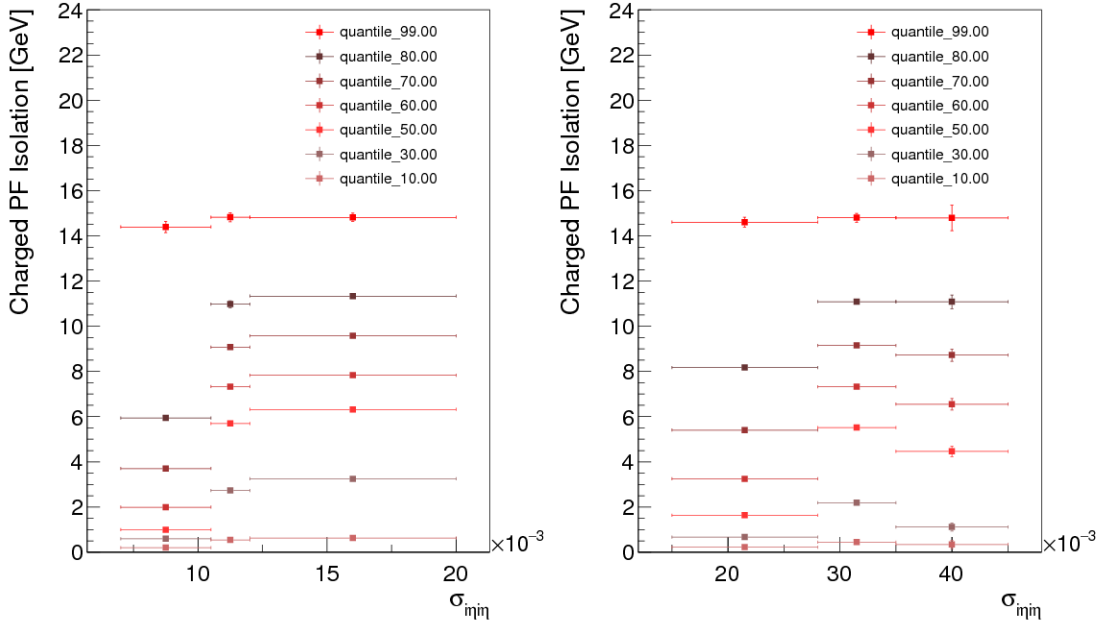
### 9.1.2 Fake template with the $\sigma_{i\eta i\eta}$ -sideband method

To build a template consisting of misidentified jets, a discriminating variable for prompt and fake photons had to be found. Here, the shower shape variable  $\sigma_{i\eta i\eta}$  was chosen as the discriminating variable. It has a broader shape for a fake photon compared to a prompt photon. Above a certain  $\sigma_{i\eta i\eta}$  value, the collection should therefore consist mostly of misidentified jets. To increase the amount of fake photons, the cut on the corrected photon isolation was also slightly relaxed.

In Chapter 5.7, it was discussed that high-energy photons with an energy of about 2 TeV can saturate the ECAL readout electronics. The  $\sigma_{i\eta i\eta}$ -thresholds for non-saturated photons in the signal regions were  $\sigma_{i\eta i\eta} < 0.0105$  for EB (0.028 for EE), and for saturated photon candidates  $\sigma_{i\eta i\eta} < 0.0112$  for EB (0.030 for EE). No saturated photons were observed in the dataset of  $16.2 \text{ fb}^{-1}$ , but needed to be accounted for in the preparation of the analysis. For the  $\sigma_{i\eta i\eta}$ -sideband definition, the candidates were therefore required to fail the higher cut of  $\sigma_{i\eta i\eta} = 0.0112$  for EB (0.030 for EE) to satisfy the definition of the signal selection for saturated photons and to avoid prompt-photon contamination from non-saturated photons in the sideband. The sideband definition of the two categories is listed in Table 9.1.

The photon candidates of the  $\sigma_{i\eta i\eta}$ -sideband were then asked to pass all high- $p_T$  photon ID cuts, except for the two discriminating variables. Since these sideband candidates satisfy the rest of the high- $p_T$  photon ID criteria, a sample of fake photons with a similar event signature as the one of prompt photons is obtained.

The sideband definition should be uncorrelated with the  $\text{Iso}_{\text{Ch}}$  variables, such that the  $\text{Iso}_{\text{Ch}}$ -shape of the sideband template is close to the one of the non-prompt photons passing the photon selection. Figure 9.6 depicts the  $\text{Iso}_{\text{Ch}}$  of the fake photons as a function of  $\sigma_{i\eta i\eta}$  in EB and EE. The  $\sigma_{i\eta i\eta}$ -distribution is subdivided in three bins, following the sideband definition of Table 9.1. For each  $\sigma_{i\eta i\eta}$ -bin the  $\text{Iso}_{\text{Ch}}$ -distribution is integrated



**Figure 9.6:** Charged particle flow isolation as a function of  $\sigma_{i\eta i\eta}$  of the MC dataset for fake single photons. Left: EB, Right: EE.

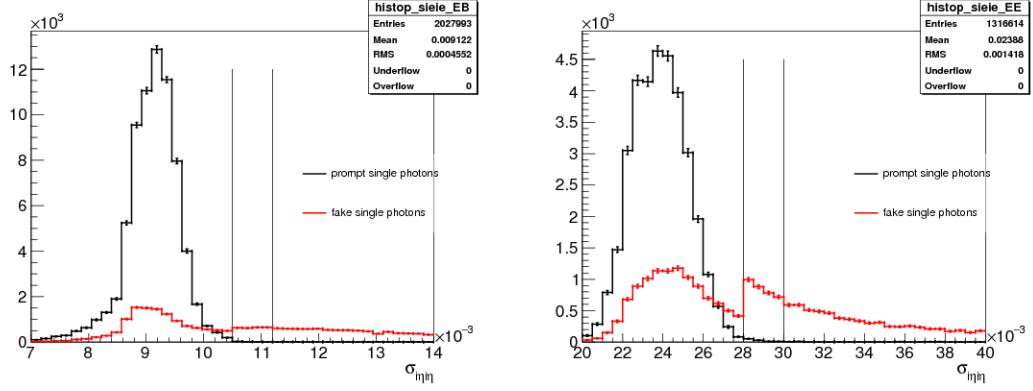
up to a certain percentage, denoted by the respective quantiles. The resulting  $\text{Iso}_{\text{Ch}}$  value is the marked  $\text{Iso}_{\text{Ch}}$  value of each quantile. For uncorrelated variables, the quantiles should be flat as a function of  $\sigma_{i\eta i\eta}$ . The observed slight upward slope is still at a manageable level and the  $\sigma_{i\eta i\eta}$  variable could be used as the discriminating sideband variable. The correlation is part of the final systematic uncertainty.

### Evaluation of $\sigma_{i\eta i\eta}$ -sideband method with single photon dataset

The discrimination power of the  $\sigma_{i\eta i\eta}$ -sideband was verified on the single photon datasets. The single photon dataset in MC was built from the full SM background dataset of Table 5.2. In data, the single photons were required to pass the following HLT triggers: HLT\_Photon50, HLT\_Photon75, HLT\_Photon90, HLT\_Photon120, HLT\_Photon165. These triggers are seeded by single photon L1-triggers. After passing the trigger selection, the single photons were required to pass the same high- $p_T$  photon ID cuts as the photons of the diphoton event in Section 5.7 plus a cut of  $p_T = 170$  GeV to avoid turn-on effects of the trigger. The  $\sigma_{i\eta i\eta}$ -distribution for prompt and fake photons, matched to their MC truth information, is depicted in Figure 9.7 for both event categories. The black vertical lines mark the end of the signal region in  $\sigma_{i\eta i\eta}$  and the start of the sideband region. The sudden increase of the fake photon distribution at the start of the sideband region at  $\sigma_{i\eta i\eta} > 0.0105$  for EB (0.028 for EE) is due to the relaxed cut of  $\text{Iso}_{\gamma^-}$ . Both figures show that the chosen  $\sigma_{i\eta i\eta}$ -sideband definition of Table 9.1 minimizes the contamination from prompt photons in the  $\sigma_{i\eta i\eta}$ -sideband to a sub-percent level.

**Table 9.1:** Sideband definition for fake photon templates.

| Category  | $\sigma_{i\eta i\eta}$ | $\text{Iso}_{\gamma}(\text{GeV})$ |
|-----------|------------------------|-----------------------------------|
| <b>EB</b> | $> 0.0112$             | $< 4.5$                           |
| <b>EE</b> | $> 0.0300$             | $< 13.5$                          |



**Figure 9.7:** The  $\sigma_{i\eta i\eta}$ -distribution of the MC dataset for true prompt and fake single photons. Left: EB, Right: EE. The sudden increase of the fake photon distribution at the start of the sideband region at  $\sigma_{i\eta i\eta} > 0.0105$  for EB ( $0.028$  for EE) is due to the relaxed cut of  $\text{Iso}_{\gamma}$ .

To study the influence of a different  $\sigma_{i\eta i\eta}$ -sideband definition, the cuts were changed to  $\sigma_{i\eta i\eta} > 0.012$  for EB and  $\sigma_{i\eta i\eta} > 0.032$ . The resulting difference in the final fit is part of the final systematic uncertainty.

### The event mixing method

With the chosen sideband definition, the two-dimensional templates for the  $\gamma j$ - and  $jj$ -component would not contain enough events to describe the background components correctly, especially for high- $p_T$  candidates. The reduction of the statistical uncertainty of the  $\gamma j$ - and  $jj$ - $\text{Iso}_{\text{Ch}}$ -templates is however crucial for the subsequent fit. The k-Nearest-Neighbor algorithm [158] can be used to reduce the statistical uncertainty of a template without modifying its shape and behavior. The algorithm selects photon candidates from a single photon selection with similar phase space values as the photons of the original diphoton event, which passed the high- $p_T$  photon ID selection. The 'n-dimensional' phase space is thereby defined by the most relevant variables of the diphoton event. Since the two photons of the diphoton event are not independent from each other, their event topology is taken into account for the subsequent assignment. Each variable of this phase space is integrated to its cumulative distribution function (cdf) to obtain a comparable metric for each phase space dimension. Each leg of the diphoton event is then paired to a single photon event with the smallest Cartesian distance defined in the space of the transformation variables by the Nearest Neighbor algorithm. To reduce

the statistical uncertainty of the template, this assignment needs to be repeated several times. The single photon selection therefore needs to provide at least a factor ten more events than the original diphoton events in the respective event category.

With this method, the  $\gamma j$  and  $jj$  templates were constructed as follows: the prompt photon candidate for the  $\gamma j$ -template was taken from the prompt single photon selection. Its  $\text{Iso}_{\text{Ch}}$  value was obtained with the random cone method. The fake photon was selected by applying the sideband photon identification to the single photons. The matching was performed in a  $n=3$  phase space, which included the most relevant variables for the diphoton events:

- **EBEB**: the logarithm of the transverse momentum of the photon ( $\log(p_T)$ ), the pseudorapidity and the number of vertices.
- **EBEE**: the logarithm of the transverse momentum of the photon, the pseudorapidity and the corrected photon isolation.

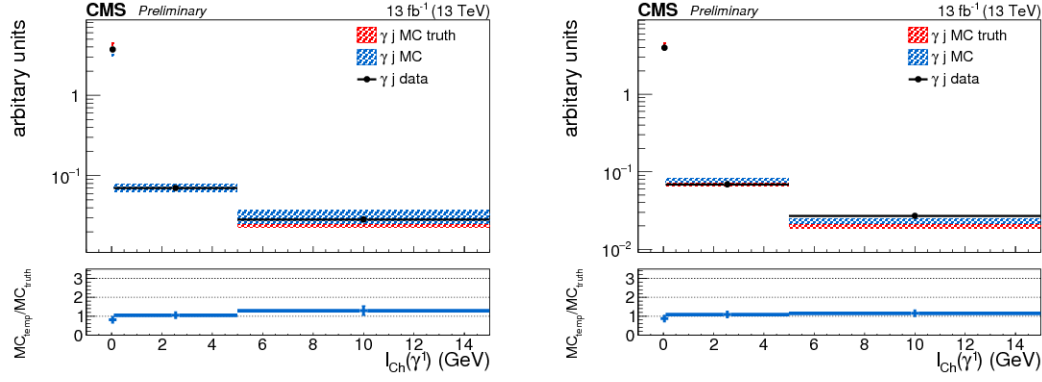
For EBEE, the  $\text{Iso}_{\gamma}$  was chosen instead of the number of vertices since the  $\text{Iso}_{\gamma}$  cut in EBEE is looser than for EBEB and is therefore slightly more relevant for the photon candidate. A sub-sample of  $k=8$  ( $k=15$ ) similar single photon events was built in EBEB (EBEE), depending on the statistics in both datasets. To account for the effect of the correlations, neglected so far, the MC truth information of the  $\gamma j$  template was analyzed:

- **$\gamma j$ -template for EBEB**: the prompt photon is with a probability of 80 % the leading photon.
- **$\gamma j$ -template for EBEE**: the prompt photon is with a probability of 56 % in the barrel.

Both values were varied by 10% for the final systematic uncertainty for the fractions of the background components. For the EBEB category, the templates variable of the leading and subleading photon is again randomly switched. For the barrel-endcaps case, the  $\text{Iso}_{\text{Ch}}$  of the barrel photon candidate is the first, the one of the endcaps photon candidate the second axis. The event mixing leads to  $\gamma j$ - and  $jj$ - templates which have  $k \times x$  more events than data and the highly enriched samples were subsequently used for the fit to determine the reducible background.

### Templates with the event mixing method

The 'event mixed'  $\text{Iso}_{\text{Ch}}$ -templates for  $\gamma j$ -events were verified against their MC truth prediction. The  $\text{Iso}_{\text{Ch}}$ -distribution of the first axis can be seen for EBEB (EBEE) in

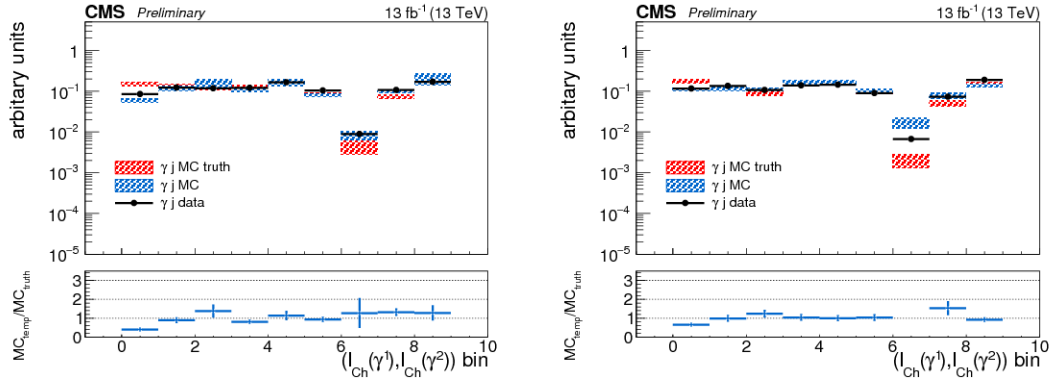


**Figure 9.8:** Projection of charged particle flow isolation of the first leg for  $\gamma j$ -templates in EBEB (left) and in EBEE (right) for the full  $m_{\gamma\gamma}$  range. For the  $\gamma j$  MC and data template the event-mixing method was used.

the left (right) panel in Figure 9.8. The charged particle flow isolation is normalized to unity and each bin and its uncertainty are then divided by the bin width. The assignment of the  $\text{Iso}_{\text{Ch}}$  values of the two candidates onto the  $\text{Iso}_{\text{Ch}}$ -axes was performed as for the  $\gamma\gamma$ -template. For the EBEB category, the random cone isolation of the leading and subleading photon is randomly switched on the axes. For the barrel-endcap case, the  $\text{Iso}_{\text{Ch}}$  of the barrel photon candidate is projected on the first (right panel in Figure 9.8), the one of the endcap photon candidate on the second axis. Both categories show a good agreement between MC truth and the enriched  $\gamma j$ -templates within  $1\sigma$  for all bins. As for the  $\gamma\gamma$ -template, the uncertainty on the MC templates and the MC truth are sometimes different due to the event weights.

The  $\gamma j$ -templates were ‘unrolled’ in one-dimension, depicted in Figure 9.9. The unrolled  $\text{Iso}_{\text{Ch}}$ -template for EBEB shows for all bins, except for the first one, an agreement within their uncertainties. The MC truth predicts a more isolated shape than it is observed by the  $\text{Iso}_{\text{Ch}}$ -templates in MC or data. In the subsequent fit, the first bin is dominated by the  $\gamma\gamma$ -component, the observed disagreement has therefore a negligible influence. The overall agreement shows that the event-mixing procedure describes the physics of the  $\gamma j$ -templates correctly. The  $\gamma j$ -templates in data could therefore be taken from the event-mixing methods. The  $\text{Iso}_{\text{Ch}}$ -distribution in data follows the MC prediction in all bins within their uncertainties.

The final template under consideration is the  $jj$ -template. The QCD single-EM enriched sample, detailed in Section 5.3, did not provide enough statistics to build true  $jj$ -templates in MC. The templates gained by the event-mixing method could therefore not be verified by a comparison to MC truth templates. As an alternative, the number of true  $jj$ -MC events were compared to the overall number of events in the MC dataset and the fraction of  $jj$ -events was estimated. The comparison is given in Table 9.2 and 9.3.



**Figure 9.9:** Projection of two-dimensional charged particle flow isolation for  $\gamma j$ -templates in EBEB and EBEE for the full  $m_{\gamma\gamma}$  range. For the  $\gamma j$  MC and data template the event-mixing method was used.

**Table 9.2:** Comparison of overall MC prediction with QCD-EM enriched events for  $1 \text{ fb}^{-1}$  for the EBEB category.

| EBEB ( $m_{\gamma\gamma} > 230 \text{ GeV}$ )     |                      |                      |
|---------------------------------------------------|----------------------|----------------------|
|                                                   | IsoCh < 5 GeV        | IsoCh < 15 GeV       |
| Truth jj-MC events                                | $1^{+2.3}_{-0.8}$    | $8^{+4.0}_{-2.8}$    |
| Truth jj-weighted MC events                       | $4^{+9.2}_{-3.3}$    | $17^{+8.4}_{-5.9}$   |
| MC events                                         | $535919 \pm 732$     | $560296 \pm 749$     |
| Weighted MC events                                | $369 \pm 0.5$        | $416 \pm 0.6$        |
| <b>Percentage of jj-events in full MC dataset</b> | $1^{+2.5}_{-0.9} \%$ | $4^{+2.0}_{-1.4} \%$ |

Thereby, the corresponding weighted events were normalized to  $1 \text{ fb}^{-1}$ . Based on these MC predictions, an approximate estimate of the jj-fraction was performed, which is listed in the last row of each table. Since the jj-MC events carry high weights, the uncertainty on the final jj-fraction, in particular for EBEE, is rather high. These listed approximate estimates of the expected number of jj-events in the full MC dataset were the only validation of the jj-component in data, but considered to be sufficient as this contribution was expected to be very small in the overall background composition.

**Table 9.3:** Comparison of overall MC prediction with QCD-EM enriched events for 1 fb<sup>-1</sup> for the EBEE category.

|                                                   | EBEE ( $m_{\gamma\gamma} > 320 \text{ GeV}$ ) |                            |
|---------------------------------------------------|-----------------------------------------------|----------------------------|
|                                                   | Iso <sub>Ch</sub> < 5 GeV                     | Iso <sub>Ch</sub> < 15 GeV |
| Truth jj-MC events                                | $6^{+3.6}_{-2.4}$                             | $15^{+5.0}_{-3.8}$         |
| Truth jj-weighted MC events                       | $19^{+11.4}_{-7.6}$                           | $40^{+13.2}_{-10.2}$       |
| MC events                                         | $412419 \pm 642$                              | $428446 \pm 655$           |
| Weighted MC events                                | $163 \pm 0.3$                                 | $193 \pm 0.3$              |
| <b>Percentage of jj-events in full MC dataset</b> | $12^{+7.0}_{-4.7} \%$                         | $21^{+6.9}_{-5.3} \%$      |

## 9.2 Estimate of purity fraction for the extended Iso<sub>Ch</sub>-range in data

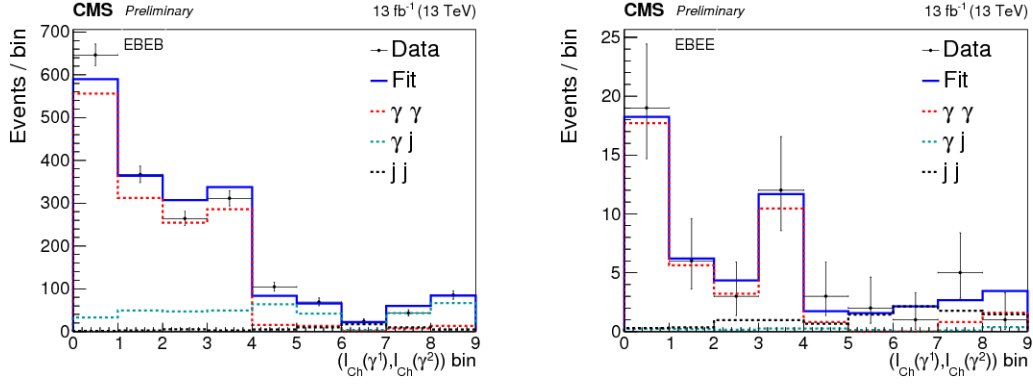
The one-dimensional 'unrolled' shapes of the three  $\gamma\gamma$ -,  $\gamma j$ -, jj-templates in data were fitted with the binned likelihood of Equation 9.1 to determine the magnitude of the background components in the extended Iso<sub>Ch</sub>-range. Due to the limited statistics of the QCD-EM Monte-Carlo sample, no jj-Iso<sub>Ch</sub>-templates could be constructed in MC and also the jj-Iso<sub>Ch</sub>-distribution in MC truth could not be evaluated. The fit in MC was therefore only performed with two components, determining  $\tilde{f}_{\gamma\gamma}$  and  $\tilde{f}_{\gamma j}$ .

The sum of the final fractions  $\tilde{f}_{\gamma\gamma}$ ,  $\tilde{f}_{\gamma j}$  (and  $\tilde{f}_{jj}$ ) for each  $m_{\gamma\gamma}$  bin was constrained to 1. The parametrization of the coefficients was defined recursively to improve the stability of the fit:

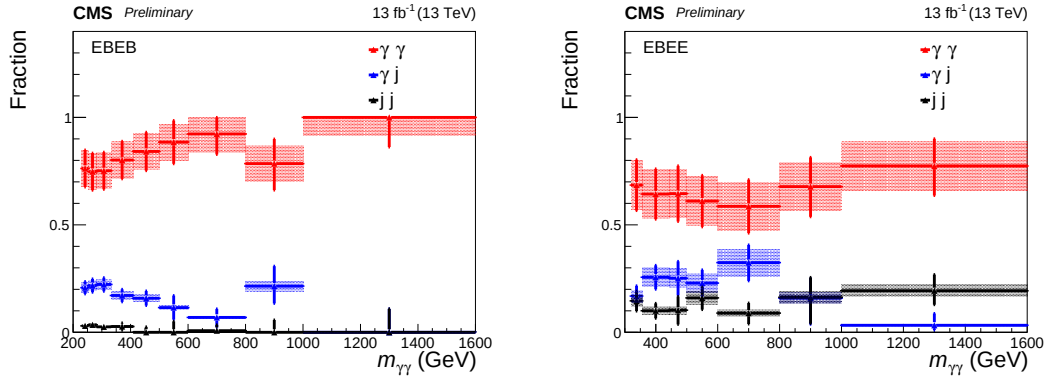
$$L(\text{data}|c_1, c_2, c_3) = c_1 \cdot \text{PDF}_{\gamma\gamma} + (1 - c_1) \cdot (c_2 \cdot \text{PDF}_{\gamma j} + (1 - c_2) \cdot c_3 \cdot \text{PDF}_{jj}) \quad (9.2)$$

Two examples fits in data for the lowest  $m_{\gamma\gamma}$  bin in EBEB and the highest  $m_{\gamma\gamma}$  bin in EBEE are shown for illustration in Figure 9.10, the rest of the fits can be found in the appendix in Figure A.5 and A.6.

The first four bins give an estimate of the  $\gamma\gamma$ -component, the last five bins are described by the  $\gamma j$ -component, which stays rather flat throughout the spectrum. The jj-component is nearly zero in all bins. The result of the fits are shown in Figure 9.11, the purity is shown with the systematical error (full area) and the total error (lines). These are not the final results as they still present the background fractions for the extended Iso<sub>Ch</sub>-range and therefore a lower  $\gamma\gamma$ -component than for the signal region. Since the shapes of the



**Figure 9.10:** Example of a fit of the  $\text{Iso}_{\text{Ch}}$ -distributions in data with the three components  $\gamma\gamma$ ,  $\gamma j$ ,  $j j$ -for the lowest  $m_{\gamma\gamma}$  bin ( $230 \text{ GeV} \leq m_{\gamma\gamma} < 253 \text{ GeV}$ ) in EBEB and highest  $m_{\gamma\gamma}$  bin ( $1 \text{ TeV} \leq m_{\gamma\gamma} < 1.6 \text{ TeV}$ ) in EBEE.



**Figure 9.11:** Fraction of the background components for  $\text{Iso}_{\text{Ch}} < 15 \text{ GeV}$  to the overall background in data for EBEB (left) and EBEE (right).

$\gamma j$ - and  $j j$ -templates are both mainly flat versus  $\text{Iso}_{\text{Ch}}$ , the minimization of the likelihood cannot distinguish very well among the two. The  $\gamma j$ - and  $j j$ -component should thus rather be added together to the reducible background fraction. It is visible that the magnitude of the  $\gamma\gamma$ -component rises towards higher  $m_{\gamma\gamma}$  values in EBEB, and stays rather flat for the EBEE category. The  $\gamma\gamma$ -component in the  $800 < m_{\gamma\gamma} < 1000 \text{ GeV}$  bin in EBEB is lower due to the  $\gamma\gamma$  template, which does not describe the observed shape for the first bin as visible in the corresponding figure in Figure A.5. This results also in a higher statistical uncertainty to these background fractions. The fit uncertainty was estimated by asymmetric uncertainties using the MINOS routine of the physics analysis tool for function minimization MINUIT [159]. As shown in Figure 9.11, the  $f_{\gamma\gamma}$  reaches nearly 1 towards higher  $m_{\gamma\gamma}$  values. In this case, the MINOS uncertainty calculation failed and the Clopper-Pearson interval [160] was used for the uncertainty calculation.

The background coefficients have an associated systematic and statistical uncertainty, which are discussed in the following section.

### 9.3 Additional uncertainties on the background component determination

The final background fractions were affected by additional uncertainties of statistical and systematic nature. The statistical limitation of the construction of the Iso<sub>Ch</sub>-templates is assessed in the first part of this section. This is followed by a short description of the systematic uncertainties, which impact the background determination.

#### 9.3.1 Statistical uncertainty of the template

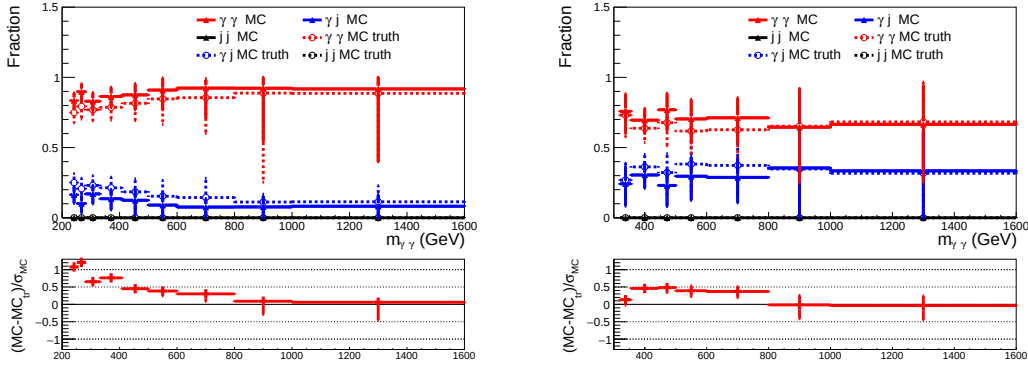
To estimate the uncertainty coming from the finite number of candidates used to populate the template, the 'jackknife resampling' is used [161]. The method can be applied to estimate the variance of statistical estimators and it proceeds as follows: given an estimator  $\Theta$  and a data sample of size 'n', several pseudo-experiments  $s(j)$  are extracted. Each pseudo-sample contains all the events in 's' except for a subset of size 'd'. Each pseudo-experiment is generated such that each event is removed once and only once. A total number of pseudo-experiments 'g', with  $g=n/d$ , can be extracted in this way. The estimator  $\Theta$  is then evaluated on each pseudo-experiment and the corresponding values are labeled as  $q(j)$ . The jackknife variance of the estimator  $\Theta$  is computed as:

$$\text{var}_J(\Theta) = \frac{g-1}{g} \sum_{j=1}^g (\bar{\Theta} - \Theta_j)^2 \text{ where } \bar{\Theta} = \frac{1}{g} \sum_{j=1}^g \Theta_j \quad (9.3)$$

In this study, the jackknife-method was used to estimate the variance of the  $\gamma\gamma$ -fraction and  $\gamma j$ -fraction for each mass bin. For the  $\gamma\gamma$ -templates  $g=10$  pseudo-experiments with 90% of the overall data events were fitted to data with the nominal  $\gamma j$ - and  $jj$ -component. For the  $\gamma j$ -templates the event mixing had to be taken into account. To describe the statistical limitation of the diphoton dataset, taken as input for the mixing, 10 pseudo-experiments were created. Additionally, 10 pseudo-experiments were created from the single photon data set. The  $\gamma j$ -pseudo-datasets were subsequently fitted to data with the nominal  $\gamma\gamma$ - and  $jj$ -templates in data.

The  $jj$ -component was not considered in the uncertainty computation as the number of events were negligible. For each fit, the final  $\gamma\gamma$ -fraction was taken and the variance was calculated according to Equation 9.3. The final variance was taken as an additional statistical uncertainty, describing the statistical limitation of the charged particle flow isolation templates.

The full statistical uncertainty is then the square root of the sum in quadrature of the



**Figure 9.12:** MC closure for  $\text{Iso}_{\text{Ch}} < 15$  GeV for EBEB (left) and EBEE (right).

statistical uncertainty in data and the total ‘jackknife’ uncertainty:

$$\sigma_{\text{tot,stat}} = \sqrt{\text{var}_{\text{JK}} + \text{var}_{\text{stat}}} \quad (9.4)$$

### 9.3.2 Closure in Monte-Carlo dataset

The agreement of the MC truth background prediction with the estimated background fractions in MC is a necessary requirement for the validation of the data-driven method. For both MC datasets only a two-component fit was possible since the QCD-EM enriched MC sample did not contain enough events to build  $m_{\gamma\gamma}$  dependent  $\text{Iso}_{\text{Ch}}$ -distributions in either case.

The  $\text{Iso}_{\text{Ch}}$ -distribution for the extended  $\text{Iso}_{\text{Ch}}$ -range ( $< 15$  GeV) of the true  $\gamma\gamma$ - and  $\gamma j$ -component in MC truth was fitted for the different bins in  $m_{\gamma\gamma}$ . It was then compared to the fit result of the MC  $\text{Iso}_{\text{Ch}}$ -templates. The comparison of the two background fractions estimates is shown with their statistical fit uncertainty in Figure 9.12 for both categories. The bottom figure shows the pull of the  $\gamma\gamma$ -MC purity values. The MC truth and MC fractions agree for most bins within their uncertainties.

For the EBEB category, the background fractions increase towards higher  $m_{\gamma\gamma}$  values. A final culprit for the general overestimation of the  $\gamma\gamma$ -component in MC for EBEB (Figure 9.12) could not be found. For EBEE, the purity is generally lower and fluctuates around a  $\gamma\gamma$ -fraction of about 70 %. The difference in scale of the two  $\gamma\gamma$ -components in MC and MC truth is one of the most dominant systematics and listed in Table 9.4. The method closes within a bias of 7 % for EBEB and 5 % for EBEE. The bias from the closure test was averaged over all mass bins as the statistics of the  $\gamma j$ -samples are limited and statistical fluctuations could have been picked up if the systematics were included per mass bin.

**Table 9.4:** Systematic uncertainties for  $12.9 \text{ fb}^{-1}$  for the  $\gamma\gamma$  fraction of the overall background in an extended charged particle flow isolation range in EBEB and EBEE.

| Absolute systematic uncertainty for $\gamma\gamma$ -fraction in % | Barrel-barrel | Barrel-endcaps |
|-------------------------------------------------------------------|---------------|----------------|
| Bias from MC closure                                              | 6.5           | 5.3            |
| Template MC fit to data                                           | 2.5           | 3.4            |
| Variation of $\text{Iso}_{\text{Ch}}$ bins                        | 2.5           | 4.1            |
| Variation of kNN algorithm parameters                             | 3.9           | 7.4            |
| Change of $\sigma_{i\eta i\eta}$ cut                              | 1.0           | 3.9            |
| <b>Systematic uncertainty</b>                                     | <b>8.4</b>    | <b>11.3</b>    |

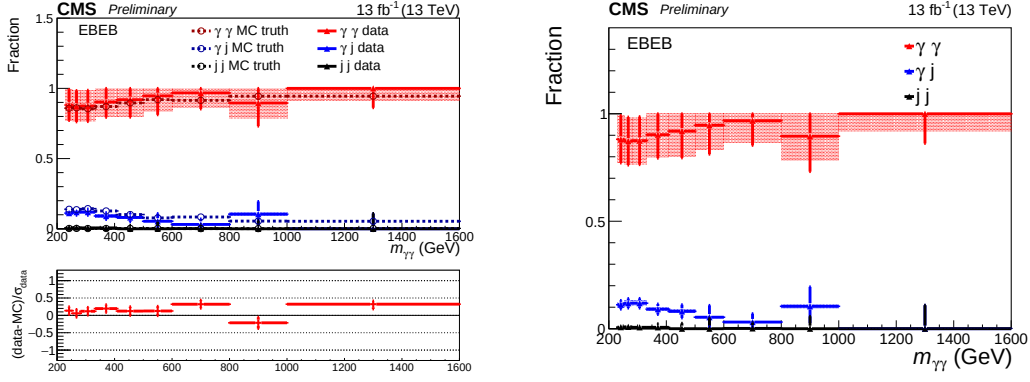
### 9.3.3 Systematic uncertainty on background fractions

Another systematic uncertainty is derived by fitting the MC templates to the data. The difference between data and MC prediction was assumed to be 50 % of this estimated difference and is around 3 %.

As an additional check, the fit in data was performed on only two components, setting the  $\text{jj}$ -component to zero. The results agree within their statistical uncertainty. A full list of all considered systematic uncertainties can be found in Table 9.4. The following systematics were studied in detail:

- the variation of the  $\text{Iso}_{\text{Ch}}$ -bins from nine to four bins for each  $\text{Iso}_{\text{Ch}}$ -axis.
- the correlations between the two photons in the event mixing. They were varied by about 10 % in each direction. The values were changed to 70 % and 90 % for EBEB as well as 50 % and 60 % for EBEE.
- the  $\sigma_{i\eta i\eta}$ -sideband cut. It was tightened to 0.012 for photons in the barrel and 0.035 for photons in the endcaps.

The systematic uncertainty of each event category was chosen to be the arithmetic mean of the systematic uncertainties of all  $m_{\gamma\gamma}$  bins. If the systematic uncertainty would have been taken bin by bin, the high weights of a few MC events could have lead to a non-physical mismatch in the final systematics. The sum in quadrature of all uncertainties leads to a total systematic uncertainty for the  $\gamma\gamma$ -fraction of 8 % for barrel-barrel and 11 % for barrel-endcaps.



**Figure 9.13:** Fraction of the background components for  $\text{Iso}_{\text{Ch}} < 5$  GeV to the overall background in MC (left) and in data (right) for EBEB.

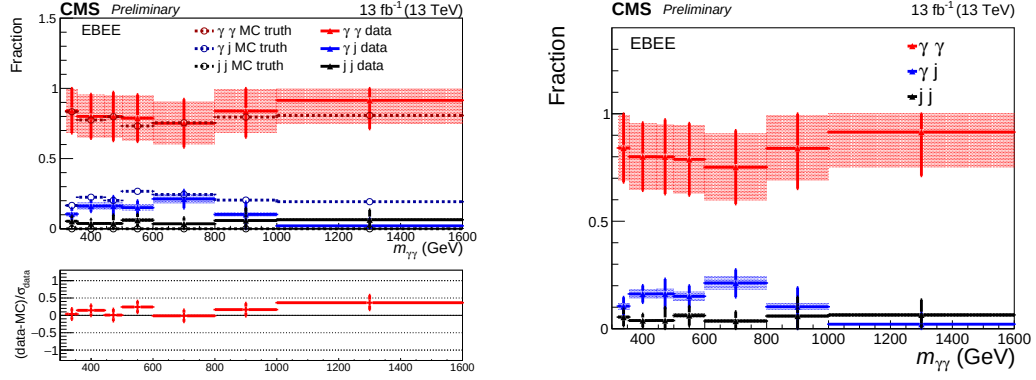
## 9.4 Extrapolation of background fractions to the signal region

The goal of this study is the background composition determination of this analysis. For this estimate, the fractions of the three components in the signal region ( $\text{Iso}_{\text{Ch}} < 5$  GeV) have to be known. So far, the background fractions in the extended charged particle flow isolation range ( $\bar{f}(\text{Iso}_{\text{Ch}} < 15$  GeV)) were determined, since the relaxed  $\text{Iso}_{\text{Ch}}$ -cut gives a better description of the fake photons according to Figure 9.1. To estimate the background fraction in the signal region, the background fractions  $\bar{f}(\text{Iso}_{\text{Ch}} < 15$  GeV) were taken and multiplied by the ratio of the integral of the respective component divided by the full background PDF:

$$f_{\text{sigRegion}} = f_{\text{fullRegion}} \cdot \frac{\int_{\text{sigRegion}} \text{PDF}_f}{\int_{\text{sigRegion}} \text{PDF}_{\text{full}}} \quad (9.5)$$

The results are shown in Figure 9.13 and Figure 9.14 for EBEB and EBEE respectively. The purity is shown with the systematic uncertainty (full area) and the total uncertainty (lines). The background fractions of the  $\gamma\gamma$ -component with their statistical and total uncertainties are summarized in Table A.6 of the appendix. The fraction of the irreducible background is higher than for the extended charged particle flow isolation range, since many fake photons are rejected by the  $\text{Iso}_{\text{Ch}} < 5$  GeV cut. It is around 90 %, increasing to a percentage above 95 % for higher  $m_{\gamma\gamma}$  values in EBEB, and 80 %, increasing to over 85 % for higher  $m_{\gamma\gamma}$  values in EBEE.

The statistical uncertainty of the background fractions in the signal region is the propagated uncertainty of the statistical uncertainty of the fractions of the full range and the jackknife uncertainty. Since the systematic uncertainty is assumed to be flat, it can be



**Figure 9.14:** Fraction of the background components for  $\text{IsoCh} < 5$  GeV to the overall background in MC (left) and in data (right) for EBEE.

calculated for the background fractions in the signal region by propagating the uncertainty from the full range. The propagation of the uncertainties is based on Equation 9.5 and underestimates the uncertainties, since the uncertainty on the integral in the nominator could not be derived. Furthermore, the uncertainty of the integral of the denominator cannot be derived if the  $\tilde{f}_{\gamma j}$  or  $\tilde{f}_{jj}$  component is absent in the signal region. Thus, the uncertainties of the background fractions the last bin in EBEB are underestimated.

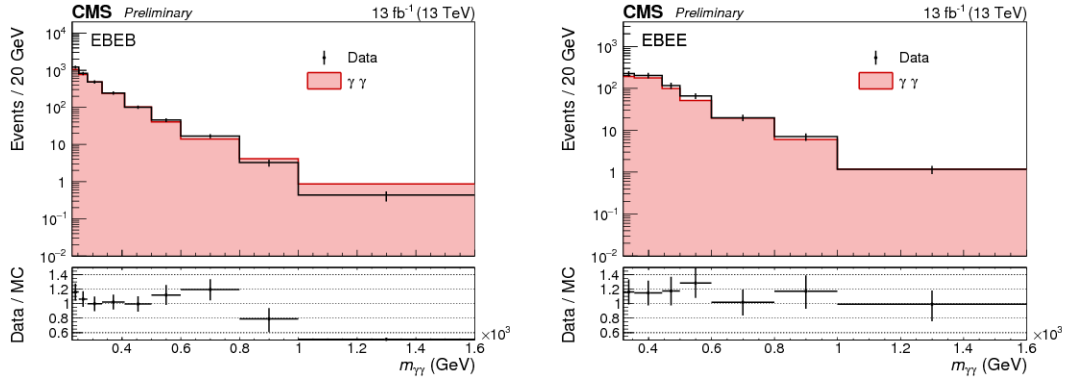
This extrapolation will be replaced by an extended likelihood fit in the future. The study could not be finished by the time of this thesis, but is discussed in the outlook of Part I of this dissertation.

## 9.5 Comparison between the measured and predicted $\gamma\gamma$ -component

Using the results of the parametric fits described above, the mass spectrum of the irreducible  $\gamma\gamma$ -background component can be extracted from data. It is the product of  $\tilde{f}_{\gamma\gamma}$  and the number of events observed in each of the  $m_{\gamma\gamma}$  bins:

$$N_{\text{data}}^{\gamma\gamma}(\text{bin}) = \tilde{f}_{\gamma\gamma} \times N_{\text{data}}(\text{bin})$$

The resulting spectrum was compared to the expectation from perturbative QCD, described in Section 5.3.3. The result of the comparison is reported in Figure 9.15. The predictions from perturbative QCD match qualitatively the observation for the EBEB category. The first mass bin shows an under-prediction in MC, while an underfluctuation in data is observed for the two highest  $m_{\gamma\gamma}$  bins. In the last bin, data is nearly a factor two lower compared to the MC prediction. A reason might be the recently discovered inaccuracies in the signal reconstruction induced by the 'gain switch' of the



**Figure 9.15:** Comparison between the predicted and measured  $\gamma\gamma$ -background spectrum. Events in the EBEB (EBEE) category are shown on the left (right).

ECAL electronics system, which was explained in Section 4.4.5 and with respect to this analysis in Chapter 6. If the electronics system switches from a higher amplification to gain-1 or also gain-6, the signal amplitude decreases [162]. This could lead to the strong underfluctuation observed for the highest  $m_{\gamma\gamma}$  bin in EBEB in data.

A small under-prediction is observed for the EBEE, which is still covered by the large uncertainties in data.

# 10

CHAPTER

## Statistical interpretation of the results

This section defines the statistical analysis used to quantify the compatibility of the observed dataset with the predicted background and signal plus background hypotheses. The results were interpreted in terms of modified frequentist limits and the background-only p-value.

### 10.1 Maximum likelihood fit to data

A simultaneous unbinned maximum likelihood (ML) fit to the invariant diphoton mass spectra was performed, for each analysis category and each signal hypothesis (S), respectively:

$$L(\mu, \theta) = \prod_{i=1}^{N_{\text{events}}} [\mu \cdot S(m_i | \theta_S)] + B(m_i | \theta_B) \cdot \text{Poisson}(N_{\text{events}} | N_B + \mu \cdot N_S) \quad (10.1)$$

In this formula, 'B' denotes the SM background model. The signal and background model depend on the mass ( $m_i$ ) of the i-th event and their respective nuisance parameters ( $\theta$ ), which model the systematic uncertainties. The parameter  $\mu$  denotes the signal strength of the considered model.

### 10.2 Statistical hypothesis testing

The standard LHC test statistic  $q(\mu)$  is used:

$$q(\mu) = -2 \ln \lambda(\mu) := -2 \ln \left( \frac{L(\mu \cdot S + B | \hat{\theta}_\mu)}{L(\hat{\mu} \cdot S + B | \hat{\theta})} \right) \quad (10.2)$$

The likelihood in the numerator denotes the tested and therefore fixed signal strength ( $\mu$ ) and the conditional ML estimator ( $\hat{\theta}_\mu$ ). For the denominator, both, the signal strength ( $\mu$ ) and the nuisance parameters ( $\hat{\theta}$ ), are floating and maximize the likelihood fit. The value of  $\lambda$  is between 0 and 1, where the latter denotes a good agreement between the observed data and the hypothesized value of  $\mu$ . Consequently, the higher the value of the test statistic  $q(\mu)$ , the higher the incompatibility between the observed data and the hypothesized signal model with signal strength  $\mu$ .

The discovery of a new diphoton resonance would appear as a localized excess of events. The signal strength need therefore to be equal to (in the case of the background-only hypothesis) or greater than zero.

### 10.3 Background-only p-value

The test statistic  $\tilde{q}(\mu = 0)$  is used to exclude the background-only hypothesis. The test statistic is based on Equation 10.2 and defined as:

$$\tilde{q}(0) = \begin{cases} -2 \ln \lambda(0) & \hat{\mu} \geq 0 \\ 0 & \hat{\mu} < 0 \end{cases} \quad (10.3)$$

The p-value is the probability to obtain  $\tilde{q}(0) > \tilde{q}_{\text{obs}}(0)$  when  $\mu = 0$ :

$$p_\mu = \int_{\tilde{q}_{\mu, \text{obs}}}^{\infty} f(\tilde{q}_\mu | \mu) d\tilde{q}_\mu \quad (10.4)$$

The p-value is the probability to obtain a result with equal or greater incompatibility to the null-hypothesis ( $H_0$ ) than the observation. The smaller the p-value, the higher the confidence in rejecting  $H_0$ , and a threshold for the rejection of  $H_0$  can be defined. The p-value can be transformed to the significance ( $Z$ ), which is defined as:

$$Z = \Phi^{-1}(1 - p)$$

with  $\Phi^{-1}$  being the inverse of the cumulative distribution function of the standard Gaussian distribution [163].

### 10.4 Exclusion limits

Upper exclusion limits on the resonant diphoton production rate under different signal hypotheses were evaluated with the modified frequentist method, which is also known

as the  $CL_s$  method [164, 165]. The hypothesis ( $H_1$ ) is set as the background plus signal hypothesis which is tested against the alternative, background-only hypothesis ( $H_0$ ). For upper limits, the test statistic  $q(\mu)$  of Equation 10.2 is defined as [163]:

$$\tilde{q}_\mu(\mu) = \begin{cases} -2 \ln \lambda(\mu) & \hat{\mu} \leq \mu \\ 0 & \hat{\mu} > \mu \end{cases} \quad (10.5)$$

with the estimated signal strength  $\hat{\mu}$  and the tested signal strength  $\mu$ . Upper exclusion limits result in one-sided confidence intervals. An upward fluctuation in data ( $\hat{\mu} > \mu$ ) is therefore not taken into account for the limit setting of the tested signal hypothesis.

The exclusion limits are set with the modified frequentist method. Two probabilities are defined, one for the signal plus background hypothesis ( $CL_{s+b} = P(\tilde{q}_\mu \geq \tilde{q}_{\mu,obs}|H_1)$ ) and one for the background-only hypothesis ( $CL_b = P(\tilde{q}_\mu \geq \tilde{q}_{\mu,obs}|H_0)$ ). The  $CL_s$  is defined as the ratio of the two probabilities and depends on the tested signal strength  $\mu$ :

$$CL_s = \frac{CL_{s+b}}{CL_b} = \frac{P_{\mu,s+b}}{1 - p_b}$$

The  $CL_s$  value needs to be smaller than a threshold  $\alpha$  to exclude the tested signal model with signal strength  $\mu$  at a confidence level (CL) of  $(1 - \alpha)$ . This threshold was chosen to be 0.05, corresponding to a 95 %  $CL_s$  limit. The above probabilities  $CL_b$  and  $CL_{s+b}$  were calculated for different values of  $\mu$ . All possible  $q_\mu$  are tested until a signal strength is found, which gives a  $CL_s$  value lower than  $\alpha = 0.05$ .

## 10.5 Methods for expected and observed sensitivity

The sensitivity of an analysis is typically reported as the median expected limit and the expected background-only p-value. This analysis employs asymptotic methods based on the theorems of Wilks [166] and Wald [167], valid in the limit of a large sample size. The distribution of the test statistic can be described as a non-central chi-square distribution with one degree of freedom [163]. With this approximation, the significance of the expected signal strength  $\mu$  is:

$$Z_\mu = \Phi^{-1}(1 - p_\mu) = \sqrt{q_\mu}$$

Another important simplification for the calculation of the expected sensitivity are Asimov datasets [163]. The Asimov dataset is a representative replacement of an ensemble of simulated pseudo-datasets. Its ML estimates of all parameters correspond to their expectation values, which are the medians of their respective distributions.

The validity of the above described methods was verified for the expected significance of

a  $2\sigma - 5\sigma$  discovery and the median expected exclusion limits for an integrated luminosity of 5 and  $10 \text{ fb}^{-1}$  [168, 169]. For both cases, the results of the asymptotic methods were tested against the estimated sensitivity employing 100,000 pseudo-experiments. The median expected exclusion limits agreed within 10 % for the narrow width hypothesis ( $\Gamma_X/m_X = 1.4 \times 10^{-4}$ ) and within a few percents for the large width hypothesis ( $\Gamma_X/m_X = 5.6 \times 10^{-2}$ ). The validity of asymptotic methods was also tested for the background-only p-value of a statistical fluctuation at  $m_X = 750 \text{ GeV}$ . An agreement within 10 % was found.

# 11

## CHAPTER

# Background model

The background model was determined by an unbinned maximum likelihood fit to the invariant diphoton mass spectrum in data. A data-driven technique was chosen to have a robust background model. Possible inaccuracies, especially for high masses, were quantified by a method detailed in the following.

The choice of the functional form determines the accuracy of the background prediction and the sensitivity of the analysis. It was estimated by the following MC-driven procedure:

- the true underlying distribution  $h(m_{\gamma\gamma})$  was constructed from MC events in  $m_{\gamma\gamma}$ .
- unbinned pseudo-datasets  $t_i$  were extracted from  $h(m_{\gamma\gamma})$ . The total number of events was determined by a Poisson distribution whose mean was set equal to the observation in data.
- an Ansatz functional form  $g(m_{\gamma\gamma})$  was chosen to parametrize the background. The tested functional forms were able to describe a falling distribution in a double logarithmic spectrum. These families of functions were chosen as the signal would show as a localized excess on top of a continuum SM background.
- an unbinned maximum likelihood fit determined  $\hat{g}_i(m_{\gamma\gamma})$  for each of the pseudo-experiments.
- the number of events predicted by  $\hat{g}_i(m_{\gamma\gamma})$  was compared to the true value prediction  $\int_w h(m_{\gamma\gamma}) dm_{\gamma\gamma}$  in several mass test regions  $w_j$ . To quantify the agreement, pull test statistics were constructed as:

$$p_i^j = \frac{N_{\hat{g}_i}^{w_j} - N_h^{w_j}}{\sigma(N_{\hat{g}_i}^{w_j})}$$

where  $\sigma(N_{\hat{g}_i}^{w_j})$  accounted for both normalization and shape uncertainties on  $\hat{g}_i$ .

The parametrization  $g(m_{\gamma\gamma})$  was considered accurate, when the following relation applied:

$$b^j = |\text{median}(p_i^j)| < 0.5 \quad (11.1)$$

The threshold of  $b^j = 0.5$  signifies that the uncertainty on the mean number of estimated background events to be underestimated by at most 10 %:

$$\sqrt{\sigma_{\text{stat}} + \sigma_{\text{stat}} \cdot (0.5)^2} \approx 1.10 \cdot \sigma_{\text{stat}} \quad .$$

Including only the statistical uncertainty  $\sigma(N_{\hat{g}_i}^{w_j})$ , the criterion of Equation 11.1 could not be met for any of the tested background shapes. The uncertainty in the denominator of the pull test statistics is increased by an additional uncertainty, the bias term  $\beta_{I(w_j)}$ :

$$\tilde{p}^{ij} = \frac{N_{\hat{g}_i}^{w_j} - N_h^{w_j}}{\sqrt{\sigma^2(N_{\hat{g}_i}^{w_j}) + \beta_{I^2(w_j)}}} \quad (11.2)$$

The chosen functional form which gave the least bias was:

$$g(m_{\gamma\gamma}) = m_{\gamma\gamma}^{a+b \log(m_{\gamma\gamma})} \quad . \quad (11.3)$$

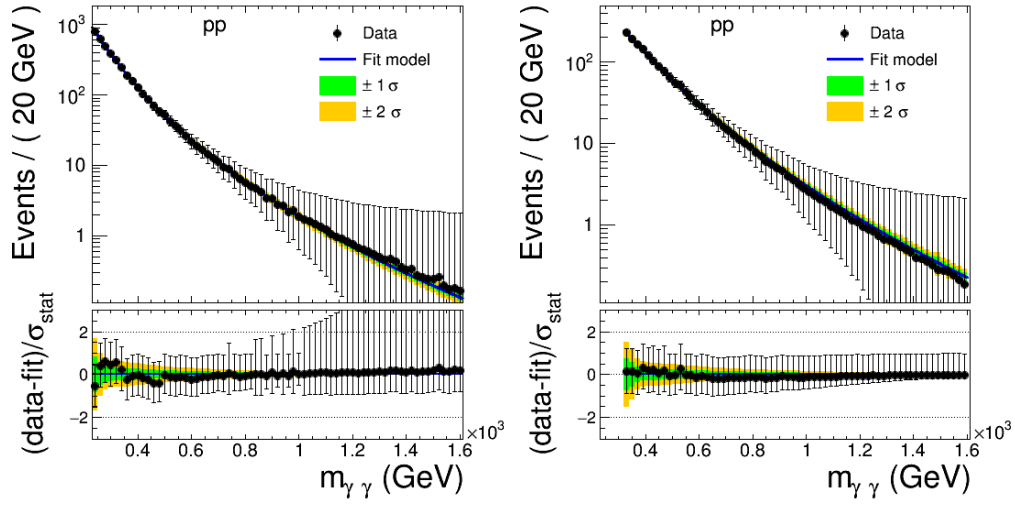
In the statistical analysis, the coefficients 'a' and 'b' were maximized by a likelihood fit of  $m_{\gamma\gamma}$  in data, for each event category and each dataset separately. The coefficients entered the hypotheses tests as unconstrained nuisance parameters and are of statistical nature.

The size of the background mismodeling entered the hypothesis test as the only systematic uncertainty of the background model. The shape of this additional bias was assumed to have a similar form as the signal PDF ( $s(m_{\gamma\gamma})$ ) and was therefore modeled as a Gaussian of mean zero and with a width, that reflected the size of the bias. It was added to the background description via the following equation in which  $N_{\text{bkg}}$  ( $N_\beta$ ) are the number of background (bias) events:

$$\begin{aligned} \tilde{g}_{\text{sig}}(m_{\gamma\gamma}|\theta_\beta) \cdot \text{PDF}(\theta_\beta) = \\ \left( \frac{N_{\text{bkg}} - \theta_\beta N_\beta(\text{sig})}{N_{\text{bkg}}} g(m_{\gamma\gamma}) + \frac{\theta_\beta N_\beta(\text{sig})}{N_{\text{bkg}}} s(m_{\gamma\gamma}) \right) \cdot \text{Gauss}(\theta_\beta|0, N_\beta(\text{sig})) \end{aligned} \quad (11.4)$$

The bias term  $\beta(m_{\gamma\gamma})$  was chosen such that the integral of the bias term was equal to the FWHM (Full Width Half Maximum) of the tested signal shape:

$$N_\beta(\text{sig}) = \int \beta(m_{\gamma\gamma}) \cdot s(m_{\gamma\gamma}) dm_{\gamma\gamma} \sim \beta(m_{G,S}) \cdot \text{FWHM}(\text{sig}) \quad .$$



**Figure 11.1:** Fit to the  $\gamma\gamma$  MC spectrum, for the EBEB (left) and for the EBEE category (right) with the background parametrization  $g(m_{\gamma\gamma}) = m_{\gamma\gamma}^{a+b \log(m_{\gamma\gamma})}$ . The mass window up to 1.6 TeV is shown. The statistical uncertainty is reflecting the expected uncertainty in data for  $10 \text{ fb}^{-1}$ . The fit uncertainties shown account for shape and normalization uncertainties only and are not used in the bias study [149].

The results on the accuracy of the background model for the first public result at 13 TeV can be found in Ref. [170]. It was newly evaluated for the 2016 dataset, targeting an integrated luminosity of  $10 \text{ fb}^{-1}$ . The recent results are detailed in the following section.

## 11.1 Accuracy of the background prediction

The dominating background source of this analysis is the irreducible diphoton SM background. The true underlying distribution  $h(m_{\gamma\gamma})$  of the diphotons events was therefore chosen to only consist of prompt  $\gamma\gamma$  events. The distribution, covering a range of  $60 \text{ GeV} < m_{\gamma\gamma} < 13 \text{ TeV}$  was simulated by the SHERPA 2.1 event generator. The used MC samples are listed in Table 5.2. The leading-order cross-section was scaled by a factor of 1.4 to take into account higher order corrections. The resulting predicted background model and its fit with the functional form of Equation 11.3 is shown in Figure 11.1.

This approach might however not have given the true underlying distribution to full accuracy. To assess a possible systematic bias in modeling  $h(m_{\gamma\gamma})$ , several variations of the spectrum were taken into account. The above described procedure was performed for each of the following modifications:

- the  $m_{\gamma\gamma}$  spectrum as predicted by the SHERPA 2.1 MC (“default”).

| category | $m_{\gamma\gamma}$ range | $\beta(m_{\gamma\gamma})/L$ (fb/ GeV)                                                       |
|----------|--------------------------|---------------------------------------------------------------------------------------------|
| EBEB     | $> 230$ GeV              | $0.1 \times m_{\gamma\gamma}^{(2.2-0.4 \times \log(m_{\gamma\gamma}))}$                     |
| EBEE     | $> 320$ GeV              | $0.01 \times \left(\frac{m_{\gamma\gamma}}{600 \text{ GeV}}\right)^{-5} + 2 \times 10^{-6}$ |

**Table 11.1:** Bias parametrization  $\beta$  divided by the integrated luminosity for the two analysis categories.

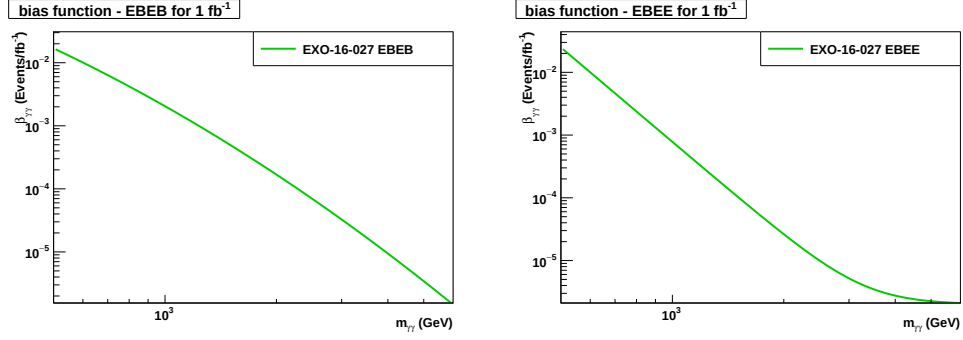
- the  $m_{\gamma\gamma}$ -dependent k-factor from Chapter 5.3.3 was added to the leading-order SHERPA 2.1 prediction to take into account higher order corrections up to NNLO (“pNNLO”).
- the contribution from the reducible background was estimated and added to the leading-order SHERPA 2.1 prediction. Its approximate fraction was taken from the results of the 2015 dataset (“pFakes”).
- one further spectrum was generated, subtracting the k-factor from the default MC spectrum (“mNNLO”).

For all of these  $h(m_{\gamma\gamma})$  spectra, three sets of test regions  $w_j$  with different spacings in  $m_{\gamma\gamma}$  were considered:

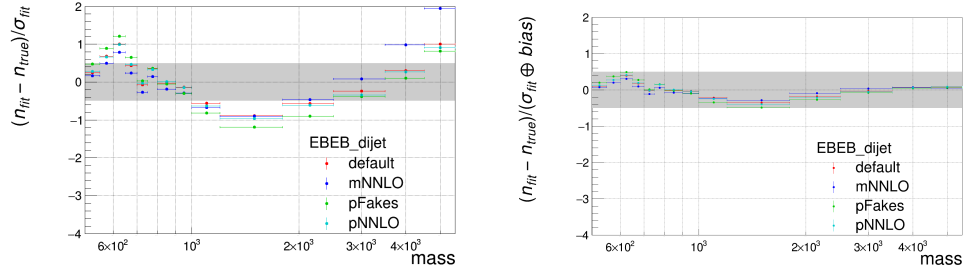
- with a relative bin width of 5 % with respect to the central  $m_{\gamma\gamma}$  bin value, listed in Table A.3 in the appendix.
- with a relative bin width of 10 % of the central  $m_{\gamma\gamma}$  bin value, listed in Table A.4 in the appendix.
- a third set with a bin width of 50 GeV up to  $m_{\gamma\gamma} = 800$  GeV and with increasing bin widths for higher  $m_{\gamma\gamma}$  values. The exact bin widths are listed in Table A.5 in the appendix.

A bias parametrization  $\beta$  which fulfills Equation 11.1 for all above MC spectra  $h(m_{\gamma\gamma})$  and test regions  $w_j$  had to be found. The  $\beta$  parametrization is reported in Table 11.1 and illustrated in Figure 11.2.

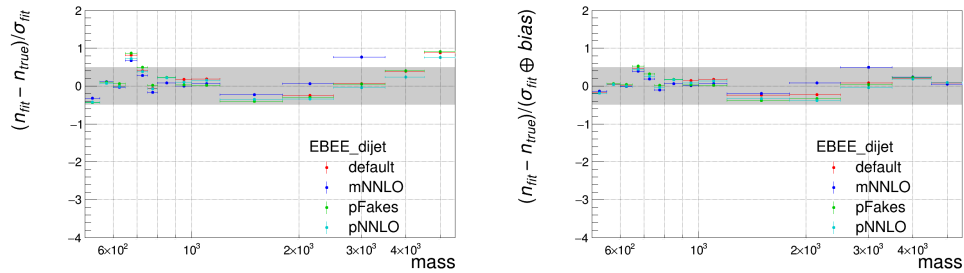
The median of the pull and modified pull of the default test region of Table A.5 can be found in Fig. 11.3 (Fig. 11.4) for the EBEB (EBEE) category, respectively. The results for the set of test regions with a 5 % and 10 % width are shown in Fig. A.1 – Fig. A.4 in the appendix. The chosen bias term parametrization covered all MC shape variations and different sets of test regions. Its magnitude is roughly the one of the one standard deviation bands in Fig 8.1.



**Figure 11.2:** Comparison of the bias parametrization  $\beta$  divided by the integrated luminosity, obtained for the published results of Ref. [1]. Left and right figures show the EBEB and EBEE categories respectively [149].



**Figure 11.3:** Median of the pull ( $p$ ) and modified pull ( $\tilde{p}$ ) for all considered test regions according to Tab. A.5 for EBEB. Different datasets correspond to different MC shape variations as specified in the text [149].



**Figure 11.4:** Median of the pull ( $p$ ) and modified pull ( $\tilde{p}$ ) for all considered test regions according to Tab. A.5 for EBEE. Different datasets correspond to different MC shape variations as specified in the text [149].

| Signal hypothesis |                    | $\frac{N_\beta}{\varepsilon \cdot A \cdot L}$ (fb) |      | Signal hypothesis |                    | $\frac{N_\beta}{\varepsilon \cdot A \cdot L}$ (fb) |      |
|-------------------|--------------------|----------------------------------------------------|------|-------------------|--------------------|----------------------------------------------------|------|
| $m_G$ (GeV)       | $\Gamma_X/m_X$ (%) | EBEB                                               | EBEE | $m_G$ (GeV)       | $\Gamma_X/m_X$ (%) | EBEB                                               | EBEE |
| 500               | 5.6                | 2.54                                               | 6.75 | 2000              | 5.6                | 0.04                                               | 0.04 |
| 750               | 5.6                | 0.94                                               | 1.71 | 3000              | 5.6                | 0.01                                               | 0.04 |
| 1000              | 5.6                | 0.43                                               | 0.59 | 4000              | 5.6                | 0.004                                              | 0.07 |
| 1500              | 5.6                | 0.12                                               | 0.15 |                   |                    |                                                    |      |

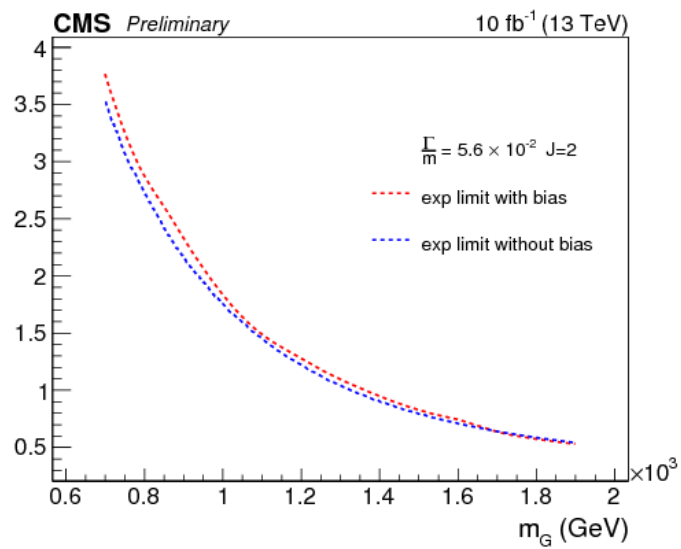
**Table 11.2:** Equivalent cross-section of the bias uncertainty for the widest signal hypothesis  $\Gamma_X/m_X = 5.6 \times 10^{-2}$  tested in the analysis for  $J = 2$  [149].

### 11.1.1 Effect of the bias term on the analysis sensitivity

The size of the background mismodeling for the  $12.9 \text{ fb}^{-1}$  dataset is detailed in this section. The equivalent cross-sections of  $N_\beta(\text{sig})$  for the widest mass hypotheses ( $\Gamma_X/m_X = 5.6 \times 10^{-2}$ ) of this search are reported in Table 11.2. Further studies, aiming to quantify the accuracy of the background model can be found in the appendix of Ref [149].

The bias term is included as a nuisance parameter of the background model in the hypothesis test. The impact of the bias term on the analysis sensitivity was studied by including or removing it from the background model. Two metrics were considered: the expected 95 %  $\text{CL}_s$  on the signal strength for different RS-graviton masses  $m_G$ , as well as the expected significance for a mass of  $m_G = 750 \text{ GeV}$  with a cross-section of  $\sigma = 7 \text{ fb}$ . Both quantities were computed, using frequentist statistics in the asymptotic approximation and assuming an integrated luminosity of  $10 \text{ fb}^{-1}$ .

A comparison of the median expected limit for the largest width RS-graviton hypothesis is shown in Figure 11.5. With regard to the expected significance, the mass hypotheses for which the effect is largest were the widest ones ( $\Gamma_X/m_X = 5.6 \%$ ) at the low end of the search region ( $m_G \sim 500 - 800 \text{ GeV}$ ). In this range, a 5 – 15 % worsening of the analysis sensitivity was estimated. The expected significance for a mass of  $m_{\gamma\gamma} = 750 \text{ GeV}$  was reduced by up to 3 % for the narrowest and largest signal width hypotheses. The impact of the bias on the expected sensitivity decreases for higher mass hypotheses. For the narrow width (largest width) hypothesis the effect was at most 1 % for masses above 1 TeV (1.6 TeV).



**Figure 11.5:** Comparison of the median expected limit for the largest width and spin-2 hypothesis in the mass range of  $700 \text{ GeV} < m_{\gamma\gamma} < 2 \text{ TeV}$  [149].



# 12

CHAPTER

## Signal model

For the first published results with  $3.3 \text{ fb}^{-1}$ , a non-parametric signal model was used for the interpretation [12]. In this approach, the theoretical mass and width of the resonant signal are described by histograms. For the updated results with an integrated luminosity of  $16.2 \text{ fb}^{-1}$ , the signal was defined by a parametric model [1], in which the resonance mass and the signal width are parametrized by an analytic function. The change allowed a finer scan in mass around interesting points without generating a large number of signal models. For both models, the shape of the signal as a function of the diphoton invariant mass was modeled by the convolution of the intrinsic shape of the hypothetical resonance with the CMS detector response.

The theoretical signal line shape was simulated by the leading-order PYTHIA 8.2 event generator for a grid of mass points, listed in Chapter 5.3. For the parametric model, these MC histograms were fitted with a double-sided crystal ball function. This choice of functional form was verified by fitting the theoretical signal line shape also with a relativistic Breit-Wigner (BW) function. The BW function is the theoretical prediction of a resonance with mean  $m_X$  and natural width  $\Gamma_X$ . It describes the theoretical signal line shape well, except for high mass signals with large couplings. These signals show a pronounced off-shell tail due to the large gluon-gluon PDF and the BW approximation cuts off the signal around  $10 \times \Gamma_X$ . The fit of the double-sided CB and the BW agreed within their uncertainties and the former was taken for the subsequent convolution with the detector response.

The detector response was taken from fully simulated signal samples, listed in Chapter 5.3 and the energy resolution corrections of Chapter 6 were applied. This detector response was fitted by a double-sided crystal ball function. The parametric detector response was then convoluted with the parametric description of the theoretical signal line shape. The mass resolution of the convoluted signal shape was defined as the FWHM of the peak divided by 2.35. It is about 1 % (1.5 %) for the EBEB (EBEE) category.

For the former non-parametric description, the different widths of the theoretical signal line shape were instead described by a binned histogram. For these histograms and the detector response, taken from fully simulated signal samples, a 'moment morphing' technique [171] was used to interpolate among the available points.

In order to determine the signal normalization, the efficiency of the final event selection (see Chapter 5) was combined with the kinematic acceptance as shown in Figure 12.1. The total combined efficiency and acceptance ( $\epsilon \times A$ ) for a magnetic field configuration of  $B = 3.8$  T varies between 0.5 – 0.7 (0.6) for the spin-2 (spin-0) model. The EBEB category has a higher sensitivity than the EBEE category and contributes to the overall  $\epsilon \times A$  with more than 50 % for lower  $m_X$  values and up to 85 % for high  $m_X$  values. Since the diphoton selection efficiency stays flat over the  $m_{\gamma\gamma}$  spectrum (see Figure 5.8), any visible trends are mainly driven by the signal acceptance.

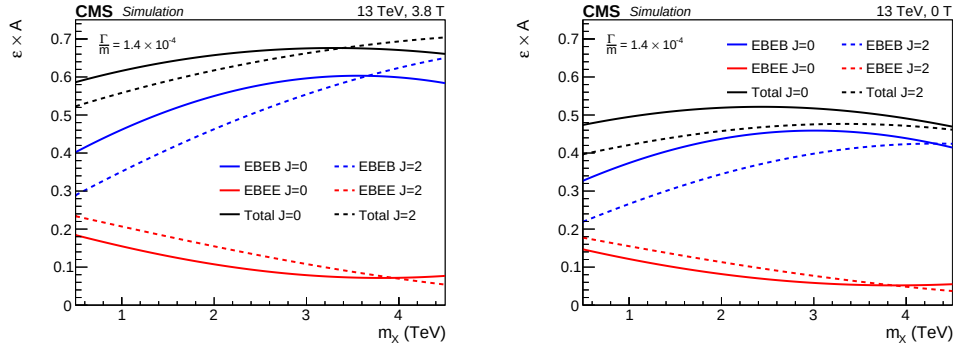
The acceptance of the spin-0 signal model stays mostly flat over the  $m_X$  spectrum, whereas for the spin-2 signal it rises with higher  $m_X$  values. This can be explained by the  $\cos(\theta_{CS}^*)$  distribution of the two:  $\theta^*$  is the angle of the diphoton rest frame, between the two photons and the Collins-Soper axis, which bisects the beams:

$$\cos(\theta_{CS}^*) = 2 \times \frac{E_2 p_{z1} - E_1 p_{z2}}{m_{\gamma\gamma} \sqrt{m_{\gamma\gamma}^2 + p_{T\gamma\gamma}^2}} \quad (12.1)$$

This distribution changes with the spin of the resonance. The  $|\cos(\theta_{CS}^*)|$  distribution for a spin-0 resonances is expected to be flat, whereas the distribution of spin-2 resonances rises towards higher values. Equation 12.1 shows that the variable is strongly correlated with the pseudorapidity, which is identical to the rapidity ( $y$ ) in the case of photons:

$$y = \frac{1}{2} \ln \left( \frac{E + p_z}{E - p_z} \right) \quad (12.2)$$

The rise in acceptance for the spin-2 resonance as a function of  $m_{\gamma\gamma}$  can therefore be explained by a larger production of forward photons. Finally, the  $\epsilon \times A$  for the spin-0 hypothesis decreases towards high  $m_{\gamma\gamma}$  values. This is due to the production of off-shell signals, which show a decrease in the efficiency due to the selection cuts. This decrease is not visible for the spin-2 resonance since it is produced to 10 % via  $q\bar{q}$  annihilation, which PDFs have a high contribution for high Bjorken scaling variables (see Chapter 2).



**Figure 12.1:** Fraction of events selected by the analysis categories for  $0.5 < m_X < 4.5$  TeV and the narrow width hypothesis  $\Gamma_X/m_X = 1.4 \times 10^{-4}$ . Curves for both spin-0 and RS-graviton resonances are shown, in the left figure for the 3.8 T sample and in the right one for the 0 T sample [12].



# 13

CHAPTER

## Systematics

This brief chapter summarizes the systematic uncertainties included in the subsequent hypothesis test. It is important to note that in this analysis the statistical uncertainties dominated over the systematic ones.

In addition to the bias uncertainty on the background model, described in Chapter 11, uncertainties associated to the signal model were included in the hypothesis test. The uncertainties impacting the signal normalization were assigned to the overall signal yield and were the following:

- **Luminosity uncertainty:** a 6.2 % uncertainty was assigned to the knowledge of the total integrated luminosity for the part of the dataset with  $B = 3.8$  T. This uncertainty was taken from updated beam scan studies, performed after recording the analyzed dataset of  $12.9 \text{ fb}^{-1}$  in 2016 and employing methods described in Ref. [138]. For the  $B = 0$  T dataset, an uncertainty of 12 % was assigned.
- **Parton distribution functions:** a 6 % uncertainty accounted for the variation in the kinematic acceptance of the analysis originating from the use of alternative PDF sets. As described in Chapter 7, the default PDF set is the NNPDF2.3 [140], as alternatives, the MSTW08 [172] and CT10 PDF sets were used [141].
- **Selection efficiency uncertainties:** a 6% uncertainty (3 % per photon) reflected the uncertainty on the data to MC scale factors for  $B = 3.8$  T as detailed in Chapter 5.7. For the  $B = 0$  T dataset, an uncertainty of 16 % was included.
- **Photon energy scale uncertainty:** a 1 % energy scale uncertainty was assigned according to Chapter 6. As described there, this uncertainty was determined by extrapolating the energy scale of very high transverse momentum electrons of  $Z \rightarrow e^+e^-$  events. For the  $B = 0$  T dataset, an additional 1 % uncertainty was assigned to account for possible differences between the energy scales of the 3.8 and 0 T datasets.

- **Photon resolution uncertainty:** a 10 % uncertainty was assigned to the extra smearing on the photon uncertainty. This was estimated by varying the Gaussian energy smearing of  $Z \rightarrow e^+e^-$  events by  $\pm 0.5$  %. The 0.5 % value reflected the statistical uncertainty on the extra smearing term measured in Chapter 6.

The uncertainties on the signal model as well as the bias uncertainty were taken to be fully correlated for the two 13 TeV datasets at  $B = 3.8$  T. For the combination with the 0 T dataset as well as with the 8 TeV datasets, the PDF uncertainty was assumed to be fully correlated. For the photon energy scale uncertainty, a linear correlation of 0.5 was taken for the 0 T dataset as well as for the 8 TeV datasets. In case of the 0 T dataset, all further systematic uncertainties were assumed to be fully correlated. For the combination with the 8 TeV dataset, all other systematic uncertainties were assumed to be uncorrelated.

# 14

CHAPTER

## Results of the search for resonant production of high mass photon pairs

This chapter summarizes the results of the search for a diphoton resonance at 13 TeV and the statistical combination with results obtained at a center-of-mass energy of 8 TeV. For the interpretation of the results, frequentist statistics were used in conjunction with asymptotic formulas as explained in Chapter 10. The search targeted two spin hypotheses:

- spin-0 resonances, produced via gluon-gluon fusion
- spin-2 resonances, benchmarked by the RS-graviton model

For the RS-graviton model, which is the chosen benchmark model for the spin-2 resonance, the width of the resonance is defined by the dimensionless coupling parameter  $\tilde{k}$  as explained in Chapter 3.1. The intrinsic width  $\Gamma_X$  of the resonance with mass  $m_X$  was simulated for three benchmark values:

- $\Gamma_X$  is much narrower than the detector resolution:  $\tilde{k} = 0.01$ .
- $\Gamma_X$  is of the same size as the detector resolution:  $\tilde{k} = 0.1$ .
- $\Gamma_X$  dominates over the detector resolution:  $\tilde{k} = 0.2$ .

For the relative width ( $\Gamma_X/m_X$ ) of the spin-0 resonance this corresponds to

$$\Gamma_X/m_X = \frac{\tilde{k}^2}{1.4} = 1.4 \times 10^{-4}, 1.4 \times 10^{-2} \text{ and } 5.6 \times 10^{-2}$$

as described in Chapter 3.1 and Ref. [76].

## 14.1 Combination with searches for diphoton resonances at 8 TeV

To further improve the sensitivity of the search, the results of the 13 TeV dataset were combined statistically with results obtained by the CMS collaboration at 8 TeV. Two searches for resonant diphoton production were performed with this dataset, employing an integrated luminosity of  $19.7 \text{ fb}^{-1}$ :

- the first one, published in Ref [95], searched for spin-0 and RS-graviton resonances in the mass range of 150 – 850 GeV.
- the second one, presented in Ref [96], focused on RS-graviton searches in the mass range of 500 GeV – 3 TeV.

At each  $m_X$ , the analysis with the most stringent expected 95 %  $\text{CL}_s$  on resonant diphoton production was taken for the final combination. The corresponding expected 95 %  $\text{CL}_s$  exclusion limits as a function of the graviton mass for the narrow width RS-graviton hypothesis is depicted on the left of Figure 14.1. It shows the three analyses entering the combination. For resonance masses below  $m_X = 850 \text{ GeV}$ , the event selection of Ref. [95] entered the combination, for masses above 850 GeV the event selection of Ref. [96] was taken.

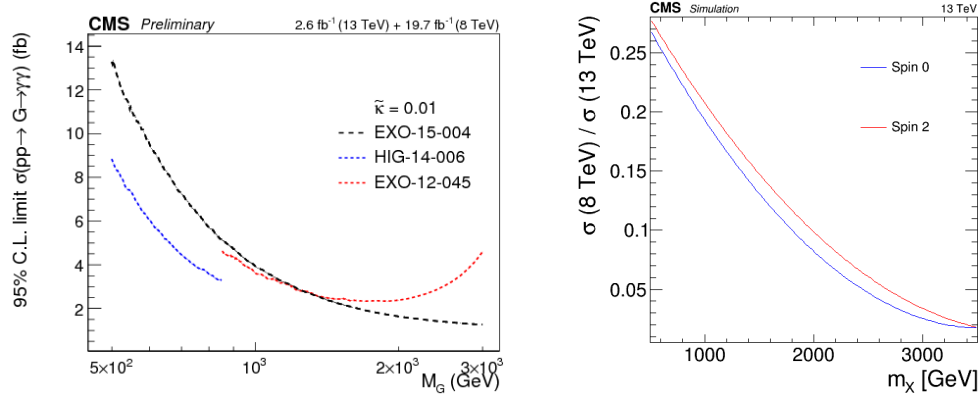
For the combination of the results, the signal production cross-section at 8 TeV had to be scaled to the equivalent cross-section at 13 TeV. The  $\sigma_{8 \text{ TeV}} / \sigma_{13 \text{ TeV}}$  ratio was computed with the PYTHIA 8.2 event generator under the narrow width signal hypothesis and is depicted on the right in Figure 14.1. The uncertainty on this ratio was determined by using alternative PDF sets and found to have a negligible impact on the results.

For the first search [95], the background model was determined with a similar data-driven method as for the search at 13 TeV. This search employed two further categories by dividing the events according to their  $R_9$  value: (EBEB, EBEE)  $\times$  ( $R_9 < 0.94$ ,  $R_9 > 0.94$ ). The background of this analysis was parametrized by:

$$g(m_{\gamma\gamma}) = m_{\gamma\gamma}^{-c} e^{-d \cdot m_{\gamma\gamma}} \quad .$$

The coefficients 'c' and 'd' were determined by a fit on data for each event category and different  $m_{\gamma\gamma}$  intervals were used for each  $m_X$  [12, 95].

The second search [96] used a different approach to determine the background model, which relied on the MC description of the  $\gamma\gamma$ -SM background component. It only analyzed the EBEB category and its statistical treatment was employing Bayesian methods.



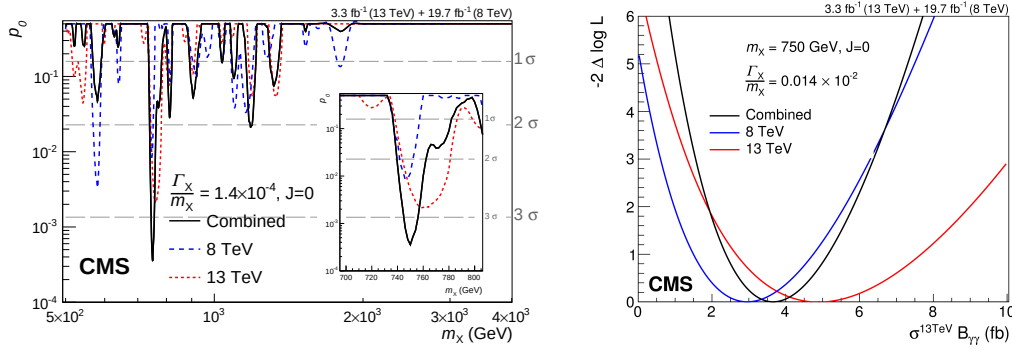
**Figure 14.1:** Left: Expected 95 % CL<sub>s</sub> exclusion limits of the RS-graviton hypothesis for the three analyses entering the combination as a function of the graviton mass. Right: ratio of the spin-0 and spin-2 production cross-section at 8 TeV and 13 TeV as a function of the resonance mass [148, 173].

For the statistical combination with the dataset at 13 TeV, the statistical analysis was repeated using the modified frequentist approach and using the background parametrization and the signal models of the latter. The combined result was obtained by a simultaneous fit to the  $m_{\gamma\gamma}$  spectra in all event categories, assuming a common signal strength modifier for all categories.

## 14.2 Combined results of the 13 TeV dataset with the $3.3 \text{ fb}^{-1}$ and the 8 TeV datasets

In December 2015, the first results on the search for high mass diphoton resonances at 13 TeV were presented, exploring a mass range of 500 GeV – 4.5 TeV with an integrated luminosity of  $3.3 \text{ fb}^{-1}$ . The result is published in Ref. [12]. As mentioned in the introduction, the most significant excess with respect to the background-only hypothesis was observed around a mass of 750 GeV. This excess could not be confirmed as detailed in the subsequent Section 14.3. Due to the interest given to the excess, the combined results of the first 13 TeV dataset with the 8 TeV analyses are highlighted in the following.

The background-only p-value ' $p_0$ ' for the narrow width spin-0 hypothesis is depicted on the left side of Figure 14.2 and shows a local significance of 3.4 standard deviations. The individual contributions from the 8 TeV and 13 TeV datasets are visible and in particular the insert shows that both dataset contribute with a similar weight to the excess at  $m_X = 750 \text{ GeV}$ . As discussed in Chapter 6, it was recently discovered that the non-linearity of the electronics system near the gain saturation is not covered by the newly developed 'multi-fit' electromagnetic signal reconstruction for the dataset at 13 TeV. This leads to an incorrect reconstruction of electromagnetic particles at very



**Figure 14.2:** Left: observed background-only p-values for narrow-width scalar resonances as a function of the resonance mass  $m_X$ , from the combined analysis of the 8 and 13 TeV data. The results for the separate 8 and 13 TeV data sets are also shown. The inset shows an expanded region around  $m_X = 750$  GeV. Right: likelihood scan for the cross-section corresponding to the largest excess in the combined analysis of the 8 and 13 TeV data sets assuming a scalar signal [12].

high energies and is being investigated and corrected. The effect on the 750 GeV excess is however relatively small and the mass scale shifts only by about 1.8 %, which is twice its systematic uncertainty. The worsening of the resolution is still covered by its systematic uncertainty. The overall observed limits and p-values are well within the  $1\sigma$ -uncertainty band with the currently provided energy scale corrections and are therefore presented in this chapter as published in the respective references.

On the right side of Figure 14.2, the likelihood scan for the cross-section at  $m_X = 750$  GeV under the scalar narrow width hypothesis of the two analyses and their combination is depicted. The 8 TeV results were scaled to the cross-sections at 13 TeV according to Chapter 14.1. It verifies that the cross-sections  $\sigma_S^{13\text{ TeV}} \cdot \mathcal{B}_{\gamma\gamma}$  of the two datasets were compatible with each other. The ATLAS collaboration reported for the same mass value a local significance of 3.8 (3.9) standard deviations for the large width spin-2 (spin-0) hypothesis ( $\Gamma_X/m_X = 6.0 \times 10^{-2}$ ) [13].

These quoted local significances do not take the probability into account, that a statistical fluctuation could happen anywhere in the search range and for any of the signal hypotheses. This problem is the so-called 'look elsewhere effect'. By adding these corrections to the local significance, the global significance can be estimated.

### 14.2.1 Global significance

For the 13 TeV analysis, the global significance was computed in the following way:

- an ensemble of background-only pseudo-experiments was generated.

- for each pseudo-experiment, the local p-value was determined for all signal hypotheses and for the full search range. The maximum p-value ( $\max(p_{0,pe})$ ) was extracted per pseudo-experiment (pe) and its corresponding global significance ( $Z_{\text{global},pe}$ ) was computed.
- each global significance per pseudo-experiment was filled in a histogram as a function of the global significance ( $Z$ ).
- the final global significance ( $Z_{\text{gl},\text{obs}}$ ) of an observed excess ( $Z_{\text{obs}}$ ) could then be found by integrating the  $Z_{\text{global},pe}$  distribution from the observed local significance up to the last bin of the distribution:  $Z_{\text{gl},\text{obs}} = \int_{Z_{\text{obs}}}^{Z_{\text{max}}} Z_{\text{global},pe} dZ$

The global significance of the 13 TeV dataset with  $3.3 \text{ fb}^{-1}$  was estimated to be less than one standard deviation.

For the global significance of the 8 and 13 TeV combination a different method had to be utilized. The 8 TeV analysis of Ref. [95] used a sliding window technique and therefore partially overlapping data regions to search for different mass hypotheses in the same mass region. In order to calculate the global significance as above, the fit of the mass spectrum with the sliding window technique would have needed to be repeated for each toy. The realization of this procedure was not trivial and the global significance was instead estimated by asymptotic formulas, using the so-called trial factor. The trial factor gives the ratio of the probability  $P(q(\hat{m}) > c)$  of observing an excess at a certain mass, e.g.  $\hat{m} = 750 \text{ GeV}$ , to the probability  $P(q(m) > c)$  of observing an excess anywhere in the signal region [174]:

$$f_{\text{trial}} = \frac{P(q(\hat{m}) > c)}{P(q(m) > c)} \quad (14.1)$$

where  $P(q(\hat{m}) > c)$  is the tail probability of the maximum of the test statistic,  $q(\hat{m})$ . The test statistic 'q(m)' depends on a nuisance parameter 'm' which exists for the signal hypothesis, for instance the location parameter of a resonance in the  $m_{\gamma\gamma}$  spectrum, but not for the background hypothesis. The distribution of this test statistic 'q(m)' can then be described as a  $\chi^2$  distribution with one degree of freedom [175]. The calculation of the probability of  $q(\hat{m})$  to be above a level 'c', for instance  $3\sigma$ , is normally subject to intensive pseudo-experiment studies. With the above assumptions and according to Ref. [174],  $P(q(\hat{m}) > c)$  can instead be calculated by:

$$\begin{aligned} P(q(\hat{m}) > c) &\leq P(\chi_s^2 > c) + \langle N(c) \rangle \\ &\leq P(\chi_s^2 > c) + \langle N(c_0) \rangle \times \left( \frac{c}{c_0} \right)^{(s-1)/2} e^{-(c-c_0)/2} \end{aligned} \quad (14.2)$$

where the expectation of the number of 'upcrossings' at the level  $c, \langle N(c) \rangle$ , by the process  $q(\hat{m})$  can be replaced by the expectation value  $\langle N(c_0) \rangle$  at a lower level  $c_0$ , e.g.  $c_0 = 0.5$ , plus a correction factor.

The corrective trial factor for the 8 and 13 TeV analysis combination was then estimated in the following way:

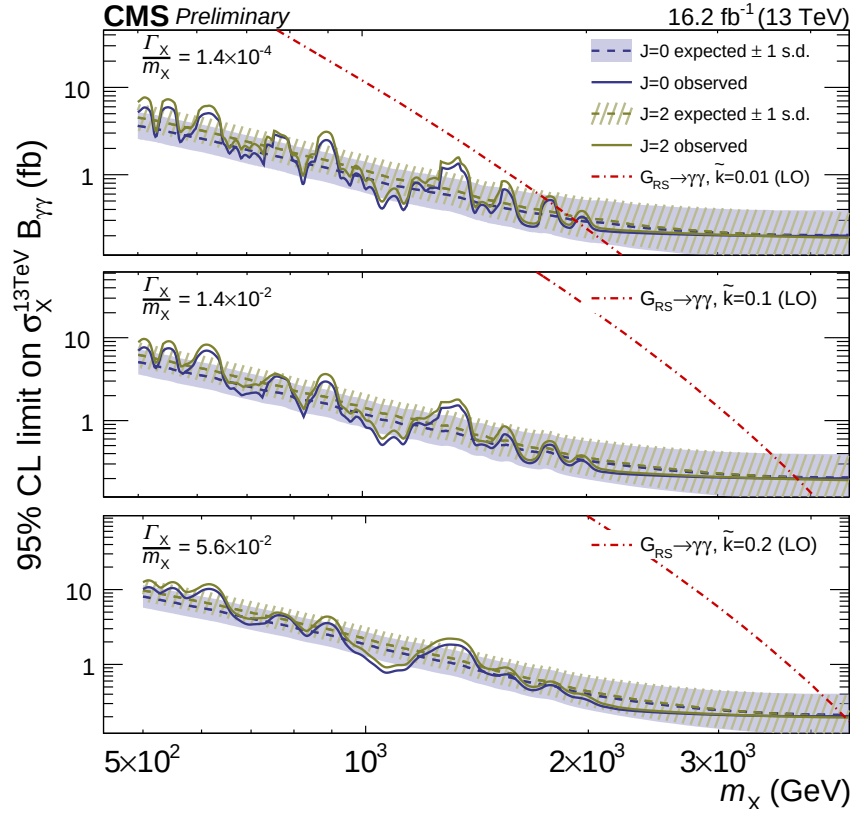
- the probability of observing an excess similar or more significant than what was observed in data for the narrow width hypothesis  $\tilde{k} = 0.01$  was calculated for the 8 and 13 TeV using the method of Ref. [174].
- the  $\max(p_0)$  sampling distribution for the 13 TeV analysis was employed to estimate the additional trial factor emerging from testing all different signal hypotheses. The additional factor was estimated to be around 30% on top of the above trial factor.
- the local p-value of 3.4 standard deviations was corrected by the resulting trial factor of 160.

The probability of observing at least one excess more significant than that in the full search range and among all considered models of this analysis was found to be about 1.6 standard deviations [12].

## 14.3 Search for diphoton resonances at 13 TeV with $16.2 \text{ fb}^{-1}$

### 14.3.1 Combination of the datasets recorded at 13 TeV

The results of the search at 13 TeV employed a dataset of  $16.2 \text{ fb}^{-1}$ , combining the results of the dataset with  $3.3 \text{ fb}^{-1}$  and the one with  $12.9 \text{ fb}^{-1}$ . Since the data-taking conditions were similar and the shapes of the respective  $m_{\gamma\gamma}$  spectra of both datasets agreed within their uncertainties, the same functional form from Equation 11.3 was chosen for both datasets. The normalization coefficients were assumed to be independent. The correlations between the datasets is detailed in Chapter 13. The search range of the 13 TeV dataset covered the mass range of  $500 \text{ GeV} < m_X < 4.5 \text{ TeV}$  and no significant excess was found as detailed in the following.



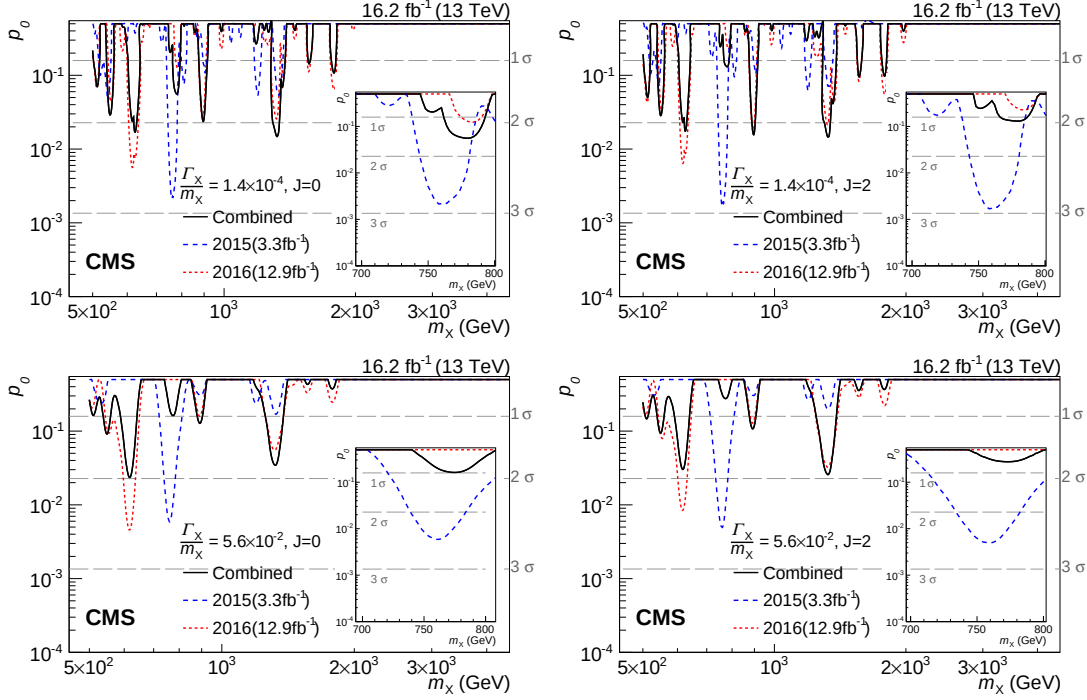
**Figure 14.3:** The 95 %  $\text{CL}_s$  upper limits on the production of diphoton resonances as a function of the resonance mass  $m_X$ , from the combined analysis of data recorded in 2015 and 2016. The blue-gray (darker) curves and the green (lighter) ones correspond to the scalar and RS-graviton signals, respectively. Solid (dashed) curves represent the observed (expected) exclusion limit. The expected results are shown with their 1 standard deviation dispersion bands. The leading-order RS-graviton production cross-section is shown by the red dot-dashed curves. The results are shown for (upper) a narrow, (middle) an intermediate-width, and (lower) a broad resonance, with the value of the width  $\Gamma_X/m_X$ , relative to the mass, indicated in the legend of each figure [1].

### 14.3.2 Results with the full 13 TeV dataset

The expected and observed 95 %  $\text{CL}_s$  exclusion limits on the product of the production cross-section  $\sigma_X^{13\text{TeV}}$  for scalar and RS-graviton resonances and the branching fraction to two photons ( $\mathcal{B}_{\gamma\gamma}$ ) are reported in Fig. 14.3. RS-graviton signals were excluded for 3.85 and 4.45 TeV for  $\tilde{k} = 0.1$  and 0.2, respectively, employing leading-order PYTHIA 8.2 MC signal samples. For the narrow width hypothesis ( $\tilde{k} = 0.01$ ), graviton masses below 1.95 TeV were excluded, except for the region between 1.75 TeV and 1.85 TeV. The expected and observed 95 %  $\text{CL}_s$  exclusion limits for scalar resonances are comparable.

The background-only p-values for the RS-graviton and a spin-0 resonance for the narrow and largest width hypotheses are depicted in Figure 14.4. They show the largest excess at  $m_X = 1.3$  TeV with a local significance of 2.2 standard deviations for the two

respective narrow width signal hypotheses. The global significance of this excess was found to be less than one standard deviation.



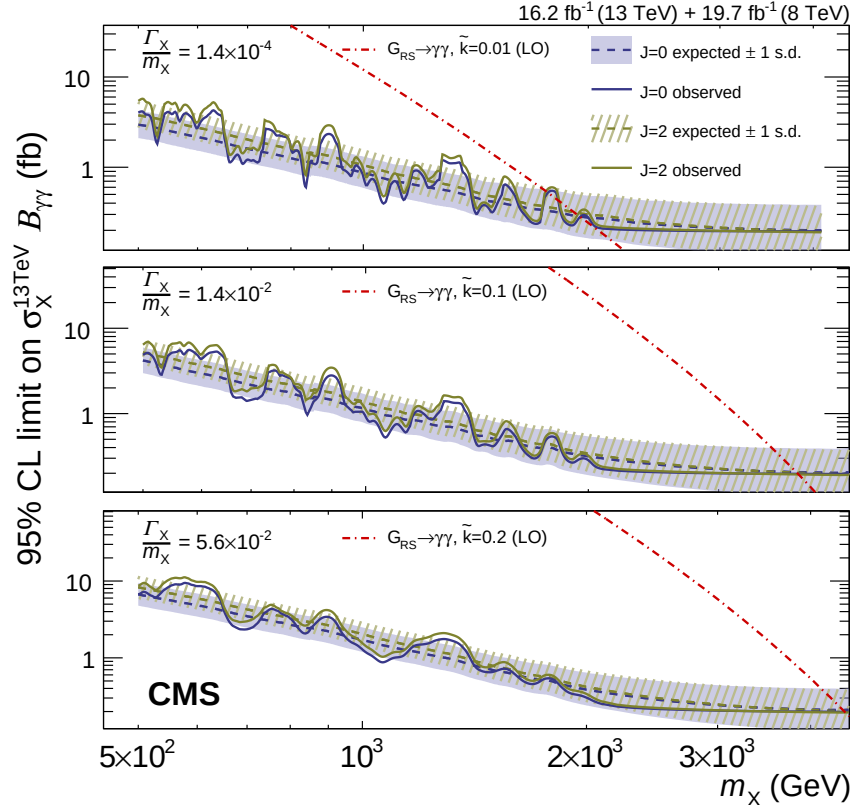
**Figure 14.4:** Observed background-only p-values for resonances with (upper)  $\Gamma_X/m_X = 1.4 \times 10^{-4}$  and (lower)  $5.6 \times 10^{-2}$  as a function of the resonance mass  $m_X$  from the combination of the 2015 and 2016 dataset with  $16.2 \text{ fb}^{-1}$ . The results obtained for the two individual data sets are also shown. The curves corresponding to the scalar and RS-graviton hypotheses are shown in left and right columns, respectively. The insets show an expanded region around  $m_X = 750 \text{ GeV}$  [1].

## 14.4 Combined results of the full 8 TeV and 13 TeV datasets

The expected and observed 95 % CL<sub>s</sub> exclusion limits on the equivalent 13 TeV diphoton resonance production cross section,  $\sigma_{G,S}^{13 \text{ TeV}} \cdot \mathcal{B}_{\gamma\gamma}$ , for the combined analysis are depicted in Figure 14.5 for all studied signal hypotheses of this analysis. For  $m_{\gamma\gamma}$  values below  $m_X < 850 \text{ GeV}$ , Ref. [95] was used, above this value Ref. [96] was employed. Due to the less stringent limit of the latter, a slight shift in the expected limits is visible at  $m_X = 850 \text{ GeV}$ . The comparison with Figure 14.3 shows an improvement of about 10 % for lower masses due to the combination. For masses above 1.5 TeV, the exclusion limits were mainly driven by the sensitivity of the 13 TeV analysis and the benefits of the combination were negligible. The observed exclusion limits remain therefore the ones

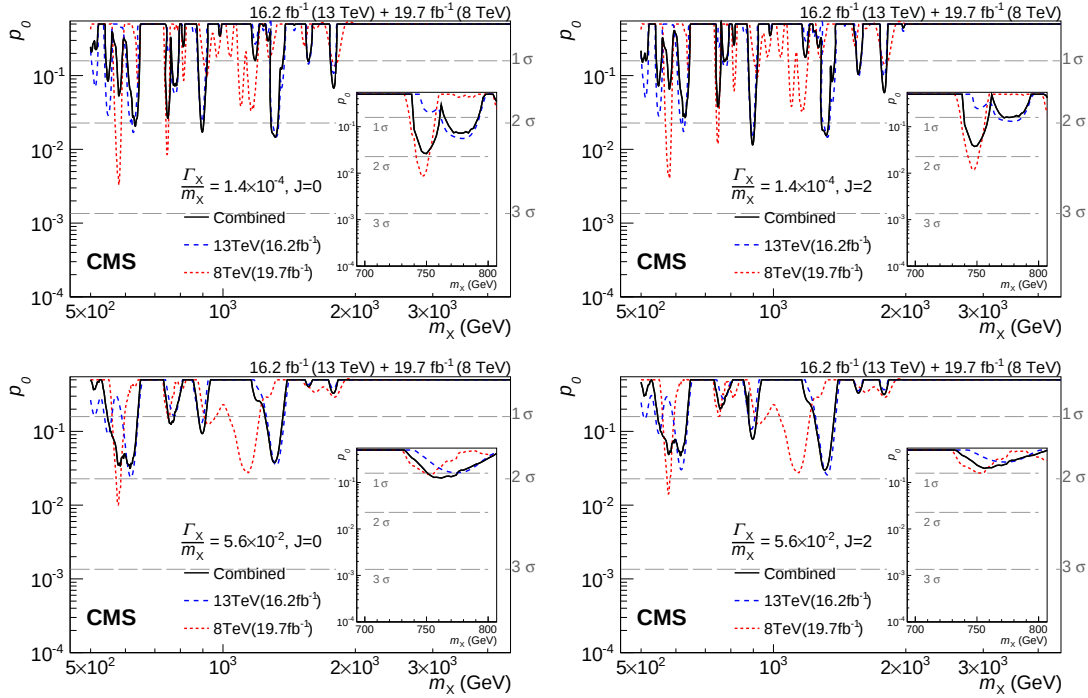
quoted in Chapter 14.3.

The background-only p-value for both spin and the narrow and largest widths hypotheses



**Figure 14.5:** The 95 %  $\text{CL}_s$  upper limits on the production of diphoton resonances as a function of the resonance mass  $m_X$ , from the combined analysis of the 8 and 13 TeV data. The 8 TeV results are scaled by the ratio of the 8 to 13 TeV cross-sections. Exclusion limits for the scalar and RS-graviton signals are given by the gray (darker) and green (lighter) curves, respectively. The observed limits are shown by the solid lines, while the expected limits are given by the dashed lines together with their associated 1 standard deviation uncertainty bands. The leading-order production cross-section for diphoton resonances in the RS-graviton model is shown for three values of the dimensionless coupling parameter  $\tilde{k}$  together with the exclusion upper limits calculated for the corresponding three values of the width relative to the mass,  $\Gamma_X/m_X$ . Shown are the results for (upper) a narrow width, (middle) an intermediate-width, and (lower) a broad resonance [1].

are shown in Figure 14.6. The largest excess with a mass of 850 GeV was observed for the narrow width hypotheses with approximately 2.2 standard deviations. The corresponding global significance was estimated to be less than one standard deviation. The excess at  $m_X = 750$  GeV for a subset of the 13 TeV dataset as reported in Chapter 14.2 was reduced to 1.9 standard deviations.



**Figure 14.6:** Observed background-only p-values for resonances with (upper)  $\Gamma_X/m_X = 1.4 \times 10^{-4}$  and (lower)  $5.6 \times 10^{-2}$  as a function of the resonance mass  $m_X$  from the combination of the 8 and 13 TeV data. The results obtained for the two individual data sets are also shown. The curves corresponding to the scalar and RS-graviton hypotheses are shown in left and right columns, respectively. The insets show an expanded region around  $m_X = 750$  GeV [1].

# Summary and prospects

The presented search studies a new energy range of 13 TeV, employing two datasets: a first dataset with  $3.3 \text{ fb}^{-1}$  and a second with  $16.2 \text{ fb}^{-1}$ . The search region for new heavy resonances started at 500 GeV, for which photons with a transverse momentum above 75 GeV were selected. The diphoton invariant mass spectrum was interpreted in terms of spin-0 and spin-2 resonances, which are among others motivated by extended Higgs and RS-graviton models, respectively.

The results at 13 TeV were statistically combined with results obtained at 8 TeV with  $19.7 \text{ fb}^{-1}$ . For the first dataset of  $3.3 \text{ fb}^{-1}$  an excess of 3.4 standard deviations with respect to the background-only hypothesis at a mass of 750 GeV was observed. The significance of this excess decreased to 1.6 standard deviations for the CMS analysis after taking the probability into account to observe such an excess anywhere in the search range and for any of the signal hypotheses. The ATLAS collaboration reported a similar excess of 2.1 standard deviations in their high mass diphoton search around the same mass value of 750 GeV. After analyzing a larger dataset ( $16.2 \text{ fb}^{-1}$  for the CMS collaboration), this excess could not be confirmed by both collaborations.

The production of RS-gravitons can be excluded at a 95 %CL<sub>s</sub> up to 3.85 and 4.45 TeV for  $\tilde{\kappa} = 0.1$  and 0.2, respectively, employing leading-order PYTHIA 8.2 MC signal samples. For the narrow width hypothesis ( $\tilde{\kappa} = 0.01$ ), graviton masses below 1.95 TeV are excluded, except for the region between 1.75 TeV and 1.85 TeV. The expected and observed 95 %CL<sub>s</sub> exclusion limits for scalar resonances are comparable. No significant excess was observed for the larger dataset.

After the disappearance of the 750 GeV diphoton excess and the ICHEP 2016 publication, our analysis group is now 'on the way to new horizons', realizing a new analysis version for spring 2017. The search is now targeting two different goals:

- an improved analysis strategy, employing the full 2016 dataset.
- an extension of the physics scope, including a search for wider resonances and non-resonant signals.

The full 2016 dataset ( $37.82 \text{ fb}^{-1}$ ) is roughly two times larger than the dataset analyzed for ICHEP 2016. This does not improve the sensitivity of the analysis as strongly as for instance the change in center-of-mass-energy from 8 TeV to 13 TeV. However, it will still be an important reference result for this search in the upcoming years. The sensitivity can be further improved by an updated version of the analysis and a few aspects are detailed in the following paragraph.

Since the ICHEP 2016 results, two developments corrected or improved the photon reconstruction. As discussed in Chapter 6, it was recently discovered that the non-linearity of the electronics system near the gain saturation is not covered by the newly developed 'multi-fit' electromagnetic signal reconstruction for the 13 TeV dataset. This leads to an incorrect reconstruction of electromagnetic particles at very high energies and is being investigated and corrected.

Secondly, a larger dataset enables us also to explore a higher  $m_{\gamma\gamma}$  range. With that, the likelihood increases to select high energy photons, for which the ECAL readout electronics saturated. A new regression for the photon and electron reconstruction takes the effect of saturation properly into account.

At the analysis level, several aspects can be improved. It was found that the discrepancy of the observed and predicted photon isolation was probably the main culprit of the 3 % (6 %) efficiency scale factor between data and MC in EB (EE) of Chapter 7. The (corrected)  $\text{Iso}_\gamma$  variable changed the most among all analysis variables during the run-II data-taking, since it is dependent on the additional activity originating from pile-up decay products in the detector as well as the transverse momentum of the photon. The observed discrepancy in EB may therefore be due to the pile-up dependence.

For EE, the pile-up dependence of the  $\text{Iso}_\gamma$  variable was overcorrected, which leads to an increasing efficiency versus pile-up of the order of 5 %. Additionally, the  $\text{Iso}_\gamma$  variable also exhibited a run-time dependence. These disagreements need to be corrected and the high- $p_T$  photon ID will be revised.

Two aspects of the background composition determination (Chapter 9) should be improved. The extrapolation of the background fraction from the extended charged particle flow isolation range to the signal region is an estimate. Due to this extrapolation, the associated uncertainties are in some points slightly underestimated. A more precise approach would be to determine the background components with an extended likelihood fit: in contrast to the maximum likelihood method, the normalization of the probability distribution function is allowed to vary [176]. This approach benefits from the larger discrimination power of the enlarged  $\text{Iso}_{\text{Ch}}$  range, but would be able to determine the number of events in the signal range by minimizing the extended likelihood. This would in consequence also give a correct uncertainty calculation.

When the corrections for the electromagnetic signal reconstruction due to the gain switch

are determined, the comparison of the observed and predicted prompt diphoton background of Section 9.5 should be repeated. The corrected photon energy assignment should account for the observed underfluctuation of the  $\gamma\gamma$ -component in data.

For an updated analysis, the uncertainty on the background prediction accuracy (Chapter 11) needs to be revised. This uncertainty is a nuisance parameter in the final profile likelihood and increasingly limits the sensitivity of the analysis, since, for a larger dataset, the statistical uncertainty decreases and the size of this nuisance parameter has a larger impact.

For the first dataset with  $3.3 \text{ fb}^{-1}$ , the statistical uncertainty dominated over this systematic one. The larger size of the dataset with  $16.2 \text{ fb}^{-1}$  already required a new and thorough evaluation of the background accuracy, since the nuisance parameter describing the uncertainty on the background accuracy had a greater impact on the final analysis sensitivity. With  $37.82 \text{ fb}^{-1}$ , this nuisance parameter will be the limiting factor among all for low mass and wide resonances. As it is planned to include the interpretation of wider resonances with  $\Gamma_X/m_X$  of 6 % and up to 10 % in the search, an improved assessment of the background accuracy is even more important.

One solution is an alternative background model with a different determination of the background prediction accuracy. For the ICHEP 2016 results, an alternative background model was already studied, adapting the background model of the  $H \rightarrow \gamma\gamma$  analysis for high diphoton masses. This discrete profiling method [177] treats the functional form for the background description as a discrete nuisance parameter. This reduces the arbitrariness of the background model choice, since ultimately the background model with the highest maximization of the likelihood fit to the data is chosen. The final uncertainty on the background prediction is rather small. Preliminary results did not show a significant improvement of the analysis sensitivity and the method suffered from a bias due to the low-populated tail of the distribution at high  $m_{\gamma\gamma}$  values. It is nevertheless worth considering this background model for an improved version of the analysis.

Another possible alternative background model is similar to the one used for the RS-graviton search in the high mass diphoton final state at 8 TeV [96]. A full NNLO calculation for diphoton production at the LHC [63], including contributions at  $\mathcal{O}(\alpha_s^3)$ , was recently published and will improve the accuracy of this approach. The method also benefits from an improved estimate of fake-photons.

A possible extension of the physics scope would be the interpretation of the diphoton events in terms of a non-resonant signal. The ADD model, described in Chapter 3, predicts a tower of KK-particles which can be detected at the TeV scale. These ADD signals would in contrast to the RS-resonance not appear as well separated resonances with  $\mathcal{O}(100 \text{ GeV})$  spacing among them. The signal would instead appear as a continuous increased number of events at high  $m_{\gamma\gamma}$  values due to the fact that the KK resonances

would only have a spacing of  $\mathcal{O}(\text{meV})$  among each other. For this model, interference effects need to be taken into account.

The current background model, which tests the distribution of diphoton events only as a function of their mass, is likely to work also robustly for this interpretation. It may however be combined with the method presented for the background determination in Chapter 9. This method was originally not only aimed for a determination of the different background fractions, but its goal was to combine this two-dimensional fit with the one to the  $m_{\gamma\gamma}$  spectrum for a more precise estimate of the high  $m_{\gamma\gamma}$  tail of the spectrum. An improved version of the analysis will benefit from all of the above outlined plans and first results are expected for spring 2017.

## PART II

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*Radiation studies of the  
electromagnetic calorimeter in CMS  
for the  
high-luminosity upgrade of the LHC*

*There is nothing more wonderful than being a scientist, nowhere I would  
rather be than in my lab, staining up my clothes and getting paid to play.*

Marie Curie

The current electromagnetic calorimeter in CMS is a homogeneous and hermetic calorimeter. It consists of about 76,000 lead-tungstate crystals and is divided in a barrel and two endcap regions. The endcap calorimeter will not be able to sustain the current performance after the high-luminosity upgrade of the LHC. The increased luminosity leads to a harsh radiation environment in the detector, especially in the forward region. The following Chapter 16 first motivates the desired replacement of the forward ECAL and the upgrade of the electronic readout system of the ECAL barrel. Thereafter, the Monte-Carlo simulation program FLUKA, which was used for the subsequent radiation studies, is described in Chapter 17.

For the upgrade of the ECAL barrel electronic readout system, the radiological hazard for personnel working on the detector during the upgrade has to be assessed. As ECAL contact person for FLUKA simulation studies, I worked on the prediction of the residual dose, which was crucial for the planning of the upgrade and is presented in Chapter 18. One studied solution of a new endcap ECAL was the 'Shashlik' sampling calorimeter with alternating layers of a heavy inorganic scintillator and an absorber material. First, different scintillator materials are studied to assess their suitability for the harsh-radiation environment in CMS at the HL-LHC. The measured residual dose rate of hadron-irradiated scintillating crystals is compared to my FLUKA simulations in Chapter 19. Based on these results, the induced fluence of proton-irradiated scintillating crystals is compared to the induced fluence of a Shashlik calorimeter in the CMS environment in Chapter 20. The radiation damage as well as the radioactivity of a Shashlik calorimeter in CMS is studied and it is discussed if the radiation from decaying isotopes may lead to a prohibitive background signal for the ECAL readout.

# 16

CHAPTER

## Expected performance of the CMS experiment at the HL-LHC

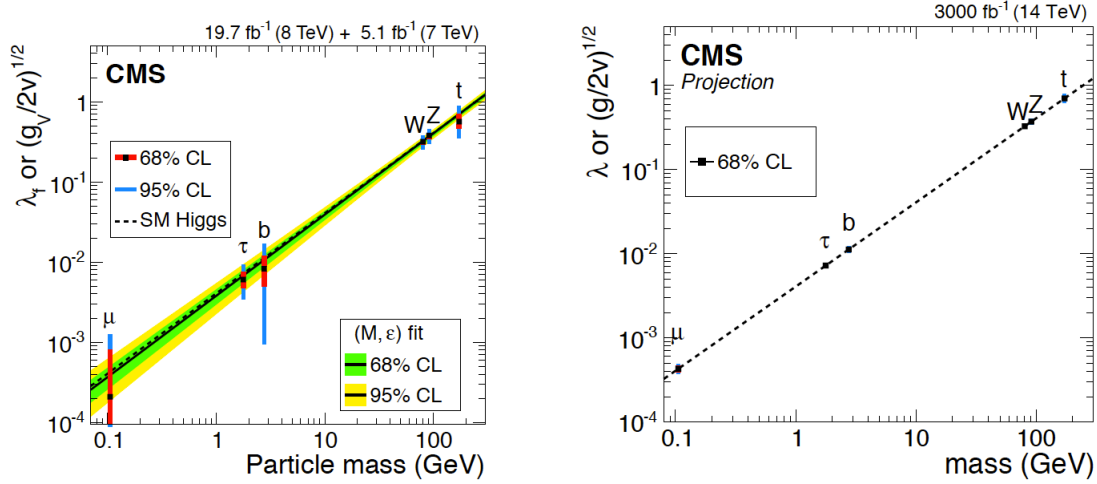
The aim of this introductory chapter is to highlight the reasons and goals for the CMS ECAL upgrade at the HL-LHC and the FLUKA simulation studies performed in this context. The harsh radiation environment and its impact on the ECAL is specified.

### 16.1 The high-luminosity upgrade

The phase-I program of the LHC is expected to finish in the year 2024, ensued by a long shutdown 3 (LS3) to equip the accelerator and its detectors for the phase-II upgrade of the HL-LHC, providing a higher instantaneous luminosity. The planned luminosity levels and the final integrated luminosity are described in the introductory Chapter 4.1, in particular in Figure 4.2. With this increase in luminosity many searches for new physics and precision measurements of the standard model of particle physics [17] will have an increased discovery potential.

The excellent performance of the LHC allowed the discovery of the Higgs boson in run-I by the ATLAS and CMS collaboration [44, 45]. Until now, new measurements of the Higgs boson and its properties do not show any deviations from the standard model expectations. These measurements still have large statistical uncertainties of up to 20% associated to them as shown on the left panel of Figure 16.1. It displays the current measurements of run-I Higgs boson couplings [178] to fermions ( $\lambda_f$ ) and bosons ( $g_v/2v^{1/2}$ ). On the right side of the same Figure 16.1, the expected results for 3000 fb<sup>-1</sup> with  $\sqrt{s}=14$  TeV are depicted [179]. Due to the high integrated luminosity, a few percent precision for most Higgs coupling measurements is expected.

Details about the envisaged upgrades for the LHC and the CMS detector can be found in Ref. [17]. The higher luminosity will be accomplished by a new proton bunch-forming scheme in PS, a new injector chain for high-intensity and low-emittance bunches



**Figure 16.1:** Observed and projected precision on Higgs boson couplings as a function of boson or fermion masses. [178, 179]

**Table 16.1:** Design values for phase-I and phase-II data-taking [17].

| Parameter                                                                 | Phase-I   | Increase    | Phase-II           |
|---------------------------------------------------------------------------|-----------|-------------|--------------------|
| Instantaneous luminosity $\mathcal{L}$ ( $\text{cm}^{-2} \text{s}^{-1}$ ) | $10^{34}$ | $\times 5$  | $5 \times 10^{34}$ |
| Integrated luminosity $\mathcal{L}$ ( $\text{fb}^{-1}$ )                  | 300 – 500 | $\times 10$ | 3000               |
| Average pile-up $\langle PU \rangle$                                      | 40 – 60   | $\times 5$  | 140 – 200          |

and new low- $\beta$  quadrupole triplets, focusing colliding beams. Additionally, new crab-cavities will optimize the bunch overlap in the interaction region. In the upcoming years, the LHC team also aims to increase the center-of-mass energy from 13 TeV to 14 TeV. Table 16.1 compares the luminosity of phase-I to phase-II. The increase of instantaneous luminosity by a factor five and the large amount of integrated luminosity imply a challenging radiation environment for the CMS experiment. In the following, the consequences for the electromagnetic calorimeter are highlighted.

## 16.2 The electromagnetic calorimeter at the HL-LHC

The current electromagnetic calorimeter was designed for an integrated luminosity of  $500 \text{ fb}^{-1}$  over ten years of data-taking with  $\mathcal{L} = 2 \times 10^{34} \text{ cm}^{-2} \text{s}^{-1}$  [11]. The higher luminosity in phase-II leads however to a harsh radiation environment with high hadron fluences and ionizing dose rates for calorimetry, especially in the forward region. To guarantee an excellent ECAL performance, the design of the ECAL, especially for the forward region, has to be revised. Before the envisaged upgrades of the ECAL are

described, an overview of the radiation environment in CMS and its impact on the ECAL detector material is given.

### 16.2.1 Radiation environment for the ECAL

The ECAL has to withstand a mixed background field of very low energy neutrons, energetic charged hadrons, photons and electrons. This field is created by the secondary particles of high pile-up collisions, which interact with the detector material. The magnitude of the background field increases with pseudorapidity, since many proton-proton collisions are not head-on. The particles produced in these collisions lead to a high particle fluence in the forward region of the detector. The residuals from the collision can also interact with the beam pipe and their decay products then impinge on forward calorimeters at very high pseudorapidities. In the ECAL, particles can also be backscattered or escape from cascades within them. Their interaction with adjacent materials, such as the electronics or the tracker system therefore needs special attention. The highest particle fluence in the ECAL comes from charged particles. The fluence consists mainly of pions with an energy of  $\mathcal{O}(1 \text{ GeV})$ , which produces hadron showers in the material.

Electrons or photons, impinging on the  $\text{PbWO}_4$  crystals induce electromagnetic showers. Photons from  $\pi^0$ -decays can interact with the beam pipe or tracking system, produce  $e^\pm$ -pairs and therefore induce electromagnetic cascades in the ECAL.

Neutrons travel a long distance in the detector material without interaction, since they only interact with nuclei and in contrast to charged particles not via Coulomb interaction with the shell electrons. Most neutrons have an energy below 20 MeV and therefore not enough energy to create a displacement of lattice atoms in the detector material. They are instead slowed down via elastic scattering processes until they are thermalized and can then be captured by the nuclei. Since they do not have to overcome the Coulomb barrier, they can interact directly with the nucleus down to very low energies (meV). The most common neutron reaction is the radiative capture, where the neutron is captured and the excitation energy is emitted by photon radiation. The neutron-nucleus reaction can also result in the creation of radionuclides. These may lead to a prohibitive long-time background in the detector readout and are therefore discussed in Section 20.2.1. Detector materials can be shielded against neutrons by a layer of material consisting of very light elements. Polyethylene for instance is a hydrogen-rich element and is used in CMS to thermalize neutrons. If the neutrons need to be also captured by the shielding material,  $^{10}\text{B}$ -doped polyethylene can be used.

The radiation environment in the ECAL is characterized by the following quantities:

- the absorbed dose ( $D$ ), measured in Gy, which is the deposited energy by ionizing radiation per unit mass of the medium.
- its corresponding induced dose rate ( $\dot{D}$ ), measured in Gy/h.
- the integrated fluence, measured in  $\text{cm}^{-2}$ , expresses a density of particle tracks: the fluence is the time integral of the flux density  $\Phi$ , which can be expressed as the product of the particle density  $n(r,v)$  and the particle velocity ( $v$ ). The integrated fluence can therefore be evaluated based on the tracklength ( $dl$ ) of the particle trajectory:

$$\Phi(E) = n(r,v) \times dl \quad .$$

The ionizing damage, induced by electromagnetically interacting particles, scales with the  $e^\pm$ -fluence ( $\Phi_e$ ).

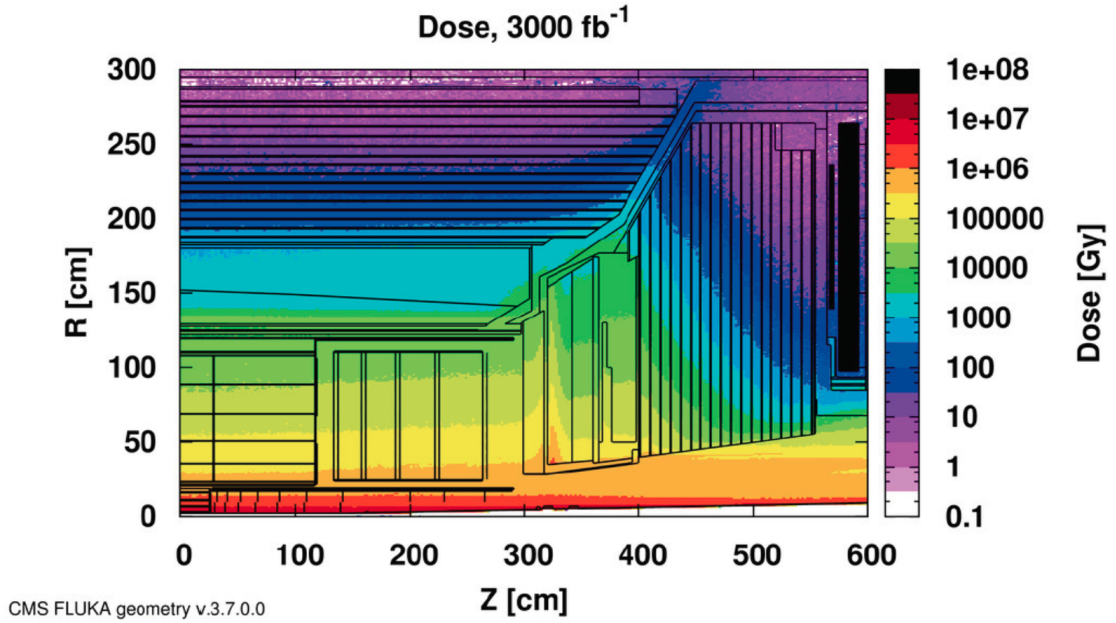
- the density of inelastic hadronic interactions (stars), measured in  $\text{cm}^{-3}$ . Stars are caused by a projectile above a certain energy threshold and lead to local energy deposits which can displace lattice atoms. Stars are proportional to the charged hadron fluence ( $\Phi_{\text{ch.h.}}$ ), weighted by the inelastic pp-cross-section. They are also proportional to the induced dose rate and are a FLUKA specific quantity.

A comparison of phase-I and phase-II parameters of these quantities in the EB and the EE is given in Table 16.2. The listed values are approximate and shall only emphasize the scaling between the different situations. For exact values, the systematic uncertainties of the simulation with respect to its location in the CMS detector need to be taken into account. All simulation values in the CMS cavern are verified by measurements if possible. Most measurements can just be taken in the CMS cavern, since the detector itself is rather hermetic. A few selected measurement devices are placed inside the detector, for instance in front of the tracker. They can be read out during technical stops and shut downs.

Dose rate and fluxes scale with the delivered instantaneous luminosity, whereas integrated dose and fluence scale with the integrated luminosity. As shown in Table 16.2, the forward calorimeter has to withstand a much higher dose than the EB. This conclusion can also be derived from Figure 16.2, which illustrates the expected absorbed dose for 3000  $\text{fb}^{-1}$  for the current EE in an otherwise phase-II-upgraded CMS detector. Since a new forward calorimeter will replace the current EE and HE, this figure is aimed at scaling from the current to the situation at the end of the HL-LHC running. The prediction shows that the dose reaches up to 300 kGy in the EE, while orders of magnitude lower doses are expected for the EB. In fact, the expected dose at the end of the HL-LHC in the EB is comparable to the one expected for the EE after phase-I. To further understand the necessary upgrade of the EE, the following section discusses the hadron-induced cumulative damage in  $\text{PbWO}_4$  crystals.

**Table 16.2:** Approximate dose ( $D$ ), dose rate ( $\dot{D}$ ) and hadron fluence ( $\Phi_{\text{ch.h.}}$ ) for the EB and the EE during phase-I and phase-II data-taking. These are conservative estimates at the shower maximum. The values are taken from Ref. [17] or FLUKA simulations [180].

| Parameter                                        | Phase-I<br>$\mathcal{L} = 300 \text{ fb}^{-1}$ | Increase    | Phase-II<br>$\mathcal{L} = 3000 \text{ fb}^{-1}$ |
|--------------------------------------------------|------------------------------------------------|-------------|--------------------------------------------------|
| <b>ECAL barrel</b>                               |                                                |             |                                                  |
| $\dot{D}$ (Gy/h)                                 | 0.3                                            | $\times 5$  | 1.5                                              |
| $D$ (kGy)                                        | 1                                              | $\times 10$ | 10                                               |
| $\Phi_{\text{ch.h.}}$ ( $\text{cm}^{-2}$ )       | $2 \times 10^{11}$                             | $\times 10$ | $2 \times 10^{12}$                               |
| <b>ECAL endcaps at <math> \eta  = 2.6</math></b> |                                                |             |                                                  |
| $\dot{D}$ (Gy/h)                                 | 6                                              | $\times 5$  | 30                                               |
| $D$ (kGy)                                        | 30                                             | $\times 10$ | 300                                              |
| $\Phi_{\text{ch.h.}}$ ( $\text{cm}^{-2}$ )       | $2 \times 10^{13}$                             | $\times 10$ | $2 \times 10^{14}$                               |



**Figure 16.2:** Absorbed dose in the CMS cavern after an integrated luminosity of  $3000 \text{ fb}^{-1}$ .  $R$  is the transverse distance from the beamline and  $Z$  the distance along the beamline from the interaction point  $Z=0$  (see Figure 20.2 for details of the CMS geometry in FLUKA). Phase-II improvements like the phase-II tracking system and an aluminum beam pipe are implemented (version 3.7.0.0) [17].

### 16.2.2 Hadron-induced damage in PbWO<sub>4</sub> crystals

The radiation induced degradation of light transmission in a material is expressed by the radiation-induced absorption coefficient ( $\mu_{\text{ind}}(\lambda)$ ). It expresses the loss in optical longitudinal transmission (LT) measured through a crystal of length ( $l$ ) with respect to the initial value  $LT_0$  [181]:

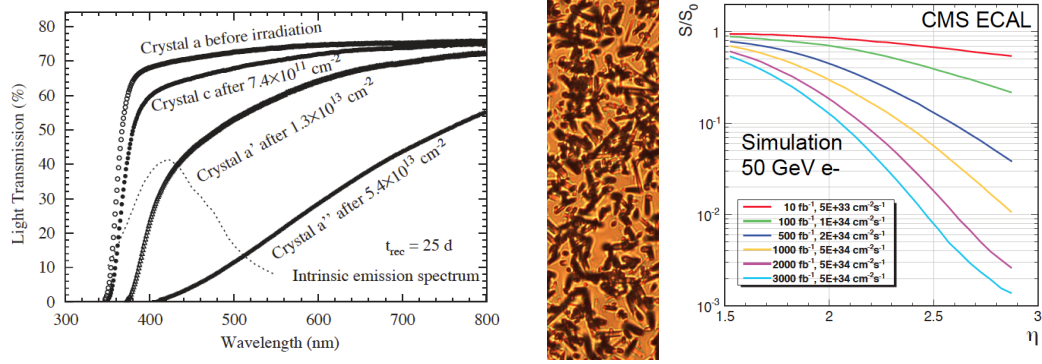
$$\frac{LT(\lambda)}{LT_0(\lambda)} = e^{-\mu_{\text{ind}}(\lambda)l} \quad (16.1)$$

The formula implies that  $\mu_{\text{ind}}(\lambda)$  is the inverse of the attenuation length. The induced absorption coefficient is dependent on the wavelength, which for PbWO<sub>4</sub>, is set to be its maximum scintillation emission wavelength of 420 nm (see Table 19.1). The ECAL design for LHC requires  $\mu_{\text{ind}}(\lambda)$  to be below  $1.5 \text{ m}^{-1}$  for dose rates of 100 Gy/h. Indeed, the absorption band induced by dedicated  $\gamma$ -irradiations shows a constant  $\mu_{\text{ind}}(\lambda)$  for stable dose rates within this limit [181].

For hadron-irradiated crystals, a different observation was made [181–183]. The loss in LT among different proton-irradiated crystals versus  $\lambda$  is depicted on the left side of Figure 16.3. With increasing hadron fluence, the LT is decreased. More importantly, the band edge of the transmission spectrum shifts to higher wavelengths. Ref. [181] reported a degradation of  $\mu_{\text{ind}}(\lambda) = 15 \text{ m}^{-1}$  after a 20 GeV/c proton fluence of  $5 \times 10^{13} \text{ p/cm}^2$ . The  $\mu_{\text{ind}}(\lambda)$  is found to increase linearly with  $\Phi_{\text{ch.h.}}$ , an effect which cannot be reproduced with  $\gamma$ -irradiations [181, 182].

The observation can be explained by energetic inelastic nuclear interactions. In the hadron shower, some particles carry an energy which is high enough to break up the nuclei (Lead or Tungsten) into fission fragments which displace a large number of lattice atoms [181]. This production of fission fragments is possible for every scintillator material made of elements with atomic numbers above 71. Ref. [181] further reports that the observed emission light is polarized and that  $\mu_{\text{ind}}(\lambda)$  is proportional to  $\lambda^{-4}$ . This behavior can be explained by damage regions, which were caused by the fission fragments and are therefore named ‘fission tracks’, acting as Rayleigh scattering centers [184]. These fission tracks are visualized in Ref. [184] and an exemplary photograph of this study is depicted in the middle of Figure 16.3.

The attenuation of the uniform light output due to the scattering centers increases the constant term of the energy resolution in Equation 4.7 and therefore worsens the energy reconstruction of electromagnetically interacting particles. It was demonstrated in further studies [183] that the scintillation mechanism itself stays unchanged, which is crucial for the ability to monitor hadron-induced damage through light injection.



**Figure 16.3:** Left: LT curves for crystals with various degrees of proton induced radiation damage. The emission spectrum (dotted line) has arbitrary normalization [181]. Middle: Visualization of the fission tracks induced by proton-irradiations [184]. Right: expectation of the relative light output  $S/S_0$  of the ECAL crystals for electron showers of 50 GeV as a function of pseudorapidity for various aging conditions, corresponding to the integrated luminosities [17].

### 16.2.3 Consequences for the ECAL performance

The previous Section 16.2.2 shows that  $\mu_{\text{ind}}(\lambda)$  increases with higher hadron fluence. Since the hadron fluence also scales with the integrated luminosity, a decrease of relative light output  $S/S_0$  for higher integrated luminosities is expected. The right graph of Figure 16.3 shows the degradation of  $S/S_0$  as a function of the pseudorapidity. It is visible that the relative light output for the EB will be reduced by a factor two until the end of phase-II data-taking, while a reduction down to more than  $1/10$  of  $S/S_0$  has to be expected for  $|\eta| > 2$ . The loss in light output impacts the stochastic term ( $\propto \sqrt{S_0/S}$ ) and the noise term ( $\propto S_0/S$ ) and is mainly due to the damage from ionizing radiation. On top of that, the constant term of Equation 4.7 increases with  $\propto \frac{d(S/S_0)}{dz}$  due to the cumulative hadron damage. A replacement of the EE is therefore desirable and is detailed below in Section 16.2.4.

For the EB, the degradation of the relative light output is still at a manageable level. However, the increased pile-up, especially the out-of-time pile-up, challenges the ECAL electronics and the reconstruction of electromagnetically interacting particles. An upgrade of the EB electronics system is planned to update the trigger acceptance rate (750 kHz L1 acceptance rate with 12.5  $\mu\text{s}$  L1 latency), to improve the pulse shape information and to add possible timing information. Everything will be exchanged for this upgrade, except for the  $\text{PbWO}_4$  crystals, the APD photodetectors and the motherboards. To implement the upgrades during LS3, it will be necessary to remove the supermodules from the CMS detector. The planning of the intervention also has to take the radiological hazard into account. Studies of the predicted residual dose rates, which I performed in collaboration with the BRIL project of CMS are discussed in Chapter 18.

#### 16.2.4 Choice of a new ECAL forward calorimeter

A new calorimeter in the forward ECAL region has to provide:

- high density, to stop the high momentum electrons or photons and to match the current dimensions of the EE.
- high light yield to ensure a good electromagnetic energy reconstruction.
- high radiation tolerance, especially against hadron fluence.

A sampling calorimeter with radiation-tolerant active layers satisfies these requirements. Its short light path also reduces the effects of radiation damage to the ECAL signal readout, compared to a homogeneous crystal calorimeter.

The final choice for a new endcap ECAL had to be taken among two different proposed sampling calorimeter designs [18]:

- a 'HGCAL' (High Granularity CALorimeter), a silicon based calorimeter [17].
- a 'Shashlik' scintillator based sampling calorimeter with a separate solution for the hadronic forward calorimeter [18].

The ETHZ group and its collaborators developed in this context a Shashlik calorimeter and were interested in the behavior of this sampling calorimeter in a harsh radiation environment. This was the focus of my work and is detailed in Chapter 19. For these studies, I am using the Monte-Carlo simulation program FLUKA [185, 186], which is introduced in the subsequent Chapter 17.

In 2015, the CMS collaboration selected the high-granularity and longitudinally segmented silicon calorimeter as their solution for a new endcap ECAL [17]. The research program of the ETHZ group and collaborators for the Shashlik sampling calorimeter design is being completed at the moment.

# Radiation simulations with the particle physics Monte-Carlo simulation package FLUKA

The radiation environment at CMS is described in the previous chapter. The Monte-Carlo simulation program FLUKA (FLUkturierende KAsakade) [185, 186] is designed for a general estimation of the radiation environment of an experiment and is described in the first part of this chapter, since the simulation studies of the subsequent chapters are performed with this particle physics simulation toolkit. The studies themselves are either performed by myself or in collaboration with the BRIL project, which is among others responsible for radioactivation measurements and the simulation of radiation levels in the CMS detector and its cavern. BRIL is therefore also responsible for the maintenance of the CMS detector description in FLUKA. The FLUKA CMS geometry and the corresponding FLUKA simulation settings are detailed in the second part of this chapter. The studies in this dissertation use consistent FLUKA simulation settings, where possible.

In the final part of this chapter, the followed official recommendations for radioactivation studies by BRIL and the radiation protection group of CERN are detailed.

## 17.1 Monte-Carlo simulation program FLUKA

My radiation studies were performed with the fully integrated particle physics Monte-Carlo simulation program FLUKA. If not otherwise stated, the FLUKA version 2011.2b.5 is used within this thesis. A detailed description of FLUKA and its relevance for the CMS experiment can be found in the appendix of Ref. [17] and in Ref. [187]. The FLUKA simulation program is well designed for average radiation results, recorded in a 3-dimensional coordinate system. In contrast to other particle physics MC simulation toolkits, its focus is not on the prediction of a single particle behavior in the detector, but

the general particle rates and their consequences. It is a preferred toolkit for the simulation of flux maps, energy depositions and radiological studies as will be demonstrated later. The geometry is efficiently modeled to obtain these averaged results and is built from averaged material composition and simplified geometries.

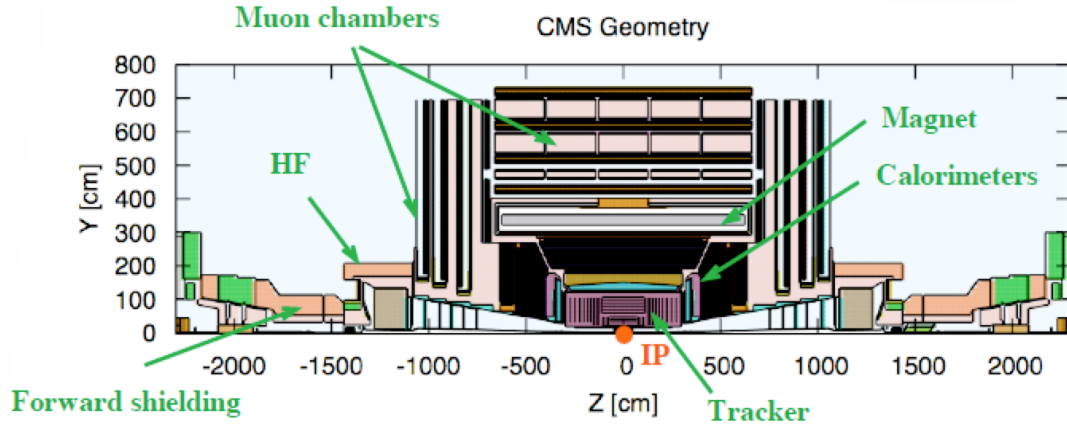
For radioactivity studies however, a precise knowledge of potentially highly radioactive material components is crucial. Even impurities at the permille level have to be known. For these studies, the detector surfaces need to be modeled with great precision as their location within the overall geometry and the resolution of the surface is important for the radioactivity results. For a precise simulation of the residual nuclei, FLUKA includes a profound thermal neutron cross-section library, which consists of 260 datasets from energies of 0.01 meV, the simulation cutoff, up to 20 MeV.

A primary event of the MC-program FLUKA is in the following either a primary proton or a pp-collision event. The simulation results are then averaged over all simulated primary events, which need to be more than 3,000 events to avoid statistical fluctuations in the MC simulation results. All primary events are normalized to one single event. This simulation result per primary event can then be normalized either to values per unit time, for an instantaneous luminosity, or normalized to an integrated luminosity.

All secondary particles are generated and transported until a predefined energy cutoff. One of the main output options used in the subsequent chapters are track length estimators, where the path length for a particle, passing through a specified volume, is recorded. The secondary particles are weighted by their assigned particle trajectories and their angle, the likelihood to escape the detector volume and their decay or creation probability. FLUKA also provides many user defined output formats and specific features for radioactivity studies.

## 17.2 CMS description in FLUKA

The CMS collaboration has an official CMS detector description in FLUKA, maintained by the BRIL project. Radiation simulation results are benchmarked with residual dose measurements, either in the CMS cavern or at specific points in the detector itself. The first development of this CMS representation is published in Ref. [189], details about recent developments can be found in Ref. [190] and Ref. [187]. The CMS description in FLUKA is subject to constant improvements and incorporation of planned detector upgrades and therefore follows an official versioning scheme with typically four digits. Each new study has its own version number assigned to it. The first two digits of the version number mark improvements in the description of the detector or official CMS detector upgrades [188]. The third digit denotes modification studies for potential future configurations, for instance a forward sampling calorimeter. The fourth digit represents



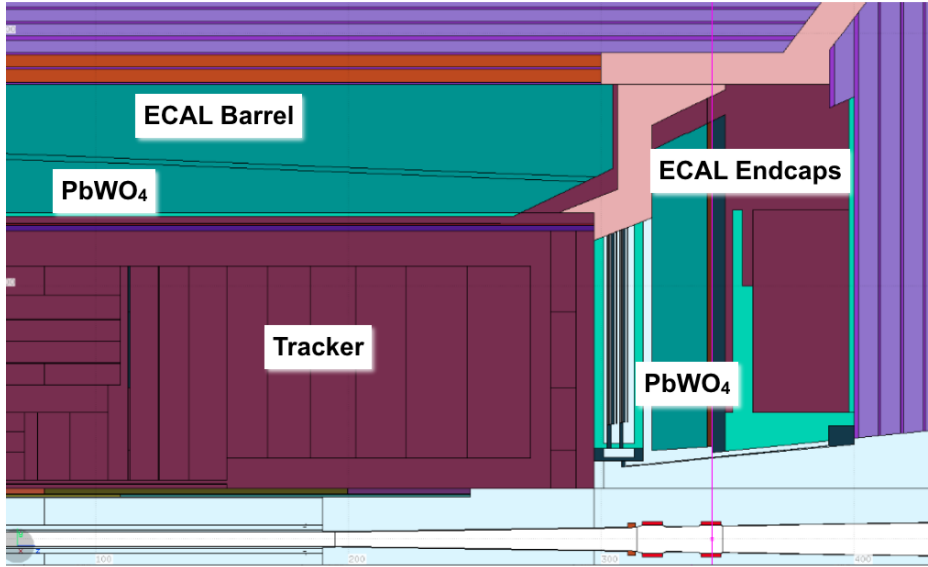
**Figure 17.1:** CMS implementation in FLUKA, version 1.0.0.0.  $R$  is the transverse distance from the beamline and  $Z$  is the distance along the beamline from the interaction point  $Z = 0$  [188].

dedicated minor modifications. The official 'CMS version' at the time of the studies presented in the following was 1.0.0.0 [188] and is illustrated in Figure 17.1.

Other FLUKA predictions in this thesis are versioned by 3.0.0.0, which is the most recent released version for run-II as of January 2016. It reflects the post LS1 situation and includes, among other upgrades, the newly installed beampipe and an updated cavern description.

The phase-II upgrade is represented by version 3.7.0.0. For this version, the ECAL was among others extended to  $|\eta| = 3$  and the preshower was replaced by a boron-polyethylene absorber as an additional shielding device for the tracking system. All of these recently released official results were performed with the FLUKA version 2011.2b.6. The binning grid typically used in general purpose CMS FLUKA simulations is  $\phi$ -symmetric with a uniform binning of 4 cm in the  $R$ - and 2 cm in the  $Z$ -direction. If the CMS detector is divided in 16 sectors of uniformly positioned  $\phi$ -bins, the binning in  $R$  and  $Z$  enlarges to 10 cm for each dimension.

The FLUKA description of ECAL is depicted in a  $R$ - $Z$  plane in Figure 17.2. It can be best compared to the sketch of the tracker and calorimeter system of CMS in Figure 4.4 of the introductory Chapter 4. All detector regions are mainly described by large volumes containing averaged materials, which are listed in Table 17.1. In the barrel part, the tracker system (purple) is shielded against slow neutrons from the  $\text{PbWO}_4$  crystals by a thin moderator layer of polyethylene (light green). Polyethylene slows down neutrons, but does not absorb them. Behind the dark-green  $\text{PbWO}_4$  crystal volume, the electronics of the supermodules are described by the material 'Ecal<sub>AV</sub>'. In the endcap region, the preshower is correctly described by layers of silicon and lead absorbers, cooling screens and neutron moderators, and supporting elements. The endcap calorimeter is described by the  $\text{PbWO}_4$  crystal volume, followed by an aluminum plate, representing the holding structure of the crystals. A layer of polyethylene shields the electronics from



**Figure 17.2:** Electromagnetic calorimeter in FLUKA CMS description, version 1.0.0.0 as described in Ref. [188].

**Table 17.1:** Material descriptions of the CMS FLUKA description

| Material            | Density $\rho$ (g / cm <sup>3</sup> ) | Elements                                                                 |
|---------------------|---------------------------------------|--------------------------------------------------------------------------|
| Trk <sub>AV</sub>   | 0.047                                 | 30 % Fe, 23 % Al, 30 % C, air                                            |
| Ecal <sub>AV</sub>  | 1.28                                  | 45 % Al, 22 % Fe, 6 % Cr, 5 % C,<br>5 % O, 6 % Cu, 2 % Ni, 4 % Si, 1 % H |
| Cable <sub>AV</sub> | 0.88                                  | 43 % Cu, 5 % Al, 7 % C <sub>6</sub> F <sub>14</sub> , 8 % PE, 44 % Steel |
| Aluminum            | 2.7                                   |                                                                          |
| Polyethylene        | 0.95                                  |                                                                          |

low neutron flux, originating from EE and the beam pipe. The EE electronics region (purple) is described by a low density material ('Trk<sub>AV</sub>').

### 17.2.1 The FLUKA settings for radiation studies in the CMS detector

To simulate the primary events of pp-collisions in the CMS detector, the recommended event generator DPMJET III [191] version 3.0-6 was used. The inelastic cross-section of 80 mb was taken from EPOS LHC simulations [192]. The assumed values for the luminosity normalizations are listed in Table 17.2. The 'precision' setting of the FLUKA simulation code is used throughout. For the ECAL endcap region, the thresholds during irradiation were the following: hadrons 100 keV, neutrons down to thermal energies of 0.01 meV, photons 50 keV and electrons 100 keV. In the surrounding regions, photons and electrons have higher cutoffs, 100 keV and 300 keV respectively.

**Table 17.2:** Simulation assumptions and normalizations for proton-proton collisions in FLUKA

| Quantities                                                      | HL-LHC                | Activation |
|-----------------------------------------------------------------|-----------------------|------------|
| Per proton-energy ( TeV)                                        | 7                     |            |
| Center-of-mass energy ( TeV)                                    | 14                    |            |
| Peak luminosity $\mathcal{L}$ ( $\text{cm}^{-2}\text{s}^{-1}$ ) | $5 \times 10^{34}$    |            |
| Rate at $\mathcal{L}$ (pp-int/h)                                | $1.44 \times 10^{13}$ |            |
| Collisions in 3000 $\text{fb}^{-1}$                             | $2.4 \times 10^{17}$  |            |
| Vertex spread ( cm)                                             | 5                     |            |
| Number of primary events (pp-collisions)                        | > 3000                |            |
| Inelastic cross-section $\sigma_{inel}$ ( mb)                   | 80                    | 100        |
| Integrated luminosity $\mathcal{L}$ ( $\text{fb}^{-1}$ )        | 3000                  | 2475       |

### 17.2.2 Radiological studies with FLUKA in the CMS detector

The knowledge about dominant drivers of residual radiation in material is interesting from a detector point of view as the radiation from radioactive isotopes may lead to a constant background for the readout of the ECAL. It is also important for the assessment of human exposure to radiological hazard. The residual dose ( $\mathcal{D}$ ) is for that purpose insufficient as it does not contain the extent of exposure to ionizing radiation on the human body. Every tissue (T) of the human body reacts differently to the various types of radiation (R). The effective dose (E) quantifies the body exposure as the weighted sum over all tissues and all radiation types:

$$E = \sum_T \sum_R w_R \times \mathcal{D}_{T,R} \quad (17.1)$$

Since this effective dose in humans is not measurable, the operational quantity of radioactivity measurement instruments is the ambient dose equivalent ( $\dot{H}^*(10)_{ind}$ ). The International Commission on Radiation Units and Measurement (ICRU) defined a phantom sphere of tissue-equivalent material to quantify the residual dose in an area. The ambient dose equivalent corresponds to the dose measured in the ICRU sphere at a depth of 10 mm.

In FLUKA, the ambient dose equivalent is based on results of particle fluence simulations. The fluence is converted to the ambient dose equivalent by a defined AMB74 set of coefficients [193]. Due to this derivation of  $\dot{H}^*(10)_{ind}$ , the comparison of a measured and simulated  $\dot{H}^*(10)_{ind}$  can also be used to disentangle the impact of different sources of background fluences to the residual dose.

The residual dose and its dominant drivers are calculated with a two-step method in FLUKA [194]:

- the first (prompt) step is the irradiation. The radionuclides, mainly  $\gamma$  and  $\beta$  emitters, are produced in the material and saved for the subsequent step.
- in the second (decay) step, the residual dose and the residual nuclei are simulated. In most scenarios, the irradiated material is taken out of the irradiation environment for that step. This is realized in FLUKA by setting all surrounding materials to vacuum.

For my radioactivation studies in CMS, the FLUKA settings from Table 17.2 were used. To employ the best activation models in FLUKA, the coalescence and the evaporation of heavy fragments were enabled in the first step. The electromagnetic transport was switched off for the prompt radiation as it is very CPU expensive, but switched on for the decay. The transport and production thresholds were taken to be the same as for the first step, except for electrons and photons, which were simulated down to 100 keV and 10 keV, respectively.

Radioactivation studies for CMS are typically performed by BRIL and the radiation protection group of CERN. The radioactivation studies described in this thesis follow the recommendations of both groups. In the following chapters, two different irradiation cycles were used to describe the pp-collisions until LS5, which are typically based on the official LHC plans at the respective time and in agreement with the technical coordination. The first one, which is listed in Table B.1, was used for our radioactivation studies for the EB electronics upgrade during LS3 [195], detailed in Chapter 18. Since this study is currently being updated, the irradiation cycle is based on the official LHC recordings and plans of the year 2016. For my radioactivation studies in Chapter 20.4.2, I used the irradiation cycle of Table B.2 [195, 196]. It results in an integrated luminosity of  $2827.5 \text{ fb}^{-1}$  ( $2475 \text{ fb}^{-1}$ ) with respect to the start of the LHC (starting from LS3) and follows the official LHC plans from 2014 [197].

Irradiation cycles for FLUKA simulations are built in the following way: The FLUKA pp-collision rate for each run is chosen to be 75 % of the peak luminosity. These irradiation periods are simulated immediately before a respective shut-down and therefore effectively overpredict the instantaneous luminosity. Since the exact  $\mathcal{L}$ -profile is not predictable, this irradiation profile conservatively assumes that all particles and their associated radiation are produced at the end of each irradiation period. As the production of short-lived residual nuclei increases with the instantaneous luminosity, the amount of short-lived radioactive nuclei is enhanced, giving a conservative prediction.

For the irradiation cycle of Table B.2 an inelastic cross-section of 100 mb is assumed.

This cross-section is higher than for in-situ CMS simulations and was the recommended value of the radiation-protection group at the time of the studies. It is a conservative estimate as it increases the instantaneous luminosity and as such the amount of short-lived radionuclides.

For the irradiation cycle of the EB supermodule study (Table B.1), an inelastic cross-section of 75 mb was taken for the irradiation up to LS1, which was based on measurements. For the irradiation situation after LS1, an inelastic cross-section of 80 mb was employed, relying on the prediction of the EPOS LHC program.

Long-lived radioactive residuals increase with the integrated luminosity and become therefore more important towards the end of phase-I.

After data-taking periods, the residual dose in the cavern is comparable to natural background radiation ( $\approx 0.07 \mu\text{Sv h}^{-1}$ ) due to the self-shielding of the closed CMS detector. Only when the detector is opened, the personnel is exposed to high residual dose rates.

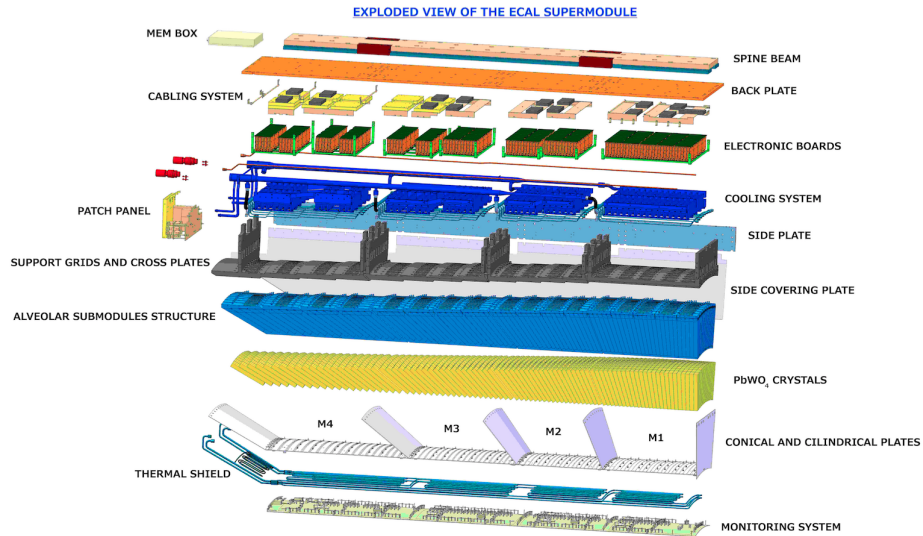


## **Studies of human exposure to radioactivity during the ECAL barrel upgrade**

This and the following chapters focus on the work, which was motivated in Chapter 16 and uses the Monte-Carlo simulation program FLUKA, described in the previous Chapter 17. For a continuous excellent performance of the EB during the HL-LHC, the EB supermodule electronic readout system need to be exchanged during LS3. For this upgrade, the supermodules need to be dismantled from the CMS detector and worked on for a long time period, requiring an appropriate radioprotective shielding. The prediction of the residual radiation within and around the EB supermodules was therefore crucial for the planning of the LS3 and the finalization of the technical proposal (TDR) of CMS for the HL-LHC [17].

In my role as the ECAL contact for FLUKA simulations, I reviewed the ECAL barrel description in FLUKA and found several items that needed to be optimized. In close collaboration with the CMS ECAL group and the BRIL project, I recommended corrections to the FLUKA EB description. The advised changes are shortly summarized in Section 18.1, highlighting to which detail the individual materials in FLUKA need to be known for radioactivation studies.

Due to time constraints, our LS3 activation study for the TDR and the now updated results were still based on the old EB implementation. If the activation study would have shown alarming levels of residual dose, the EB description would have needed to be improved immediately. An improved description of the EB, taking into account all advised changes, is being implemented in FLUKA at the time of writing this thesis. Recently, an improved version of the activation study was performed by the BRIL project. This study is based on our previous studies, but employs a new version of the FLUKA geometry, still with the not-updated EB description. The updated results are shown in Section 18.2 and present our current expectations of the residual dose rate of the EB supermodules during LS3.



**Figure 18.1:** Sketch of the different components of the ECAL supermodule[199].

## 18.1 Improvement of the EB description in FLUKA

The extensive improvements of the ECAL description in FLUKA are highlighted for two examples: the EB supermodule description and a hot-spot region, found in the cable region of FLUKA [198].

Two illustrations of the EB and its supermodules (SM) can be found in the introductory chapter to CMS, in Figure 4.6 and 4.7, respectively. The verifications of the EB description in FLUKA concentrated on its dimensions in CMS and the material composition. An overview of the different components of the EB SM is given in Figure 18.1. The material 'Ecal<sub>AV</sub>', defined in Table 17.1, averages these different components together with the SM backplate to one material based on their mass fractions. Nearly one third of this averaged material is stainless steel (70 % iron, 20 % chrome and 10 % nickel) from screws and the backplate of the SM. The quality of the stainless steel need to be precisely known as it may lead to highly radioactive elements at a sub-percent level. These can still be dominant drivers in the residual dose next to the well-known chromium. The screws in the SM have qualities of A2 and A4, the backplate of 316L. The latter contains up to 2 % manganese, 0.045 % phosphorus and 0.03 % sulfur. The implementation of the right fraction of these sub-percent elements is a necessary improvement of the EB FLUKA description.

The cable region between the EB and EE in FLUKA (pink region in Figure 17.2) showed a more than a factor ten higher residual dose compared to the surrounding regions. This hot-spot could not be explained by the ECAL group and was likely to be an inaccuracy in the simulation [198]. Cross-checks of the material composition of individual cables from the tracker and calorimeter did not reveal an unknown impurity

or false composition [200]. An investigation of the dominant nuclei revealed that silver isomers had a high contribution to the overall radioactivity [200]. The silver content in the cables itself was however correctly simulated. In its ground state, silver has only a half-life of 24.6 s, but during irradiation an isomer ( $^{110}\text{Ag}$ ) is produced with a long half-life of 249.95 days. The current released version of FLUKA (2011) is generally well benchmarked by comparisons to actual measurements, for instance the radioactivation in material from hadronic cascades [185]. However, for a few elements, among them silver, the production of the ground state and isomers is not precisely modeled. The isomer production model has been implemented in a simplified manner using an equal share among ground and isomeric states, rather than following the exact isomer production model. The latter would require spin and parity dependent calculations in the evaporation. The fraction of the  $^{110}\text{Ag}$  isomer is overestimated by this model and is therefore the main driver of the residual dose during long-shutdowns. In the yet to be officially released version of FLUKA, an improved isomer production model is implemented. The simulation was run by the FLUKA group at CERN with the development version and the hotspot disappeared [195].

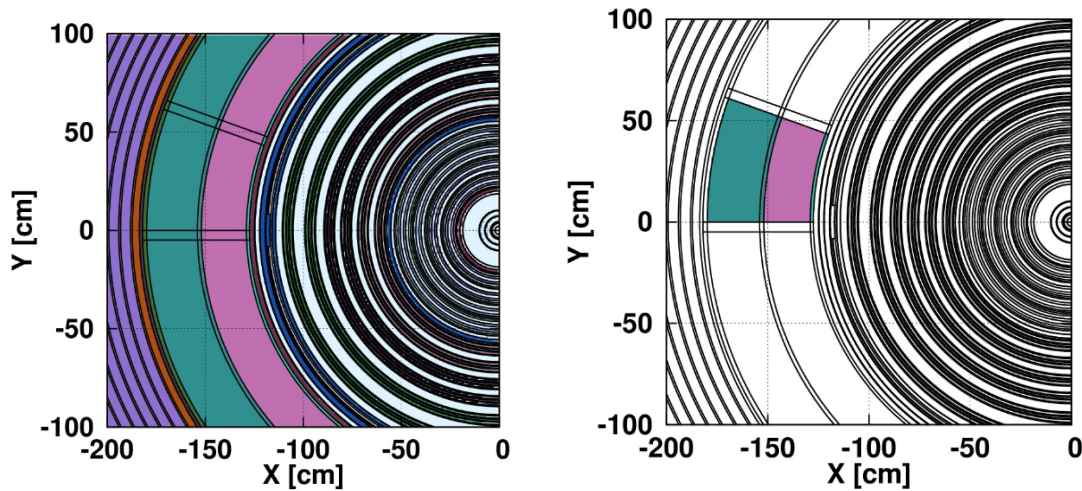
## 18.2 Activation simulations for an EB supermodule

The simulation of the residual dose for the supermodule intervention involves two scenarios:

- the residual dose in an 'open CMS' scenario, when the forward regions of CMS and the tracker system are removed and the SM is accessible.
- the residual dose of a SM outside of the CMS area for the actual work on the SM electronics system in a laboratory.

The former scenario can be simulated with a new software development of the BRIL group. It enables the separation of the prompt and decay simulation steps and the transformation of the geometry models in between. This includes the ability to rotate, translate, remove and add (shielding) components [201].

For the latter scenario, we edited the nominal CMS FLUKA geometry to form a separate supermodule and studied its residual dose in a second step by setting the surrounding regions to vacuum: in the nominal FLUKA model, the ECAL barrel region is assumed to be  $\phi$ -symmetric. To form the supermodules in the FLUKA model, the  $\phi$ -symmetry was broken into 18 bins, representing the 18 supermodules. Since we are only interested in the residual dose of one supermodule, one  $\phi$  bin was separated. Figure 18.2 shows the



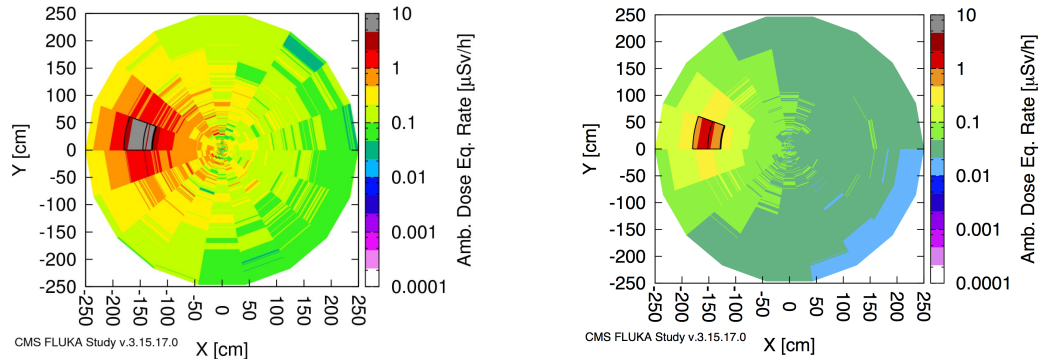
**Figure 18.2:** CMS FLUKA model for prompt (left) and decay radiation (right) simulation steps viewed in the X-Y plane. For the decay simulation step, a single super module with  $\text{PbWO}_4$  crystals (pink) and SM electronics (green) is activated and the remaining CMS geometry is set to vacuum (white). This simulation therefore represents a situation where the supermodule has been removed from the cavern (version 3.15.17.0).

X-Y plane with the separated supermodule during irradiation (left) and for the simulation of the residual dose (right).

According to Chapter 17.2.2, the prompt radiation from 14 TeV pp-collisions was transported through the full CMS detector. For the decay step, we only activated the supermodule region, including the polyethylene and crystal layer, and the SM electronics volume. All other CMS components were set to vacuum, representing the situation where the supermodule is removed from the CMS cavern and placed in a low radiation environment. Within the EB, the binning in the R-Z plane was performed in 1 cm steps to record the radioactive elements with high precision.

Our current activation studies for the EB supermodules, are a first, very conservative estimate as the residual dose is predicted based on the full 'Ecal<sub>AV</sub>' material. This is not realistic: as soon as the SMs are placed in a laboratory, the highly radioactive stainless-steel backplate will be removed to work on the electronics. The engineers will therefore experience a lower dose rate. An improved residual radioactivity study for this scenario by BRIL is currently being planned.

The used irradiation cycle is listed in Table B.1 of the appendix. The current technical plans state that the EB supermodules will be accessed 20 weeks after the irradiation stop. The right panel of Figure 18.3 depicts the expected ambient dose equivalent rate 20 weeks after the irradiation end. The 18  $\phi$ -bins in the X-Y plane are averaged over  $Z = 0 - 350$  cm. The borders of the 'supermodule' for which the radioactive decay step was performed is outlined in black. This volume shows the highest residual dose in the X-Y plane. The ambient dose equivalent rate after 20 weeks can be compared to the left



**Figure 18.3:** Ambient dose equivalent rates after one week (left) and 20 weeks (right) for a single activated supermodule. Results, calculated in a  $R$ - $\phi$ - $Z$  binning system, are shown averaged over  $0 \text{ cm} < Z < 350 \text{ cm}$ . The binning system is aligned with the CMS detector (even though all other components are removed for this simulation step). There are 18  $\phi$ -bins such that one bin covers exactly the range of a supermodule (version 3.15.17.0) [202].

figure, which shows the residual dose after one week. It illustrates the dominance of short-lived over long-lived nuclei, by a  $\dot{H}^*(10)_{\text{ind}}$  decreasing by one order of magnitude over this time period. The remaining maximal ambient dose equivalent rate after 20 weeks is maximal  $1.4 \mu\text{Sv h}^{-1}$  in the EB supermodule.

Figure 18.4 shows the ambient dose equivalent rate after 20 weeks as a function of  $R$  for two different  $Z$ -regions in EB, which are illustrated by the two sketches on top of the two figures. The two regions are averaged over one supermodule (the  $\phi$ -bin) and 20 cm in  $Z$  at the end of EB ( $245 \text{ cm} < Z < 265 \text{ cm}$  and  $255 \text{ cm} < Z < 275 \text{ cm}$ ), where the dose rate for the SM is maximal. The blue shaded region illustrates the extent of EB in  $R$ -direction. The maximum of the ambient dose equivalent rate after 20 weeks of the irradiation stop has a magnitude of about  $1.4 \mu\text{Sv h}^{-1}$  at the end of the  $\text{PbWO}_4$  region. This is due to the shelf-shielding of the  $\text{PbWO}_4$  crystals, which leads to a higher residual dose for larger depths in  $R$ . This interpretation is supported by the immediate decrease of the ambient dose equivalent rate at the start of the EB electronics volume. The left side of each peak shows also a second maximum in  $\dot{H}^*(10)_{\text{ind}}$ , which is created by the interaction of thermalized neutrons from the polyethylene layer upstream to the EB with the  $\text{PbWO}_4$  material. Comparing the left and right distribution, the ambient dose equivalent rate is about 10 % higher for the region-1 at higher pseudorapidity, the increase is however still covered by the statistical uncertainty of both distributions. The left distribution is also further away from the barrel boarder region and the characteristics of the tracking material are therefore more distinct in the left tail of the distribution. To estimate if the predicted  $\dot{H}^*(10)_{\text{ind}}$  is a radiological hazard to personnel, the official CERN radiation protection (RP) guidelines [203] are applied for this scenario. It is important to note that this profile distribution gives the ambient dose equivalent rate

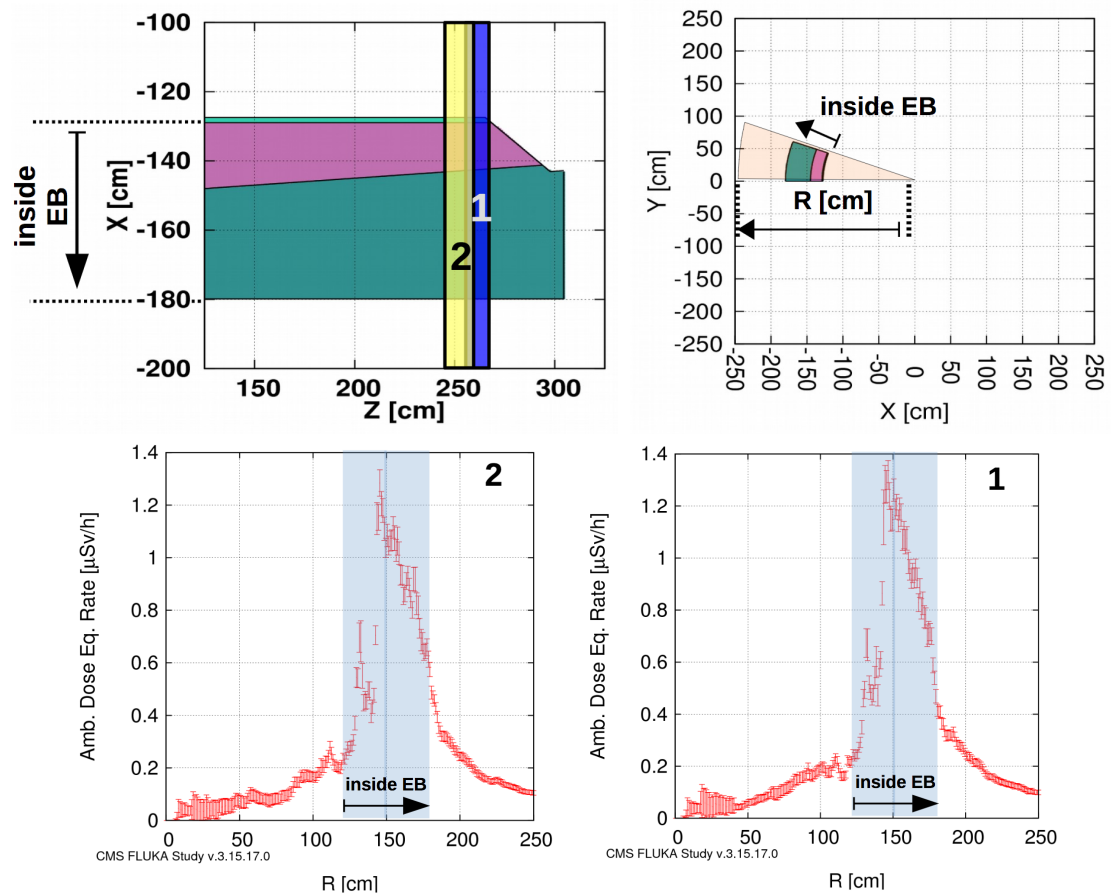
inside the SM. For personnel working on the SM, the expected  $\dot{H}^*(10)_{\text{ind}}$  outside of the SM is more important. In fact, preliminary studies show that the  $\dot{H}^*(10)_{\text{ind}}$  is slightly higher adjacent to the SM electronics ( $\mathcal{O}(1 \mu\text{Sv h}^{-1})$  after 20 weeks) compared to the area next to the  $\text{PbWO}_4$  crystals ( $\mathcal{O}(0.5 \mu\text{Sv h}^{-1})$  after 20 weeks). This is due to the self-shielding of the crystals, which results in a lower  $\dot{H}^*(10)_{\text{ind}}$  next to the crystal volume.

To estimate if the predicted  $\dot{H}^*(10)_{\text{ind}}$  is a radiological hazard to personnel, the official CERN radiation protection (RP) guidelines [203] are applied for this scenario. The RP guidelines follow the Swiss and EU law and classify the radiological hazard in different areas. The first designated area is the 'supervised radiation area' with a maximum dose limit of 6mSv/year. If a working area is exposed to this amount of dose, the shielding and installation of workplaces have to be optimized with respect to the exposure to radiation. The  $\dot{H}^*(10)_{\text{ind}}$  of the workplace area need to be below  $3 \mu\text{Sv h}^{-1}$  and a few spots with low occupancy may be exposed to up to  $15 \mu\text{Sv h}^{-1}$ .

The next level is the 'controlled radiation area' with a maximum dose limit per year of 20mSv. If personnel is working in this radiation environment, all work must be planned and optimized, including dose estimations. This area is subdivided into two classifications: for the 'controlled simple area', the  $\dot{H}^*(10)_{\text{ind}}$  of the workplace area needs to be below  $10 \mu\text{Sv h}^{-1}$  and at low occupancy spots below  $50 \mu\text{Sv h}^{-1}$ . The following two more exposed environments are the 'controlled limited stay' and 'controlled high radiation' areas with a maximum  $\dot{H}^*(10)_{\text{ind}}$  at low occupancy spots of  $2 \text{mSv h}^{-1}$  and  $100 \text{mSv h}^{-1}$ , respectively. If the dose levels reach such high values, there are dedicated limits for the different body parts.

The predicted conservative  $\dot{H}^*(10)_{\text{ind}}$  levels for the work on the supermodules in a low radiation environment ( $0.07 \mu\text{Sv h}^{-1}$ ) classifies this area most likely as a 'supervised radiation area'. Following the ALARA principles (As Low As Reasonable Achievable), personnel can be easily shielded from active elements. These are primarily the  $\text{PbWO}_4$  crystals, but also parts of the electronic system like the backplate or the respective screws, which contain chrome or stainless steel.

For the outstanding optimized simulations of the intervention in the EB during LS3 more ALARA regulations have to be fulfilled, including risk levels which measure not only the individual and collective dose and dose rate, but also the atmospheric and surface contamination.



**Figure 18.4:** The two upper geometry sketches show the location of the activated supermodule in the X-Y plane (left) and the regions of the two subsequent distributions in the Z-X plane (right). In the two bottom plots, the ambient dose equivalent rates as a function of radius (where the supermodule remains in the CMS coordinate system) are shown. The results are averaged over  $245 \text{ cm} < Z < 265 \text{ cm}$  (left) and  $255 \text{ cm} < Z < 275 \text{ cm}$  (right), and in each case, results are averaged over a single  $\phi$ -bin ( $2.44 \text{ rad} < \phi < 3.14 \text{ rad}$ ) covering the SM.



# Radiation studies for the scintillators of a Shashlik calorimeter

Several heavy inorganic scintillators were subject to proton-irradiation tests to determine their material degradation and residual dose due to high hadron fluences. The first Section 19.1 introduces suitable scintillators for such a calorimeter. The performed proton-irradiation tests and the comparison of the measured ambient dose equivalent rates of the crystals to my FLUKA simulations are focus of the second Section 19.2. As FLUKA is used to make predictions of the residual radiation environment in CMS in terms of potential dose to personnel as well as its contribution to background signals in the detectors, it is useful to first compare simulation and measured values of the residual ambient dose equivalent rates in the controlled test beam scenario. Particular attention in the simulations is given to isotopes that would contribute with a prohibitive background to the measured signal.

## 19.1 The scintillator options of the Shashlik calorimeter

The Shashlik calorimeter consists of alternating layers of an absorber, tungsten, and active plates of a heavy inorganic scintillator. Suitable candidates for the active layers, which are able to cope with the harsh radiation environment while allowing a precise signal reconstruction, are barium-doped cerium fluoride ( $\text{CeF}_3$ ), cerium-doped lutetium orthosilicate ( $\text{Ce}_{2x}(\text{Lu}_{1-y}\text{Y}_y)_{2(1-x)}\text{SiO}_5$ , LYSO) and cerium-doped yttrium orthosilicate ( $\text{Ce}_{2x}\text{Y}_{2(1-x)}\text{SiO}_5$ , YSO). The cerium in YSO and LYSO is an activator for the scintillation process, whereas the barium in  $\text{CeF}_3$  increases its radiation tolerance.

The physical properties of these scintillators are compared to  $\text{PbWO}_4$  in Table 19.1. For each quantity, the respective best scintillator choice is highlighted with the value in bold font. However, when considering the overall performance of the Shashlik calorimeter,

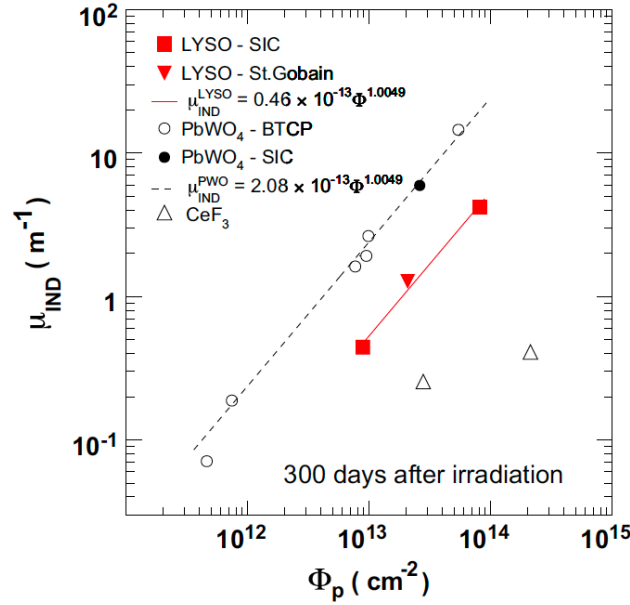
**Table 19.1:** Properties of the considered scintillator materials as used in the FLUKA simulations: density ( $\rho$ ), radiation length ( $X_0$ ), light yield (LY), scintillation decay time ( $\tau_{SC}$ ), peak emission wavelength ( $\lambda_{em}$ ). The values are taken from Ref. [8].

|                      | $\rho$<br>(g/cm <sup>3</sup> ) | $X_0$<br>(cm) | LY<br>( $\gamma$ /MeV) | $\tau_{SC}$<br>(ns) | $\lambda_{em}$<br>(nm) |
|----------------------|--------------------------------|---------------|------------------------|---------------------|------------------------|
| <b>Scintillators</b> |                                |               |                        |                     |                        |
| PbWO <sub>4</sub>    | 8.28                           | 0.89          | 200                    | 30                  | 420                    |
| YSO:Ce               | 4.53                           | 3.11          | 24000                  | 70                  | 420                    |
| LYSO:Ce              | <b>7.3</b>                     | <b>1.14</b>   | <b>32000</b>           | 40                  | 430                    |
| CeF <sub>3</sub>     | 6.16                           | 1.70          | 4400                   | <b>27</b>           | <b>320</b>             |
| <b>Absorber</b>      |                                |               |                        |                     |                        |
| W                    | 0.35                           | 19.3          |                        |                     |                        |

it is important to note that the relative advantage of these properties also depends on the other components of the sampling calorimeter.

Since the hadron-induced degradation in PbWO<sub>4</sub> is the reason for the new EE, the radiation damage in the scintillator material is of utmost importance. The induced absorption coefficient as a function of the incident proton fluence  $\Phi_p$  for PbWO<sub>4</sub>, LYSO and CeF<sub>3</sub> is depicted in Figure 19.1 and taken from Ref. [5, 182]. It illustrates that no cumulative hadron-induced damage could be found for CeF<sub>3</sub>, since it does not contain any elements with atomic numbers above the fission threshold ( $Z > 71$ ). A similar conclusion is drawn for YSO by dedicated FLUKA simulations. LYSO on the other hand contains lutetium, which atomic number is right at the fission threshold [204] and exhibits a cumulative hadron damage according to Figure 19.1. This damage is however a factor five smaller than for PbWO<sub>4</sub>.

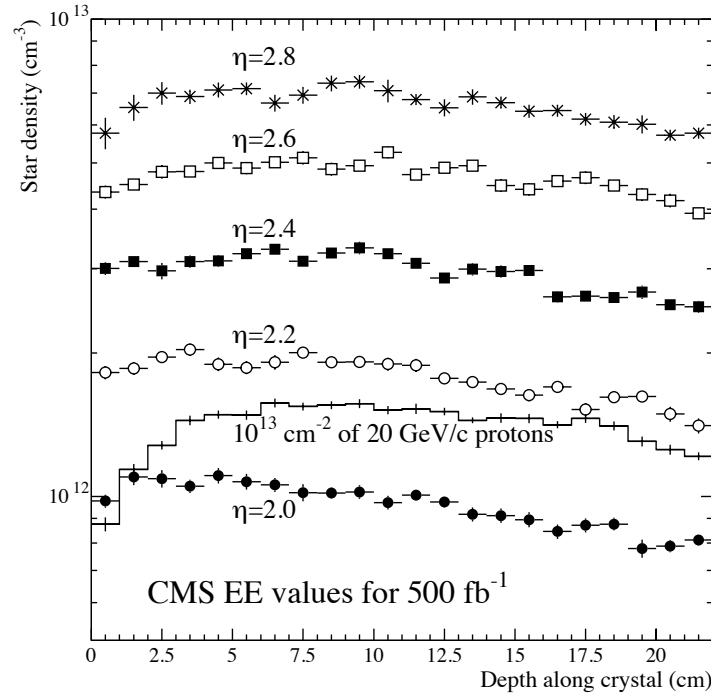
In conclusion, a CeF<sub>3</sub> based scintillating calorimeter would be the best choice with respect to a possible hadron induced damage. Since the light path of a signal to the readout is reduced in a sampling calorimeter in comparison to a homogeneous calorimeter, LYSO is also still a possible option.



**Figure 19.1:** Induced absorption coefficient  $\mu_{\text{ind}}(\lambda)$  versus proton fluence  $\Phi_p$  for  $\text{CeF}_3$ , LYSO and  $\text{PbWO}_4$  crystals of different length and origin, detailed in Chapter 19.2 [5, 182].

## 19.2 The residual dose of the scintillators after proton-irradiation tests

The Shashlik calorimeter would have to withstand a harsh radiation environment in CMS, created by a mixed particle field as described in Section 16.2 and further discussed in Section 20.2.1. Therein, the charged hadron fluence in the EE of CMS is dominated by  $\mathcal{O}(1 \text{ GeV})$  pions. The radiation tolerance and residual dose of the scintillators had to be verified by actual irradiations of the crystals, mimicking the impact of the hadron fluence in a Shashlik calorimeter in CMS. The IRRAD1 test facility at the T7 beamline of the PS accelerator at CERN [205] provides protons with an energy of up to 25 GeV and is often used as a beam facility for hadron-irradiations. These relatively high-energy protons give a good estimate of the hadron-induced degradation of  $\text{PbWO}_4$  crystals in CMS for reasons shortly outlined in the following: Ref. [206] shows experimentally that the quantification for the cumulative degradation, the star density, in  $\text{PbWO}_4$  for a 290 MeV pion-irradiation scales in the same way as for an irradiation with 20-24 GeV protons. The cumulative damage from proton-irradiations further needs to scale to LHC or HL-LHC running conditions to predict the material degradation from proton-irradiations. Figure 19.2 shows the predicted star densities in a  $\text{PbWO}_4$  crystal for a proton-irradiation of  $10^{13} \text{ p/cm}^2$  together with the star density for different pseudorapidities in CMS. It highlights that the star density can be used to scale between different proton-beam energies and pseudorapidity regions in CMS for  $\text{PbWO}_4$ . A fluence of  $10^{13} \text{ p/cm}^2$  from



**Figure 19.2:** FLUKA simulation of the star density at different  $\eta$  in the CMS endcap ECAL for an integrated luminosity of  $500 \text{ fb}^{-1}$  together with the average star density in a single crystal irradiated with  $10^{13} \text{ p/cm}^2$  in the 20 GeV/c beam line (solid line) [181].

20 GeV protons corresponds to  $500 \text{ fb}^{-1}$  at  $|\eta| = 2.1$ . This scaling is possible since a  $\text{PbWO}_4$  crystal in CMS is surrounded by other crystals of the same dense material, creating a rather uniform,  $\mathcal{O}(1 \text{ GeV})$ -pion dominated charged hadron fluence. For the proton-irradiation of a single crystal, the higher energy creates a similar charged hadron fluence since only one crystal is irradiated and part of the created hadron shower can leak out of the crystal.

Assuming that the proton-irradiations give a reliable estimate of the radiation environment in CMS, this chapter focuses on the comparison of the measurement of the ambient dose equivalent rate after proton-irradiations with FLUKA predictions. Previous results for the  $\dot{H}^*(10)_{\text{ind}}$  of  $\text{PbWO}_4$  [181] and  $\text{CeF}_3$  [182] before this thesis work are used to validate my subsequent studies. The studies of the residual dose rate for LYSO [5], other  $\text{CeF}_3$  and YSO crystals are described in more detail thereafter. The results can be used to validate the FLUKA description of the respective materials for the simulation of a Shashlik sampling calorimeter in CMS.

### 19.2.1 Experimental setup for the proton-irradiations

The FLUKA description of this setup was first developed for Ref. [181] to quantify and explain the hadron-induced damage in  $\text{PbWO}_4$  for proton-irradiations. The specifications of this proton-irradiation setup of  $\text{PbWO}_4$  crystals is listed in the first row of Table 19.2 for reference. Ref. [182] reports on the results of proton-irradiations of  $\text{CeF}_3$  crystals ( $8.4 X_0$ ), listed in the second row of Table 19.2. The simulation of the irradiation setup is thereby based on the previous setup of Ref. [181]. Before performing simulations for the new materials investigated as part of this dissertation, these FLUKA studies were repeated to check the correct use of the simulation set-up.

The irradiation zone of the IRRAD1 test facility is surrounded by steel walls at a distance of  $\mathcal{O}(40\text{ cm})$ . The back wall also serves as the beam dump, absorbing the residuals of the beam. The crystals were placed in a polystyrene box, and aligned to the beam, such that the beam was hitting the crystals perpendicular to their front face, illustrated in Figure 19.3 (corresponding to the irradiation setup of Section 19.2.4). The beam size was widened to cover the front face of the respective crystal. An aluminum foil, which was placed upstream to the crystal, was irradiated by the beam and gave as such an estimate of the beam profile. All crystal lengths were chosen to be well above one radiation length to ensure the development of a hadron shower within the material. The details of the fluence ( $\Phi_p$ ), flux ( $\dot{\Phi}_p$ ), the beam energy and the crystal dimensions of the respective irradiation can be found in Table 19.2.

The details of the beam profile during irradiation are limited, since the only available information is the one of the beam energy and its nominal size as well as the beam profile imprinted on the aluminum foil. The beam profile for the FLUKA simulations was therefore assumed to be uniformly distributed. For the first simulation setup of Section 19.2.2, the beam profile was chosen to be rectangular, assuming that the beam covers the full crystal front face uniformly. Since the aluminum foil rather showed a Gaussian beam profile, leading to a higher beam intensity in the center of the crystal than on its sides, this may have lead to an underestimation of the residual dose in the simulation: a higher beam intensity in the center of the crystal results in a higher residual dose at this point. This might however not be measurable at the sides of the crystal due to self-shielding effects of the crystal itself.

For the later simulation of the irradiation setup of Section 19.2.4, the beam profile was assumed to be Gaussian shaped to account at least partly for this effect. Non-uniformities could nevertheless not be accounted for and the limited knowledge on the beam profile during irradiation is one major uncertainty of the simulation.

Due to the position of the crystal, the induced hadron shower within the crystal is in average aligned with the beam axis. As a result, the integrated hadron fluence at the end of the crystal is about 10 times higher than the lateral one [8]. This leads to a higher

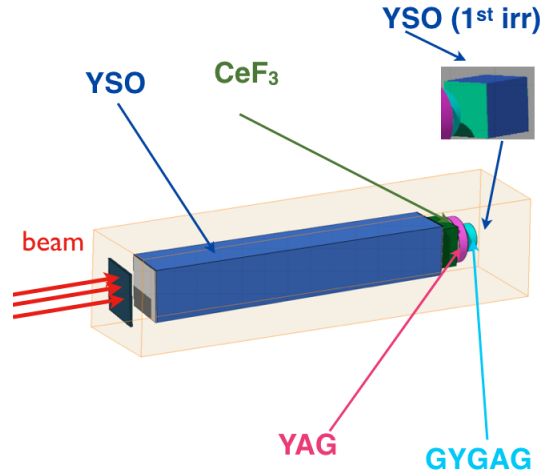
**Table 19.2:** Scintillator dimensions, beam energy, fluence ( $\Phi_p$ ) and flux for the irradiations described in Chapter 19.2. The first two rows quote results, which were performed before my thesis.

| Scintillator                                           | Volume<br>[ cm <sup>3</sup> ]                                                              | E<br>[ GeV ] | $\Phi_p$<br>[ cm <sup>-2</sup> ]                                     | $\dot{\Phi}_p$<br>[ cm <sup>-2</sup> h <sup>-1</sup> ] | Ref.  |
|--------------------------------------------------------|--------------------------------------------------------------------------------------------|--------------|----------------------------------------------------------------------|--------------------------------------------------------|-------|
| 8 <b>PbWO<sub>4</sub></b><br>crystals                  | front: $2.4 \times 2.4$<br>back: $2.6 \times 2.6$<br>length: 23.0                          | 20           | $\leq 5.4 \times 10^{13}$                                            | $\leq 1 \times 10^{13}$                                | [181] |
| <b>CeF<sub>3</sub>:</b><br>1st irr.<br>2nd irr.        | $2.1 \times 1.6 \times 14.1$                                                               | 24           | $(2.78 \pm 0.20) \times 10^{13}$<br>$(2.12 \pm 0.15) \times 10^{14}$ | $1.16 \times 10^{12}$<br>$0.94 \times 10^{13}$         | [182] |
| <b>LYSO:</b><br>1st irr.<br>2nd irr.                   | $2.4 \times 2.4 \times 23.0$                                                               | 24           | $(8.85 \pm 0.62) \times 10^{12}$<br>$(7.24 \pm 0.16) \times 10^{13}$ | $5.97 \times 10^{12}$<br>$3.82 \times 10^{12}$         | [5]   |
| <b>1st irr.:</b><br>1.YSO<br>2.YSO<br>CeF <sub>3</sub> | $1.5 \times 1.5 \times 1.7$<br>$2.5 \times 2.5 \times 15.0$<br>$2.0 \times 2.0 \times 1.0$ | 24           | $(9.96 \pm 0.74) \times 10^{12}$                                     | $4.41 \times 10^{12}$                                  | -     |
| <b>2nd irr.:</b><br>2.YSO<br>CeF <sub>3</sub>          | $2.5 \times 2.5 \times 15.0$<br>$2.0 \times 2.0 \times 1.0$                                | 24           | $(9.86 \pm 0.79) \times 10^{13}$                                     | $4.74 \times 10^{12}$                                  | -     |

amount of neutrons in the back, which can then propagate and be backscattered from the back wall. The back of the irradiation facility is therefore simulated in greater detail than the side walls as those have a less significant influence on the scintillator material. If this background wall is not precisely enough simulated, an important source of low-energy neutrons may be neglected. In the FLUKA simulation setup, I described the T7 beam dump as a volume consisting of marble (20 cm) and iron yoke parts (48 cm).

After the irradiation stop, the crystals were first locked away until the residual dose rate was at a level which allowed human handling. The crystals were then stored in a laboratory with low radiation background ( $0.07 \mu\text{Sv h}^{-1}$ ) and the ambient dose equivalent rate was measured in regular time intervals. An Automess 6150AD6 instrument [181] was used for these measurements, which has an active volume of  $1 \text{ cm}^3$ , located at a distance of 1.2 cm behind the radiation-entrance window of the device. The device was placed at 4.5 cm from the center of the long side of the crystal.

For the radioactivation simulation the settings and the two-step method, detailed in Section 17.2.2 were used. During the irradiation (first step), the radionuclides were produced in the material. The same production and transport thresholds as detailed in Chapter 17.2.1 were used, except for photons and charged hadrons which were simulated



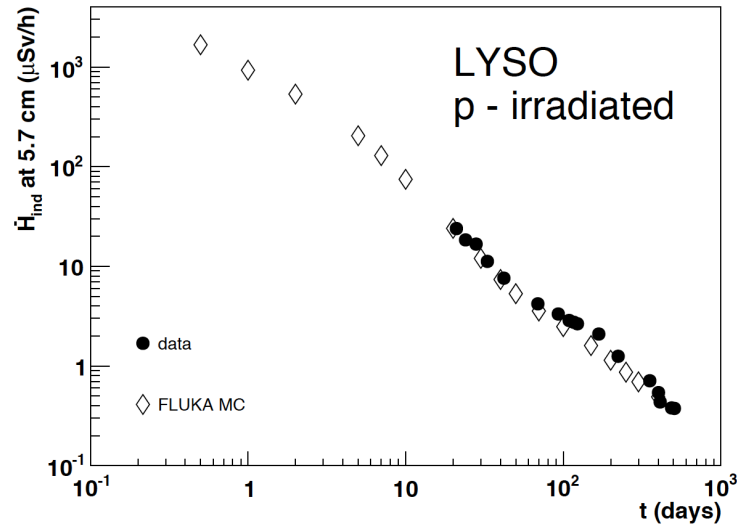
**Figure 19.3:** Geometrical setup in FLUKA for a 15 cm YSO crystal, followed by a 1 cm long  $\text{CeF}_3$  crystal, a YAG and GYGAG crystal and a 1.7 cm crystal in the back. All crystals are placed in a polystyrene box (beige) with the beam hitting the crystals perpendicular to the front face. The smaller YSO crystal is only exposed to the first irradiation.

down to 10 keV and 1 keV, respectively. The lower thresholds were possible since the simulation setup is less complex and the production and transport of secondary particles need less computing power with respect to a simulation in the CMS environment. The ambient dose equivalent rate was simulated in an active volume of  $1 \text{ cm}^3$  at a 5.7 cm distance from the longitudinal center of the crystal, taking into account the natural dose in the final estimate. In the following, all integrated fluence is normalized to  $10^{13} \text{ p/cm}^2$  to facilitate the comparison among different irradiations and materials.

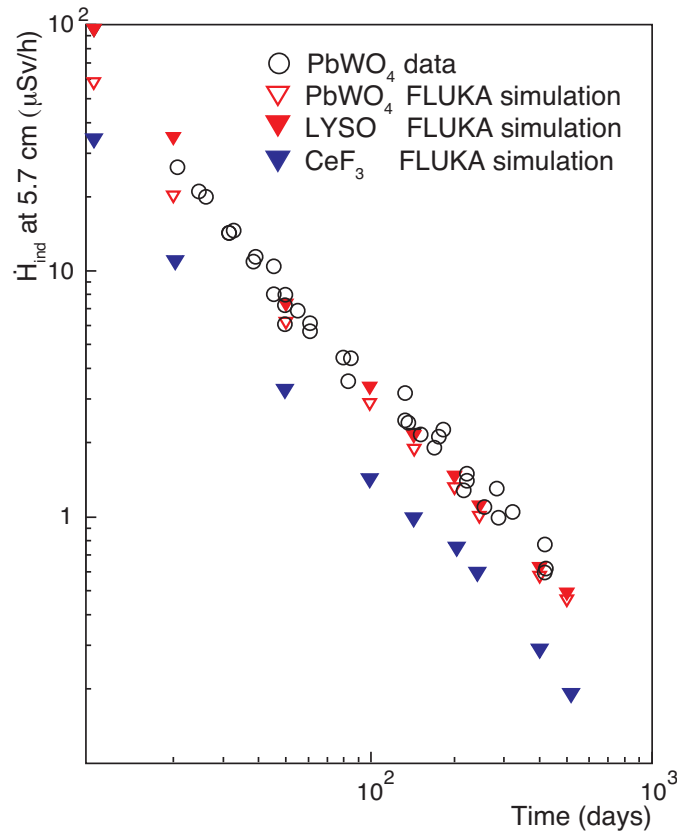
### 19.2.2 Remnant dose of proton-irradiated LYSO crystal

A cerium-doped LYSO ( $\text{Ce}_{0.003}(\text{Lu}_{0.1}\text{Y}_{0.9})_{1.997}\text{SiO}_5$ ) crystal produced by the Shanghai Institute of Ceramic (SIC) [207] with a radiation length of  $8.8 X_0$  was exposed to proton-irradiation according to the above described experimental setup, using the specifications listed in the third row of Table 19.2 and a squared and uniform beam ( $5 \times 5 \text{ cm}^2$ ) profile.

The measured and predicted  $\dot{H}^*(10)_{\text{ind}}$  after the first irradiation over time is visualized in Figure 19.4. The results agree within their uncertainties with each other over a period of one year and two orders of magnitude of the  $\dot{H}^*(10)_{\text{ind}}$ . Accounting for the statistical uncertainties of the simulation and the uncertainties associated with the dose measurements, an underprediction from the simulation is observed after 150 days. Given that the discrepancy is not visible at all cooling times, a likely cause is the current official isomer production model in FLUKA. The simulated equal share between ground and excited isomer states might underestimate the radioactivity of an isomer with a high decay activity around 150 days.



**Figure 19.4:** Measurement of  $\dot{H}^*(10)_{\text{ind}}$  as a function of time after the first irradiation, starting 20 days after irradiation and taken at 5.7 cm from the side of the crystal, compared to FLUKA simulations. Data and simulations are scaled to a fluence of  $10^{13} \text{ p/cm}^2$  [5].



**Figure 19.5:** Ambient dose equivalent rate at distance 5.7 cm from the side of the crystal as a function of time after irradiation, calculated with FLUKA for a LYSO and  $\text{CeF}_3$  crystal exposed to a fluence  $\Phi_p = 10^{13} \text{ p/cm}^2$  of 20 GeV/c protons compared to data and simulations for  $\text{PbWO}_4$  from [5, 181, 182] for the same irradiation conditions (all crystals  $26 X_0$  long).

### 19.2.3 Comparison of residual dose among scintillator options

In order to compare the residual radioactivity among all options, I normalized the scintillators to the same radiation length of  $26 X_0$ . This length corresponds to the size of the current  $\text{PbWO}_4$  ECAL crystals, since this is also the necessary depth for a potential homogeneous scintillating ECAL in CMS. A transverse area of  $24 \text{ mm} \times 24 \text{ mm}$  was used for all crystals. A radiation length of  $26 X_0$  corresponds to a length of 30 cm for LYSO and 42 cm for  $\text{CeF}_3$  due to their smaller densities, which are listed in Table 19.1. The simulation of  $\dot{H}^*(10)_{\text{ind}}$  for LYSO and  $\text{CeF}_3$  relies on the above described agreement of simulations with measurements for smaller sized crystals, since no  $\text{CeF}_3$  or LYSO crystals with a length of  $> 30 \text{ cm}$  are yet produced.

Figure 19.5 shows  $\dot{H}^*(10)_{\text{ind}}$  for these full sized crystals. The predicted  $\dot{H}^*(10)_{\text{ind}}$  for  $\text{PbWO}_4$  agrees within a factor two with measurements, and is systematically underestimated. The predicted  $\dot{H}^*(10)_{\text{ind}}$  for  $\text{PbWO}_4$  and LYSO have a similar magnitude. The simulated  $\dot{H}^*(10)_{\text{ind}}$  of  $\text{CeF}_3$  is by a factor two smaller than the predicted  $\dot{H}^*(10)_{\text{ind}}$  of  $\text{PbWO}_4$ . It is important to note, that for this comparison the transverse size was chosen to be the same for all crystals. Since  $\text{CeF}_3$  is less dense than  $\text{PbWO}_4$ , it has a larger Molière radius of 2.6 cm [182], compared to the one of  $\text{PbWO}_4$  (2.2 cm) [8]. With the same transverse size, the energy from the particle showers might have partly escaped the  $\text{CeF}_3$  scintillator material, leading to a slightly lower residual dose rate as if the transverse dimensions would have been enlarged according to their Molière radii.

In conclusion, the residual dose rate for LYSO and  $\text{CeF}_3$  is expected to be similar to the one of  $\text{PbWO}_4$  in a  $26 X_0$  deep and transversely extended calorimeter.

### 19.2.4 Radioactivation studies of YSO crystals

The last scintillator material I studied was cerium-doped YSO ( $\text{Ce}_{0.004}(\text{Y}_{1.992}\text{SiO}_5)$ ). Few yttrium isotopes have a rather high thermal neutron cross-section and their decay might add a constant noise to the readout of a future YSO based calorimeter. I compared the predicted and observed ambient dose equivalent rate and studied the created residual nuclei. In the same experimental setup as described in Chapter 4, two irradiations were performed with the specifications listed in the fourth row of Table 19.2. Two YSO crystals were irradiated, the smaller one (1.7 cm long) was only exposed to the first irradiation. The beam profile was assumed to be uniformly Gaussian shaped, with a FWHM of 1.4 cm in each direction. The setup and the positioning of the crystals is visualized in Figure 19.3. The scintillators GYGAG and YAG were also irradiated, but their results are not further discussed here.

**Table 19.3:** Dose and dose rate values for the small YSO crystal during the first irradiation and the big YSO and CeF<sub>3</sub> crystal during the 2nd irradiation.

| Quantity          | Small YSO 1st.irr       | Big YSO                 | CeF <sub>3</sub>         |
|-------------------|-------------------------|-------------------------|--------------------------|
| Dose (kGy)        | $14.8 \pm 0.1 \pm 1.1$  | $93.0 \pm 0.3 \pm 7.3$  | $162.3 \pm 1.1 \pm 12.8$ |
| Dose rate (kGy/h) | $6.1 \pm < 0.1 \pm 0.5$ | $4.5 \pm < 0.1 \pm 0.4$ | $7.8 \pm 0.1 \pm 0.6$    |

### Dose rate in YSO during irradiation

In comparison to LYSO and CeF<sub>3</sub>, the scintillator YSO is not yet well studied. Therefore various studies for YSO are planned. For example a  $\gamma$ -irradiation test, with the same applied dose and dose rate as the proton-irradiation, in order to disentangle the cause of the respective (i.e. proton and electromagnetic ionization) damage effects. With the dose (rate) of the crystals during proton-irradiation, which are calculated in this section, the estimates can be used to find a  $\gamma$ -irradiation facility providing similar dose (rates). Table 19.3 lists the dose and dose rate of the YSO crystals together with the CeF<sub>3</sub> crystal during irradiation. The predicted values include a systematic uncertainty due to the integrated beam fluence uncertainty of about 7 %. The simulation of the hadron spectra within the 15 cm YSO crystal produced at SIC [207] showed a 2-5 times lower fluence for the first millimeter compared to the last millimeter of the crystal. The hadron spectra at the end of this YSO crystal show an increase of high-energy ( $> 100$  MeV) protons, pions and neutrons, which agrees with the build-up of a hadron shower towards the end of the crystal.

### Residual activity in YSO

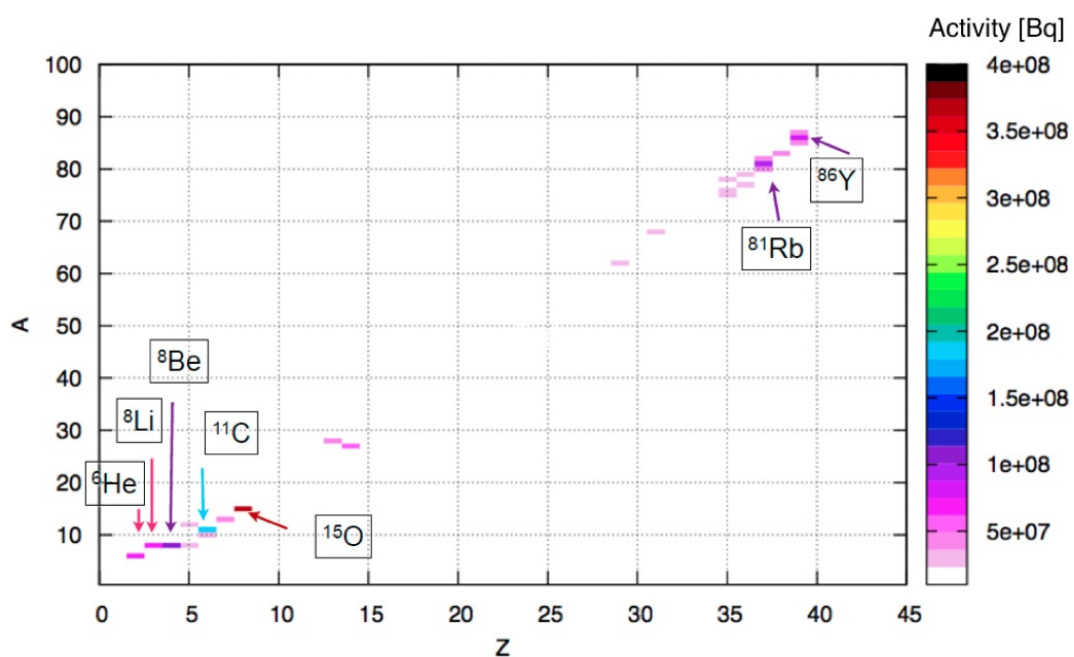
The estimated residual dose rate directly after the second irradiation was estimated to  $(10.6 \pm 0.9) \times 10^4 \mu\text{Sv h}^{-1}$  in the 15 cm long YSO crystal. After a cooling time of 43 days, the residual dose rate of the 15 cm YSO and CeF<sub>3</sub> crystal was within the radiation protection limits and  $\dot{H}^*(10)_{\text{ind}}$  could be measured. My comparison of the measured  $\dot{H}^*(10)_{\text{ind}}$  to FLUKA simulations is listed in Table 19.4. The measured and simulated values for CeF<sub>3</sub> agree within their uncertainties, but for YSO, a systematic underestimation of  $\dot{H}^*(10)_{\text{ind}}$  of up to 20 % for large times is observed. This discrepancy is however still at an expected level for FLUKA simulations. The difference may be due to the simplified representation of the irradiation facility, which might have neglected an important source of low-energy neutrons, for instance from the shielding at the sides or the back wall. This could have easily lead to an underestimate of the low energy neutron fluence of up to 20 %. If this would have been the case however, the LYSO and CeF<sub>3</sub> residual dose simulations should have shown a similar picture. As discussed above, another reason could be that the beam profile during the irradiation might not

**Table 19.4:** Residual ambient equivalent dose rate, measured and simulated for the 15 cm YSO and the  $\text{CeF}_3$  crystal. The measured value at 137 days value for YSO is an estimated, since it was not measured precisely at 5.7 cm distance, but an approximative distance.

| 1+2 irr.       | 43 days |                  | 137 days          |                | 202 days |                |
|----------------|---------|------------------|-------------------|----------------|----------|----------------|
|                | Mes     | Sim              | Mes               | Sim            | Mes      | Sim            |
| 15 cm YSO      | -       | $172.9 \pm 14.0$ | $\mathcal{O}(90)$ | $77.7 \pm 6.2$ | 68       | $49.5 \pm 6.2$ |
| $\text{CeF}_3$ | -       | $3.5 \pm 0.3$    | 1.32              | $1.1 \pm 0.1$  | 0.7      | $0.8 \pm 0.1$  |

have been as uniform as assumed in the simulation. The beam might have not covered the full crystal with uniform intensity, but might have exposed the center of the crystal to a higher proton rate. The higher radioactivity in the center of the crystal would then be shielded by the material itself, resulting in a lower measured  $\dot{H}^*(10)_{\text{ind}}$ . Another reason for the underestimate could be impurities of the YSO material. However, the relative amount of cerium in this YSO material is precisely known and other impurities would be expected to be at the permille level [207]. Even though the culprit could not be determined, the agreement between measurements and simulations was still at a level to validate the YSO FLUKA description for further studies.

I concluded my study by simulating the residual nuclei during and after irradiation. The residual nuclei were examined for different time periods after the irradiation stop to disentangle short and long-lived isotopes. The chosen times were: 0 s, 1 s, 2 s, 5 s, 30 s, 60 s, 1 h, 1 d, 43 d, 137 d and 202 d. A comparison of the deposited energy from the prompt electromagnetic shower and the deposited energy from decay products during irradiation shows that the deposited energies from the decay products is three orders of magnitude lower. This estimate suggests, that the decay products do not induce a prohibitive background to the readout of a YSO based calorimeter. Figure 19.6 depicts the residual nuclei for the full YSO crystal 0 s after the irradiation, which means that it shows the residual nuclei produced during the irradiation. To obtain the most active isotopes, a threshold of  $10^7$  Bq is applied. About nine residual nuclei with an activity (A) of  $\mathcal{O}(10^8$  Bq) were produced. All of the light elements are short-lived and only isomers with an atomic and mass number similar to yttrium are longer lived with half-times of a couple of hours. This is not unexpected since  $^{89}\text{Y}$  has a high thermal neutron cross-section of 1.28 b [208].



**Figure 19.6:** Activity of residual nuclei in the 15 cm long YSO crystal after a proton-irradiation of  $10^{14}$  p/cm<sup>2</sup> at irradiation stop. A threshold of  $10^7$  Bq is applied.

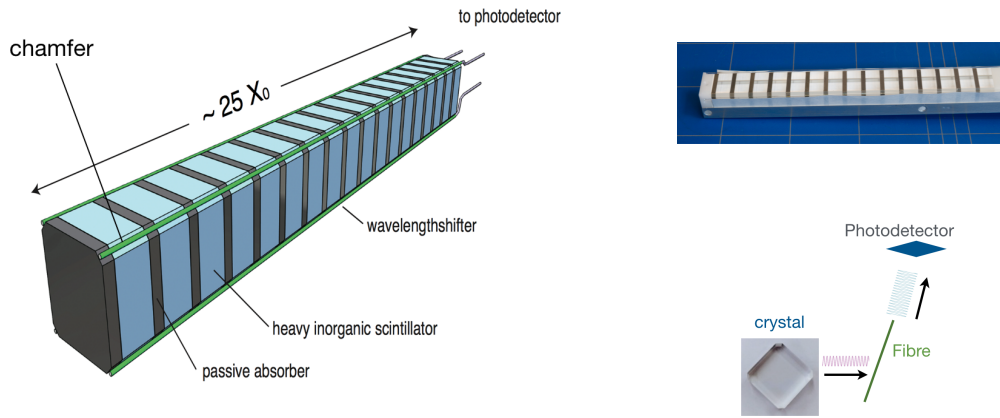
# Radiation studies for a Shashlik calorimeter in the CMS environment at the HL-LHC

After reviewing the radiation tolerance and residual dose of the scintillator options for a Shashlik calorimeter, this chapter focuses on the behavior of the full Shashlik calorimeter in the CMS environment at the HL-LHC. First, my implementation of the Shashlik calorimeter in the FLUKA CMS description is surveyed and the particle spectra in such a sampling calorimeter are discussed. Subsequently, the fluence of the previous proton-irradiations is scaled to the fluences in CMS at the HL-LHC. Finally, the radioactivation of the Shashlik calorimeter is studied. Causes of residual radiation as well as their negative impact to the ECAL readout are discussed.

## 20.1 The Shashlik calorimeter in the FLUKA CMS description

The Shashlik calorimeter, designed by the ETHZ group and collaborators, consists of alternating layers of an absorber, tungsten, and active plates of a heavy inorganic scintillator. Suitable scintillators, providing a reliable and precise performance under HL-LHC irradiation conditions were discussed in the previous chapter. The following overview of the general Shashlik calorimeter design serves the understanding of the implementation of the Shashlik calorimeter in the FLUKA CMS environment and the studies thereafter.

The relative energy loss of particles in a Shashlik calorimeter is defined by the effective radiation length ( $X_{0,\text{eff}}$ ) [210]. The radiation length of the respective scintillator has thus to be folded with the one of the absorber to compare the different options among each other. The effective radiation length, listed in Table 20.2, is in this case still driven by the



**Figure 20.1:** Sketch (left) and picture (top right) of the Shashlik calorimeter. Bottom right: sketch of a light path of an incident electromagnetic particle on the scintillating crystal, via the WLS fiber to the photodetector [3, 209].

radiation length of the scintillator as all options use tungsten as the absorber material. The energy deposited in the active layers of the Shashlik calorimeter is read out by radiation tolerant wavelength shifting (WLS) fibers, which run along depolished chamfers as illustrated on the left in Figure 20.1. These WLS fibers absorb wavelengths in the visible spectrum, shift the wavelengths and transport the light to the silicon-based photodetectors. According to Table 19.1, all previously discussed scintillator materials are well suited for a Shashlik calorimeter as their peak emission wavelengths are in the visible spectrum.

This sampling calorimeter design further minimizes the light path of the signal with respect to the current homogeneous calorimeter, and therefore reduces the effects of radiation damage. For an estimate of the signal time, the decay time of the scintillator has to be folded with the one of the chosen WLS fiber. The Shashlik calorimeter design can also be optimized with regard to the Molière radius ( $R_M$ ) to better distinguish among tracks from pile-up events.

A  $\text{CeF}_3$  Shashlik calorimeter, built by the ETHZ group, was the focus of several irradiation tests. A single-channel prototype was studied with respect to its energy resolution and uniformity, followed by a  $5 \times 5$  channel matrix, built to determine the angular dependence of the design [3, 209]. A similar LYSO Shashlik calorimeter was also studied in several irradiation tests [18].

The main requirement on the length of these Shashlik calorimeters is that the whole energy needs to be deposited in one tower of alternating layers. This determines the total depth, which is chosen to be  $25 X_0$  as for the current  $\text{PbWO}_4$  crystals. To compare the three Shashlik calorimeter options, they are scaled to the same scintillator and absorber radiation length as specified in Table 20.1. For the simulation studies, the Shashlik calorimeters start and end with a scintillator plate to detect possible effects from the CMS detector environment in these sensitive layers. The Shashlik calorimeters consist

**Table 20.1:** Dimensions of the Shashlik sampling calorimeter for the FLUKA simulation studies. The effective radiation length ( $X_{0,\text{eff}}$ ), the total radiation length of the scintillator (absorber)  $X_{0,\text{scint}}$  ( $X_{0,\text{abs}}$ ) and the number of scintillator (absorber)  $N_{\text{scint}}$  ( $N_{\text{abs}}$ ) layers is listed.

| Design     | $X_{0,\text{eff}}$ | $X_{0,\text{scint}}$ | $X_{0,\text{abs}}$ | $N_{\text{scint}}$ | $N_{\text{abs}}$ |
|------------|--------------------|----------------------|--------------------|--------------------|------------------|
| Samp.calo. | 25                 | 5                    | 20                 | 15                 | 14               |

**Table 20.2:** The total Shashlik calorimeter (SC) length ( $l_{\text{SC}}$ ), the length of an absorber (scintillator) layer  $l_{\text{abs}}$  ( $l_{\text{scint}}$ ), the Shashlik fraction ( $f_{\text{samp}}$ ), the effective radiation length expressed in cm ( $X_{0,\text{eff}}$ ), the density of the scintillator ( $\rho_{\text{scint}}$ ), the energy resolution ( $\sigma_{\text{res}}$ ) of the Shashlik calorimeter and its Molière radius ( $R_{\text{M}}$ ) of the three sampling calorimeter options.

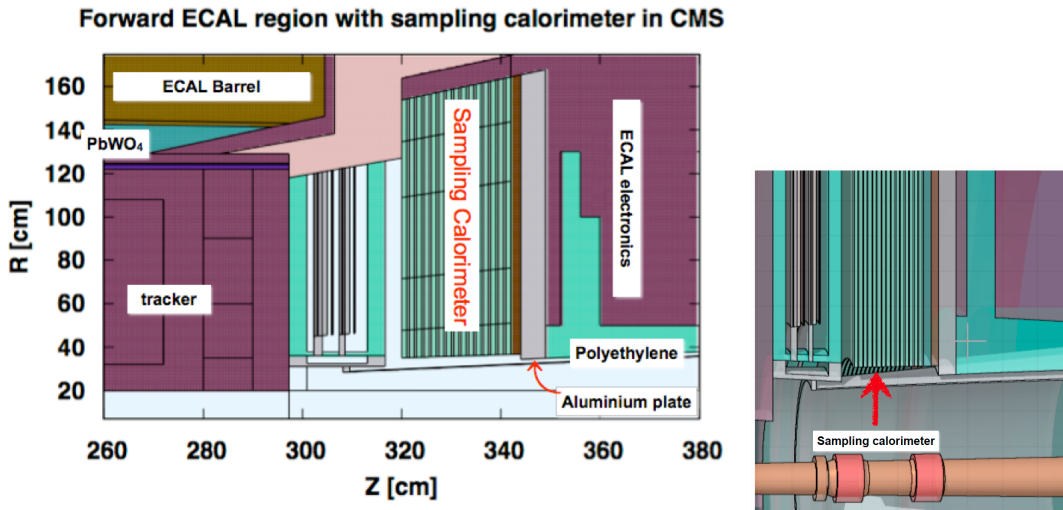
| Calorimeter         | $l_{\text{SC}}$<br>(cm) | $l_{\text{abs}}$<br>(cm) | $l_{\text{scint}}$<br>(cm) | $f_{\text{samp}}$<br>(%) | $X_{0,\text{eff}}$<br>(cm) | $\rho_{\text{scint}}$<br>(g/cm <sup>3</sup> ) | $\sigma_{\text{res}}$<br>(GeV <sup>-0.5</sup> ) | $R_{\text{M}}$<br>(cm) |
|---------------------|-------------------------|--------------------------|----------------------------|--------------------------|----------------------------|-----------------------------------------------|-------------------------------------------------|------------------------|
| YSO/W               | 22.0                    | 0.5                      | 1.00                       | 27.8                     | 0.880                      | 4.5                                           | 11 %                                            | 2.2                    |
| CeF <sub>3</sub> /W | 15.4                    | 0.5                      | 0.56                       | 23.8                     | 0.616                      | 6.2                                           | 12 %                                            | 1.7                    |
| LYSO/W              | 12.7                    | 0.5                      | 0.38                       | 21.5                     | 0.508                      | 7.1                                           | 12 %                                            | 1.5                    |

of 15 layers of scintillator material and 14 layers of tungsten. With these assumptions, the effective radiation length and the lengths of the different calorimeter parts are given in Table 20.2. These parameters are complemented by two other important quantities for a sampling calorimeter design: the sampling fraction  $f_{\text{samp}}$  and the energy resolution. The sampling fraction is defined as the percentage of deposited energy of a minimum ionizing particle (MIP) in the active part ( $E_{\text{mip}}(\text{active})$ ) with respect to the deposited energy of a MIP in the full calorimeter, consisting of active and absorber layers ( $E_{\text{mip}}(\text{active}) + E_{\text{mip}}(\text{absorber})$ ). A high sampling fraction guarantees a better signal readout [210]:

$$f_{\text{samp}} = \frac{E_{\text{mip}}(\text{active})}{E_{\text{mip}}(\text{active}) + E_{\text{mip}}(\text{absorber})} \quad (20.1)$$

The related energy resolution was predicted by our GEANT4 simulation [3, 209].

My implementation of the Shashlik calorimeter in the ECAL forward region is based on the most recent nominal CMS FLUKA model (version 1.0.0.0), available at the time. This version corresponds to the CMS cavern and detector description prior to LS1 and is described in Chapter 17.2. Only the region of the current lead tungstate crystals in the ECAL forward region was modified (320 cm - 342 cm in Z - direction).



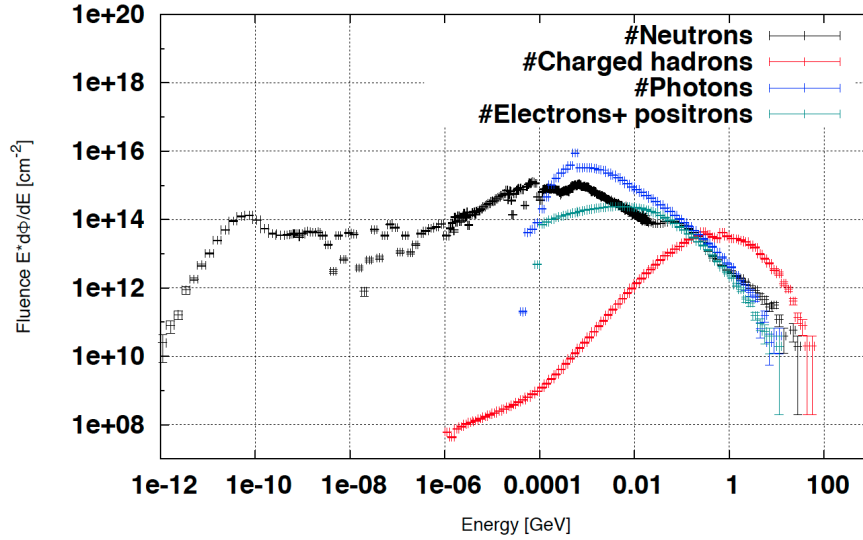
**Figure 20.2:** The top picture shows the Shashlik calorimeter implementation in the ECAL forward region in an R-Z grid of the FLUKA-CMS description (BRIL version 1.0.1-3). The bottom picture visualizes the implementation in a 3-dim perspective from the beam pipe [4].

The preshower upstream to the EE was left as a placeholder for a possible timing device and the polyethylene moderator was kept to shield the tracker from neutrons escaping the calorimeter. Directly behind the Shashlik calorimeter, the aluminum plate for the mounting of the current lead tungstate crystals was used as a placeholder for a similar support structure. If the total length of the Shashlik calorimeter was smaller than 22 cm, the rest of the volume before the aluminum plate was filled with a region of very low mass density, namely the 'Trk<sub>AV</sub>' material of Table 17.1, which reflects a region filled with cables, electronics and cooling devices. The polyethylene volume, which is placed behind the aluminum plate and shields the ECAL electronics from low energy neutrons, was kept. It is important to note, that all results based on this geometry are conservative estimates as this first design was not optimized in terms of slow-neutron shielding. The respective versions for the Shashlik calorimeter are:

- YSO/W: version 1.0.1
- LYSO/W: version 1.0.2
- CeF<sub>3</sub>/W: version 1.0.3

These versions include:

- configurable materials, number and size of the Shashlik calorimeter layers
- the division in 5- $\eta$  bins with the  $\eta$ -boarders of 1.48, 1.6, 1.8., 2.2, 2.6 and 2.9.



**Figure 20.3:** Isolethargic fluence spectra of neutrons, charged hadrons, photons and electrons and positrons for a  $\text{CeF}_3/\text{W}$  Shashlik calorimeter at  $2.2 < |\eta| < 2.6$  (version 1.0.3.0).

I verified this setup by reproducing official simulation results for the  $\text{PbWO}_4$  calorimeter. Both results agreed within the statistical uncertainties of the simulations.

## 20.2 Particle fluence in the Shashlik calorimeter in CMS

In this section, my simulation results of the overall particle spectra and their fluence in the Shashlik calorimeter at the end of the HL-LHC ( $3000 \text{ fb}^{-1}$ ) are presented. The FLUKA irradiation settings are given in Section 17.2. With the understanding of the behavior of a Shashlik calorimeter in the CMS environment, the results from Section 19.2 for the proton-irradiated scintillators can be scaled to the CMS conditions. This comparison is detailed in the subsequent Section 20.3.

### 20.2.1 The particle spectra of the Shashlik calorimeter

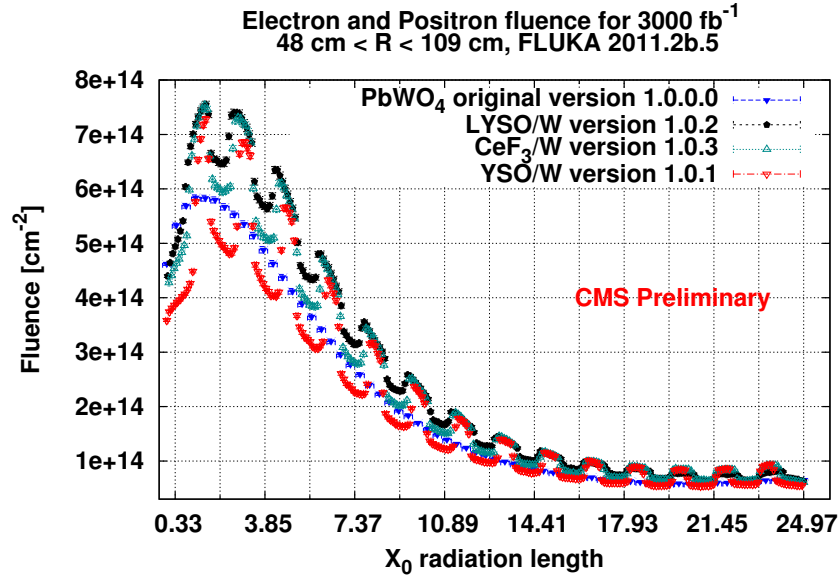
A typical isolethargic spectrum of the particle fluence in the EE of CMS is depicted in Figure 20.3. Since the spectra are similar for all scintillator options, the graph shows the one of the second layer at high pseudorapidities ( $2.2 < |\eta| < 2.6$ ) in the  $\text{CeF}_3$ -tungsten calorimeter. An isolethargic spectrum emphasizes dominant energy regions in the fluence spectra of particles. The particle fluence is simulated differentially versus its particle energy ( $d\Phi/dE$ ). The integral fluence is then calculated by multiplying each energy bin by its bin width. The various particles show quite different distributions

**Table 20.3:** Maximal Dose ( $D_{\max}$ ) and average particle fluence for electrons and positrons ( $\Phi_e$ ), photons ( $\Phi_\gamma$ ), charged hadrons ( $\Phi_{\text{ch.h.}}$ ) and neutrons ( $\Phi_n$ ) in  $1.8 < |\eta| < 2.6$  for  $3000 \text{ fb}^{-1}$ .

| Calorimeter         | $D_{\max}$<br>[Gy]                            | $\Phi_e$<br>[ $\text{cm}^{-2}$ ] | $\Phi_\gamma$<br>[ $\text{cm}^{-2}$ ] |
|---------------------|-----------------------------------------------|----------------------------------|---------------------------------------|
| YSO/W               | $1.61 \pm 0.01 \times 10^5$                   | $7.28 \pm 0.05 \times 10^{14}$   | $6.52 \pm 0.03 \times 10^{15}$        |
| LYSO/W              | $2.28 \pm 0.01 \times 10^5$                   | $7.55 \pm 0.06 \times 10^{14}$   | $6.24 \pm 0.04 \times 10^{15}$        |
| CeF <sub>3</sub> /W | $2.65 \pm 0.02 \times 10^5$                   | $7.54 \pm 0.06 \times 10^{14}$   | $6.48 \pm 0.03 \times 10^{15}$        |
|                     | $\Phi_{\text{ch.h.}}$<br>[ $\text{cm}^{-2}$ ] | $\Phi_n$<br>[ $\text{cm}^{-2}$ ] |                                       |
| YSO/W               | $6.92 \pm 0.06 \times 10^{13}$                | $4.41 \pm 0.02 \times 10^{15}$   |                                       |
| LYSO/W              | $7.13 \pm 0.07 \times 10^{13}$                | $3.60 \pm 0.01 \times 10^{15}$   |                                       |
| CeF <sub>3</sub> /W | $6.87 \pm 0.07 \times 10^{13}$                | $4.30 \pm 0.02 \times 10^{15}$   |                                       |

versus energy. Their point of lowest energy marks the production and transportation threshold in the simulations. The electrons, positrons and photons carry energies of  $\mathcal{O}(100 \text{ keV})$  up to a few GeV. The k-edge, the binding energy of the K-shell electron of an atom, and the annihilation peak at 511 keV is visible in the photon spectrum.

The charged hadron spectrum shows mostly particles (pions) with energies around 1 GeV. The neutron spectrum goes down to very low energies. In this region, the number and width of the bins is given by the thermal neutron cross-section library in FLUKA, which consists of 260 datasets. Thermal neutrons carry an energy up to a few eV with the thermal peak being between  $10^{-11} \text{ GeV}$  and  $10^{-10} \text{ GeV}$ . The neutron cross-section is proportional to the inverse of the neutron velocity for this energy region. It is followed by the resolved resonance region, where neutrons are absorbed via inelastic scattering. These resonances depend on the material, since the neutron energy has to match with the shell-structure of the nucleus. For every nuclei this can be expressed by a Breit-Wigner formula, depending on its atomic number (Z), mass number (A), spin and width. The intermediate energy region contains unresolved resonances, which are too narrow and therefore overlap. Since the neutron spectrum was simulated in the CMS environment, it shows the characteristic evaporation peak around 1-5 MeV and the knock-out peak around 100 MeV, which are typical for neutrons that have undergone several scatterings. The corresponding averaged integrated fluences for the mentioned particles are listed in Table 20.3. The particle fluences have a similar magnitude among all Shashlik calorimeter options.

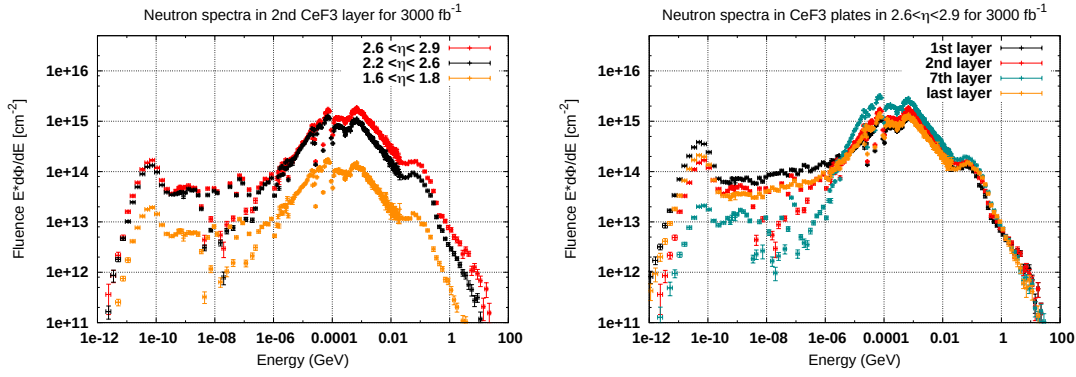


**Figure 20.4:** FLUKA estimation of the electron and positron fluence in a forward ECAL Shashlik calorimeter for  $3000 \text{ fb}^{-1}$  as a function of the radiation length  $X_0$ . The fluence is averaged over a region of  $48 \text{ cm} < R < 109 \text{ cm}$ , corresponding to  $1.8 < |\eta| < 2.6$  for  $|Z| = 320 \text{ cm}$ . The fluence for lead tungstate is depicted as a reference (version 1.0.0-3) [4].

### 20.2.2 The electron and positron fluence in a Shashlik calorimeter

My prediction of the electron and positron fluence as a function of the Shashlik calorimeter length in Z at the end of phase-II data-taking ( $3000 \text{ fb}^{-1}$ ) is depicted in Figure 20.4. To allow a comparison among the different Shashlik options, the calorimeter depth is expressed in the respective effective radiation lengths. The bin size is chosen to be 10 % of  $X_{0,\text{eff}}$  to visualize differences between the active and passive layers. The grid lines in the background of the graph indicate the end of each scintillator layer. The fluence is averaged over a region of  $48 \text{ cm} < R < 109 \text{ cm}$ , corresponding to  $1.8 < |\eta| < 2.6$  for  $|Z| = 320 \text{ cm}$ .

The Figure shows a similar overall  $e^\pm$ -fluence magnitude and shape among all options and evaluates to  $7 \times 10^{14} \text{ cm}^2$ . The predicted  $e^\pm$ -fluence will therefore be comparable to the one of the current lead tungstate crystals for  $3000 \text{ fb}^{-1}$ . The difference in density among all options and between absorber and scintillator layer is highlighted by the slight change in magnitude with respect to each layer. The development of the electromagnetic shower is evident, with the bulk part being in the first seven radiation lengths and the maximum being in the second scintillator layer.



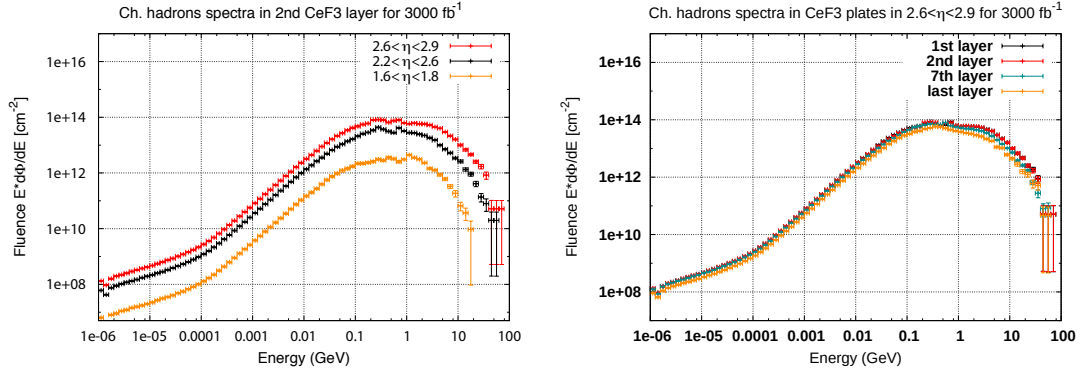
**Figure 20.5:** For  $\text{CeF}_3$ , neutron spectra in CMS for  $3000 \text{ fb}^{-1}$  in different  $\eta$  intervals (left) and different Shashlik layers for the range  $2.6 < |\eta| < 2.9$  (right), (version 1.0.3) [6].

### 20.2.3 The hadron fluence and its dependence on pseudorapidity and depth

In the following, my results on the behavior of the hadron fluence versus pseudorapidity and depth are presented on the example of the  $\text{CeF}_3$  Shashlik calorimeter. Similar results are obtained for the LYSO and YSO option. Figure 20.5 depicts the neutron fluence in three  $\eta$ -intervals and for different scintillator layers, respectively. The left graph shows that the overall magnitude of the neutron spectrum increases with higher pseudorapidity values, but also that the overall shape stays unchanged. The right side of the figure presents the variation in fluence for different depths, showing the first, second, seventh and last Shashlik layer for the highest  $\eta$ -bin. The fast neutron fluence is almost constant in depth, while the thermal and epithermal neutron fluence is higher in the first and last layer of the Shashlik calorimeter. This is due to the surrounding area in CMS, since thermal neutrons are captured by light elements or elements with a large thermal neutron cross-section and they can therefore travel long distances without interaction. The resolved resonance region is more distinct towards the middle of the calorimeter (2nd and 7th layer). This energy range depends fully on the materials the neutron is interacting with and is more pronounced the larger the surrounding volume with the same material composition is.

My results on the charged hadron fluence versus pseudorapidity and depth are illustrated in Figure 20.6. The conclusion drawn for different  $\eta$ -regions is the same as for the neutron fluence: the overall shape stays unchanged, only the magnitude increases with higher pseudorapidity values. According to the right panel of Figure 20.6, the charged hadron fluence remains independent from the Shashlik layer considered, which agrees with our expectations.

The averaged fluence for neutrons and charged hadrons is listed in Table 20.4 and 20.5 for  $\text{CeF}_3$  and LYSO, respectively. Since the particles have a different impact on the scintillator material depending on their energy, they are separated in four different



**Figure 20.6:** For  $\text{CeF}_3$ , charged hadron spectra in CMS for  $3000 \text{ fb}^{-1}$  in different  $\eta$  intervals (left) and different Shashlik layers for the range  $2.6 < |\eta| < 2.9$  (right), (version 1.0.2) [6].

**Table 20.4:** Fluence values in  $\text{CeF}_3$  for the 2nd  $\text{CeF}_3$  layer of a Shashlik CMS EE for  $3000 \text{ fb}^{-1}$  for neutrons ( $\Phi_n$ ) and charged hadrons ( $\Phi_{\text{ch.h.}}$ ).

| Energy interval                        | CMS $\Phi_n$<br>$\eta: 2.6-2.9$<br>[ $\text{cm}^{-2}$ ] | CMS $\Phi_n$<br>$\eta: 2.2-2.6$<br>[ $\text{cm}^{-2}$ ] | CMS $\Phi_{\text{ch.h.}}$<br>$\eta: 2.6-2.9$<br>[ $\text{cm}^{-2}$ ] | CMS $\Phi_{\text{ch.h.}}$<br>$\eta: 2.2-2.6$<br>[ $\text{cm}^{-2}$ ] |
|----------------------------------------|---------------------------------------------------------|---------------------------------------------------------|----------------------------------------------------------------------|----------------------------------------------------------------------|
| $E < 0.5 \text{ MeV}$                  | 4.64E+15                                                | 3.51E+15                                                | 1.25E+10                                                             | 5.54E+09                                                             |
| $0.5 \text{ MeV} < E < 20 \text{ MeV}$ | 1.93E+15                                                | 1.12E+15                                                | 1.20E+11                                                             | 5.27E+10                                                             |
| $20 \text{ MeV} < E < 200 \text{ MeV}$ | 1.37E+15                                                | 7.24E+14                                                | 7.95E+13                                                             | 3.43E+13                                                             |
| $200 \text{ MeV} < E$                  | 4.75E+13                                                | 2.43E+13                                                | 3.08E+14                                                             | 1.30E+14                                                             |

energy intervals. The fluence is listed for the two highest pseudorapidity regions,  $2.2 < |\eta| < 2.6$  and  $2.6 < |\eta| < 2.9$ , respectively. The former refers thereby to the highest  $\eta$ -bin that is still surrounded by sampling calorimeter material. As it is demonstrated later in Chapter 20.4, the latter shows in a few spots distortions due to the adjacent beam pipe and particles originating from the rest of the CMS detector. The results for the neutron fluence in Table 20.4 and 20.5 highlight that thermal and epithermal neutrons add a significant contribution to the overall fluence. An optimized geometry in terms of shielding can therefore significantly change the average neutron fluence.

### 20.3 Comparison of single crystal irradiations to CMS running conditions

The scaling of the hadron fluence spectra in single crystal irradiations from the previous Section 19.2 to the expected exposure of an endcap Shashlik calorimeter under CMS running conditions at the HL-LHC was performed in the context of the decision for a new

**Table 20.5:** Fluence values in LYSO for the 2nd LYSO layer of a Shashlik CMS EE for 3000 fb<sup>-1</sup> for neutrons ( $\Phi_n$ ) and charged hadrons ( $\Phi_{ch.h.}$ ).

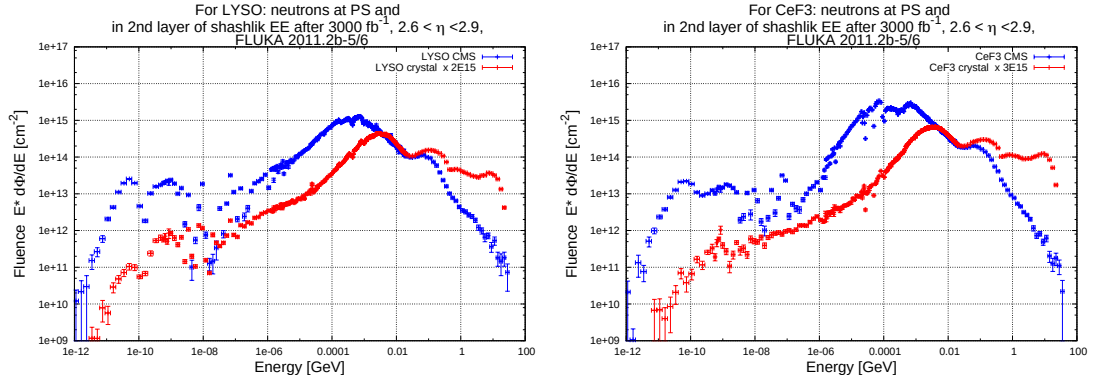
| Energy interval      | CMS $\Phi_n$<br>$\eta$ : 2.6-2.9<br>[cm <sup>-2</sup> ] | CMS $\Phi_n$<br>$\eta$ : 2.2-2.6<br>[cm <sup>-2</sup> ] | CMS $\Phi_{ch.h.}$<br>$\eta$ : 2.6-2.9<br>[cm <sup>-2</sup> ] | CMS $\Phi_{ch.h.}$<br>$\eta$ : 2.2-2.6<br>[cm <sup>-2</sup> ] |
|----------------------|---------------------------------------------------------|---------------------------------------------------------|---------------------------------------------------------------|---------------------------------------------------------------|
| E < 0.5 MeV          | 3.76E+15                                                | 2.64E+15                                                | 1.35E+10                                                      | 5.96E+09                                                      |
| 0.5 MeV < E < 20 MeV | 1.96E+15                                                | 1.11E+15                                                | 1.27E+11                                                      | 5.58E+10                                                      |
| 20 MeV < E < 200 MeV | 1.44E+15                                                | 7.50E+14                                                | 8.34E+13                                                      | 3.49E+13                                                      |
| 200 MeV < E          | 4.28E+13                                                | 2.26E+13                                                | 2.30E+14                                                      | 9.51E+13                                                      |

forward calorimeter in CMS. Hence, the CeF<sub>3</sub> and LYSO options were studied and the study is also documented in Ref. [6]. In Section 19.2 it is illustrated, that the star density in PbWO<sub>4</sub> can be used as a scale factor for the impact of hadron fluence in PbWO<sub>4</sub> from proton-irradiations to the CMS environment. The new scintillator materials do not show the same amount of hadron-induced damage, such that a different scaling for the impact of hadron fluence on the materials had to be found.

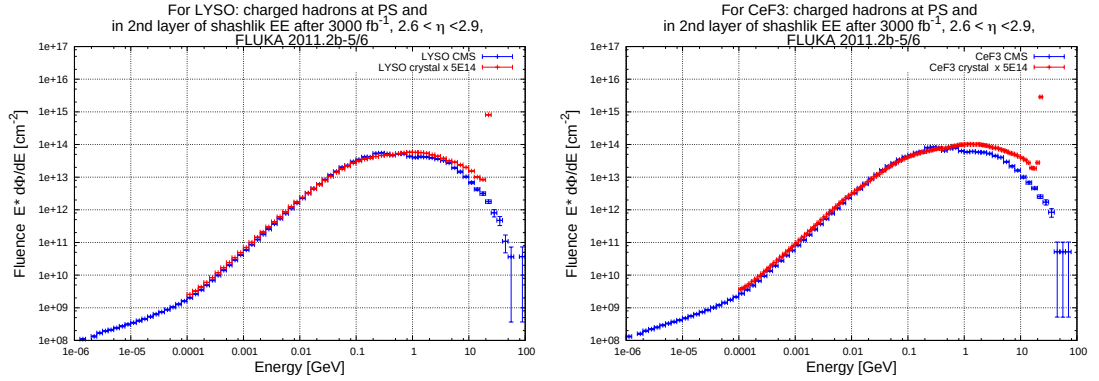
The induced hadron fluence in the respective crystal during proton-irradiation is compared to the one in the second layer of a Shashlik calorimeter EE, which is the layer of the maximum of the electromagnetic shower development as illustrated in Figure 20.4. Figure 20.7 shows the isoethargic neutron fluence spectra for both scintillator options under PS proton-irradiation for an integrated fluence of  $2\text{--}3 \times 10^{15} \text{ cm}^{-2}$  and at CMS for 3000 fb<sup>-1</sup>. It illustrates that the relative amount of thermal and epithermal neutrons is lower for the proton-irradiated crystals than for the CMS environment. It further shows that the relative amount of fast neutrons (> 100 MeV) is higher for the proton-irradiated single crystals. This can be explained by the smaller amount of surrounding materials in the IRRAD1 test facility than in CMS. A similar shape of the spectrum up to a multiplicative factor can be recognized for the four energy intervals of Table 20.4 and 20.5.

Figure 20.8 depicts the fluence of charged hadrons for the EE in CMS and the  $\Phi_{ch.h.}$  fluence of the proton-irradiation with an integrated fluence of  $5 \times 10^{14} \text{ cm}^{-2}$ . The transport and production threshold of  $\Phi_{ch.h.}$  in CMS is with 100 keV higher than for the single crystal simulation. The energy spectra have a very similar shape up to a few GeV. The relative comparison shows that the crystals in the IRRAD1 test facility are exposed to a slightly higher charged hadron fluence for energies above a few GeV due to their lack of surrounding material which could mitigate the hadron energies. For energies above  $\mathcal{O}(10 \text{ GeV})$ , the development of a hadronic shower is visible. The hadron fluence results for the PS proton-irradiation are summarized in Table 20.6 and 20.7 for CeF<sub>3</sub> and LYSO, respectively. To allow a scaling of damage measurements, the fluence values are again separated in the above defined energy intervals.

To assess the correspondence between CMS running conditions and PS irradiations,



**Figure 20.7:** Neutron shows spectra in the second layer of a Shashlik CMS EE for  $3000 \text{ fb}^{-1}$  in the pseudorapidity range  $2.6 < |\eta| < 2.9$ , and in a long crystal irradiated with 24 GeV/c protons at the CERN PS for LYSO (left, version 1.0.2) and  $\text{CeF}_3$  (right, version 1.0.3). A primary proton fluence of  $5 \times 10^{14} \text{ cm}^{-2}$  was chosen for the proton-irradiation [6].



**Figure 20.8:** Charged hadron fluence spectra in the second layer of a Shashlik CMS EE for  $3000 \text{ fb}^{-1}$  in the range  $2.6 < |\eta| < 2.9$ , and in a long crystal irradiated with 24 GeV/c protons at the CERN PS. for LYSO (left, version 1.0.2) and  $\text{CeF}_3$  (right, version 1.0.3). A primary proton fluence of  $5 \times 10^{14} \text{ cm}^{-2}$  was chosen for the proton-irradiation [6].

**Table 20.6:** Neutron ( $\Phi_n$ ) and charged hadron ( $\Phi_{\text{ch.h.}}$ ) fluence values in  $\text{CeF}_3$  for a single 24 GeV/c proton irradiation at the CERN PS.

| Energy interval                        | Neutrons<br>[ $\text{cm}^{-2}$ ] | Ch. had.<br>[ $\text{cm}^{-2}$ ] |
|----------------------------------------|----------------------------------|----------------------------------|
| $E < 0.5 \text{ MeV}$                  | 6.37E-02                         | 3.22E-05                         |
| $0.5 \text{ MeV} < E < 20 \text{ MeV}$ | 1.78E-01                         | 2.73E-04                         |
| $20 \text{ MeV} < E < 200 \text{ MeV}$ | 5.78E-01                         | 1.44E-01                         |
| $200 \text{ MeV} < E$                  | 1.84E-01                         | 1.40E-00                         |

**Table 20.7:** Neutron ( $\Phi_n$ ) and charged hadron ( $\Phi_{\text{ch.h.}}$ ) fluence values in LYSO for a single 24 GeV/c proton irradiation at the CERN PS.

| Energy interval                | $\Phi_n$<br>[cm <sup>-2</sup> ] | $\Phi_{\text{ch.h.}}$<br>[cm <sup>-2</sup> ] |
|--------------------------------|---------------------------------|----------------------------------------------|
| $E < 0.5$ MeV                  | 4.86E-02                        | 8.84E-06                                     |
| $0.5 \text{ MeV} < E < 20$ MeV | 9.73E-02                        | 1.07E-04                                     |
| $20 \text{ MeV} < E < 200$ MeV | 2.72E-01                        | 5.55E-02                                     |
| $200 \text{ MeV} < E$          | 5.46E-02                        | 3.89E-01                                     |

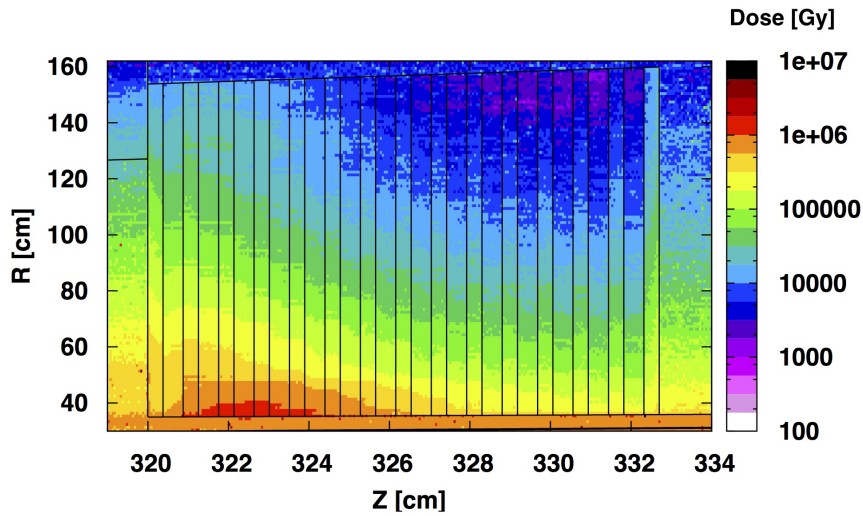
**Table 20.8:** Fluence values needed for a 24 GeV/c proton irradiation of LYSO to reach the charged hadron fluence expected for the 2nd LYSO layer in the CMS EE for the given energy range in the interval  $2.6 < |\eta| < 2.9$  for 3000 fb<sup>-1</sup> of collected data.

| Energy interval                | $\Phi_n$<br>[cm <sup>-2</sup> ] | $\Phi_{\text{ch.h.}}$<br>[cm <sup>-2</sup> ] |
|--------------------------------|---------------------------------|----------------------------------------------|
| $E < 0.5$ MeV                  | 7.7E16                          | 1.5E15                                       |
| $0.5 \text{ MeV} < E < 20$ MeV | 2.0E16                          | 1.2E15                                       |
| $20 \text{ MeV} < E < 200$ MeV | 5.3E15                          | 1.5E15                                       |
| $200 \text{ MeV} < E$          | 7.8E14                          | 5.9E14                                       |

ratios of the two situations are given for LYSO in Table 20.8. Table 20.9 displays these results in fractions, normalized to the charged hadron fluence for energies above 200 MeV. In a previous study by the ETHZ group and collaborators [181], it was shown that only neutrons above an energy of 20 MeV can deposit enough local energy to displace lattice atoms via inelastic interactions (stars). The relative amount of fast neutrons is about 11 % for  $20 \text{ MeV} < E < 200 \text{ MeV}$  and 75 % for energies above 200 MeV. Previous discussions of CeF<sub>3</sub> [182] showed that the hadron-induced damage by neutrons depends on the incident neutrons energy. The effect of thermal and epithermal neutrons is negligible and a decrease in  $\mu_{\text{ind}}(\lambda)$  is only observed for higher-energy neutrons.

**Table 20.9:** In a 24 GeV/c proton irradiation of LYSO up to  $5.9 \times 10^{14} \text{ cm}^{-2}$ , fluence fractions in different energy ranges with respect to the 2nd LYSO layer in the CMS EE in the interval  $2.6 < |\eta| < 2.9$  for  $3000 \text{ fb}^{-1}$  of collected data.

| Energy interval                        | Neutrons<br>[ $\text{cm}^{-2}$ ] | Ch. had.<br>[ $\text{cm}^{-2}$ ] |
|----------------------------------------|----------------------------------|----------------------------------|
| $E < 0.5 \text{ MeV}$                  | 0.8%                             | 39%                              |
| $0.5 \text{ MeV} < E < 20 \text{ MeV}$ | 2.9%                             | 49%                              |
| $20 \text{ MeV} < E < 200 \text{ MeV}$ | 11%                              | 39%                              |
| $200 \text{ MeV} < E$                  | 75%                              | 100%                             |



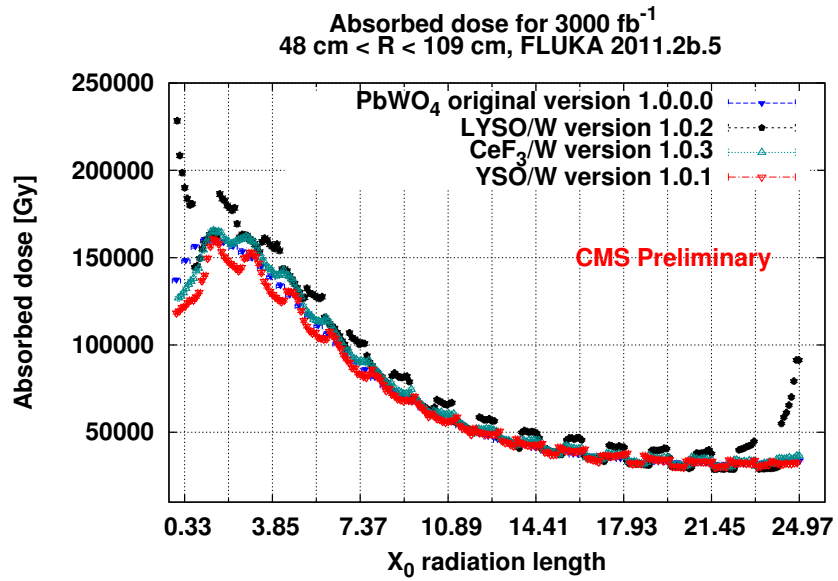
**Figure 20.9:** Monte Carlo FLUKA estimation of the absorbed dose in the R-Z plane for a LYSO/W Shashlik calorimeter after  $3000 \text{ fb}^{-1}$  (version 1.0.2).

## 20.4 Radioactivation studies for a Shashlik calorimeter at the HL-LHC

After extrapolating the exposure of hadron-irradiated crystals to the CMS running conditions and studying the particle fluence in the calorimeter, the radioactivation of the Shashlik calorimeter options in CMS at the end of the HL-LHC was analyzed. The absorbed dose among different Shashlik sampling calorimeter options and its main causes are discussed. It is determined if the activation of the residual nuclei leads to a prohibitive background signal to the EE readout. The FLUKA simulation employs the settings described in Section 17.2. Most of my results are also published in Ref. [4].

### 20.4.1 Absorbed dose in the Shashlik calorimeter at the end of phase-II

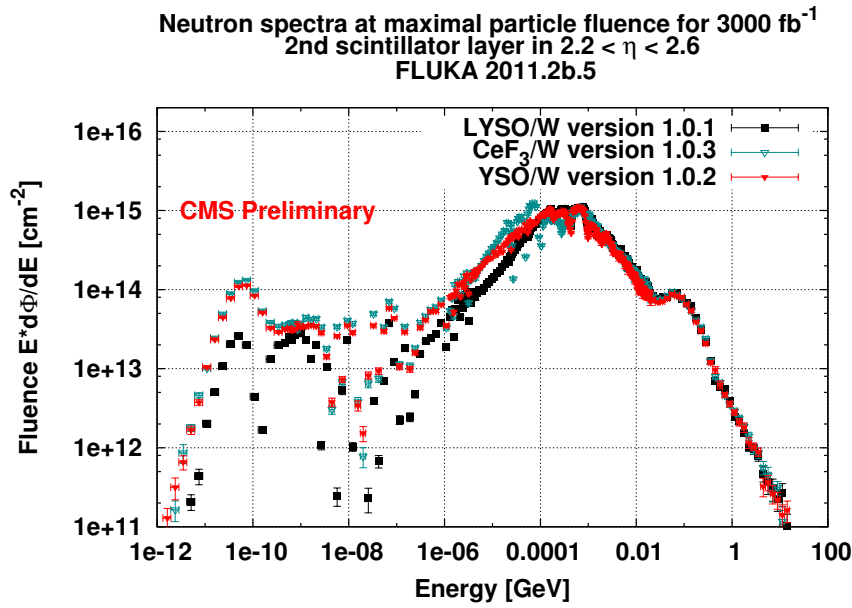
Figure 20.9 shows the absorbed dose in the R-Z plane at the end of phase-II. The absorbed dose increases with pseudorapidity, spanning more than two orders of magnitude in dose. The highest values are seen around  $|Z| = 322 \text{ cm}$  and are due to a higher flux of low energy neutrons, originating from the adjacent beam pipe, its holding structure and its surrounding volume. The low energy neutrons, produced in the beampipe or in calorimeter parts can travel through the vacuum, leading to a so-called 'crater' effect. A boron-polyethylene shielding below the calorimeter is therefore not only advisable



**Figure 20.10:** Monte Carlo estimation of the "absorbed dose" for CMS with a forward ECAL Shashlik calorimeter under HL-LHC conditions using FLUKA. The figure shows the dose absorbed in the EE for an integrated luminosity of  $3000 \text{ fb}^{-1}$  as a function of the radiation length. It is averaged over a region of  $48 \text{ cm} < R < 109 \text{ cm}$ , corresponding to  $1.8 < |\eta| < 2.6$  for  $|Z| = 320 \text{ cm}$ . The Z-coordinate is converted to radiation length by scaling with the effective radiation length for each calorimeter (version 1.0.0-3) [4].

for the protection of the calorimeter, but also for the protection of the tracker system. The profile of the absorbed dose as a function of depth among the different calorimeter options is shown in Figure 20.10. The result is presented in the same fashion as for Figure 20.4, and is averaged over the same region of  $48 \text{ cm} < R < 109 \text{ cm}$ . The dose, quantifying the deposited energy per unit mass of the medium, is in general strongly dependent on the material. Figure 20.10 shows however a similar magnitude and shape for  $\text{PbWO}_4$ ,  $\text{CeF}_3$  and YSO versus the calorimeter depth. The development of the electromagnetic shower is again recognizable due to the thereby deposited energy.

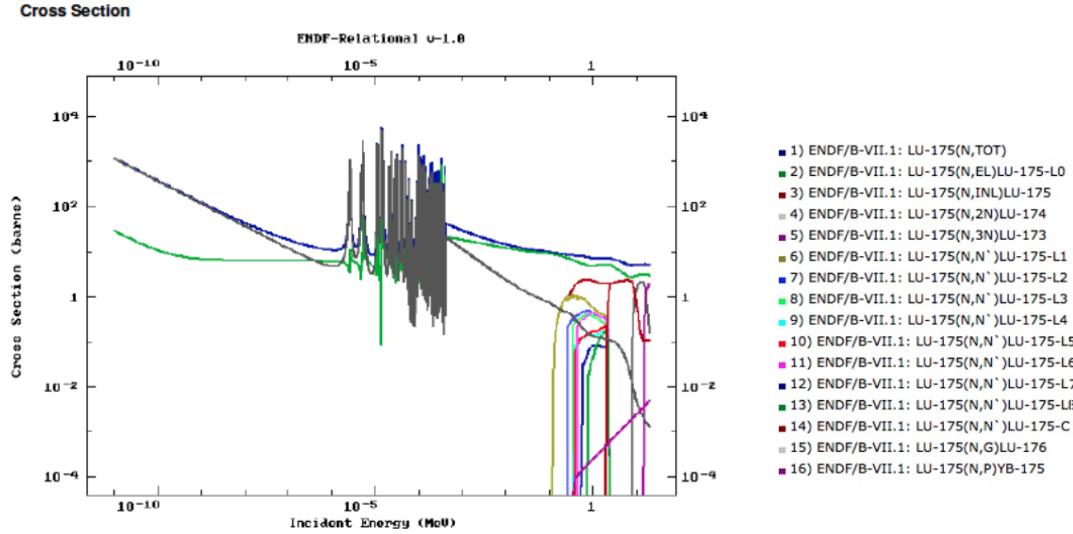
The LYSO layers experience a significantly higher absorbed dose than the rest of the scintillators, and a large increase of the absorbed dose at both ends of the LYSO-tungsten Shashlik calorimeter is observed. This can be explained by the high thermal neutron capture cross-section of  $^{175}\text{Lu}$  of  $\sigma_{\text{Lu}} = 23.1 \text{ b}$  (97.41 % isotopic signature) and  $^{176}\text{Lu}$  of  $\sigma_{\text{Lu}} = 2097.8 \text{ b}$  with a half-life of  $3.78 \times 10^{10}$  years [208]. In natural abundance, the  $^{175}\text{Lu}$  has a percentage of 97.41 % in the isotopic signature, the  $^{176}\text{Lu}$  isotope a percentage of 2.59 %. Figure 20.11 gives the isoethargic neutron fluence spectra for all Shashlik calorimeter options for  $2.2 < |\eta| < 2.6$  after  $3000 \text{ fb}^{-1}$ . This pseudorapidity region is chosen since it experiences a high dose, but is not at the boarder to the beam pipe, such that the results are less influenced by the surrounding CMS environment.



**Figure 20.11:** Monte Carlo estimation of the neutron fluence energy spectrum for CMS with a forward ECAL Shashlik calorimeter under HL-LHC conditions using FLUKA. The figure shows the fluence energy spectrum of neutrons for the maximal particle flux, which is in the second scintillator layer in  $2.2 < |\eta| < 2.6$  for 3000 fb<sup>-1</sup> (see Figure 20.9), (version 1.0.0-3) [4].

For neutrons with energies higher than 1 keV, all Shashlik options have a similar shape and magnitude. In terms of low energy neutrons however, the LYSO option shows a lower thermal neutron fluence and a much more distinctive resolved resonance region. The lutetium neutron capture cross-section with its various processes is shown in Figure 20.12 and is taken from Ref. [208]. Since the isoethargic neutron spectrum from the FLUKA simulation shows neutron fluences at all energies, all depicted reaction processes of <sup>175</sup>Lutetium of Figure 20.12 would take place in the LYSO/W calorimeter. The lutetium cross-section graph shows the dominant Lu(n,g) neutron capture process with a cross-section of about 23 b in gray. In this reaction, the slowed down neutrons are captured and the resulting excitation energy of the nucleus that captured it, is released in the form of a photon (g). This reaction is usually dominant at neutron energies of smaller than 1 eV, but can also be non-negligible at energies of a couple of eV as in the case of lutetium. The graph includes also other neutron-interaction processes as listed in the legend. It includes contributions from charged particles, for example protons (n,p) or  $\alpha$ -particles (n, $\alpha$ ). These are threshold reactions, for instance they occur only when the incident neutron is above a certain threshold energy, necessitated by the energy conservation and Q-value of the reaction. In the case of lutetium, the (n,p) reaction happens at a neutron energy of 1-10 MeV [211].

In summary, the high thermal neutron cross-section of lutetium leads to an increase of

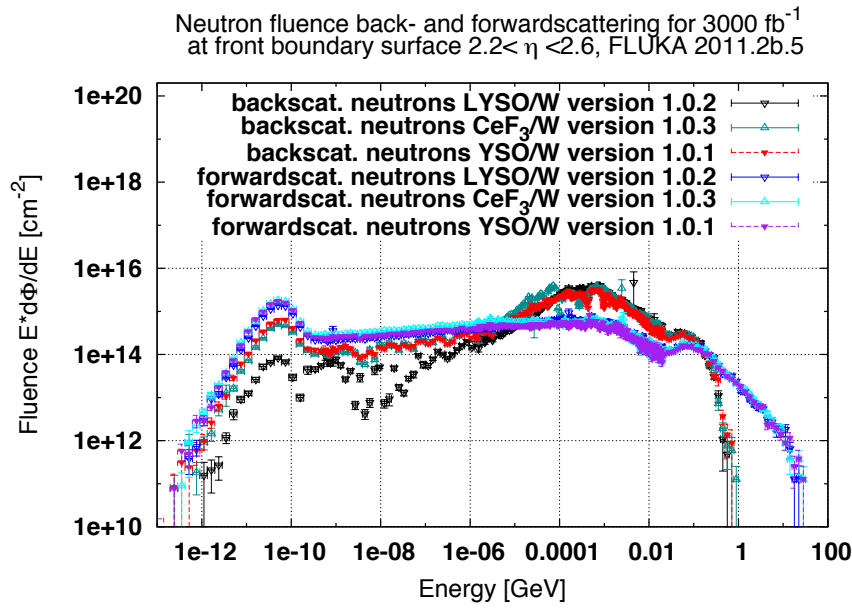


**Figure 20.12:**  $^{175}\text{Lu}$  neutron cross-section from Ref. [208] with various processes explained in the text or in the legend.

the absorbed dose rate in LYSO at both ends of the calorimeter and also in the respective scintillator layers as illustrated in Figure 20.10. This conclusion is also confirmed by Figure 20.13. It shows the backscattered and forward scattered neutrons at the front surface of the first scintillator layer of the respective Shashlik calorimeter. The first layer of the LYSO option shows already a distinctive resolved resonance region for the backscattered neutrons, due to the highly neutron absorbent lutetium, whereas the shape of the low energy neutron spectra of the  $\text{CeF}_3$  and YSO option are still comparable to the incoming neutrons. The forward scattered neutrons show a higher thermal neutron fluence and a few neutrons with energies above 1 GeV due to the surrounding CMS area, where neutrons can travel long distances without interaction. The otherwise flat isoethargic spectrum is due to the polyethylene layer before the calorimeter, which slows neutrons down by elastic collisions. The amount of backscattered neutrons is slightly higher than the one of the forward scattered neutrons at energies around 1 MeV. This is to a small fraction due to the induced hadron shower inside the  $\text{PbWO}_4$  crystals. It is therefore advisable to implement a thin absorber layer made of boron-polyethylene as this material not only moderates neutrons, but also absorbs the thermal ones.

#### 20.4.2 Prohibitive background due to decaying isotopes

The final subject of the study is if any of the created isotopes adds a constant prohibitive background to the readout of the forward ECAL. A first estimate with a proton-irradiation of  $3000 \text{ fb}^{-1}$  and subsequent simulation of residual nuclei was performed for  $\text{CeF}_3$  and YSO with the two-step method of FLUKA, described in Section 17.2.2.



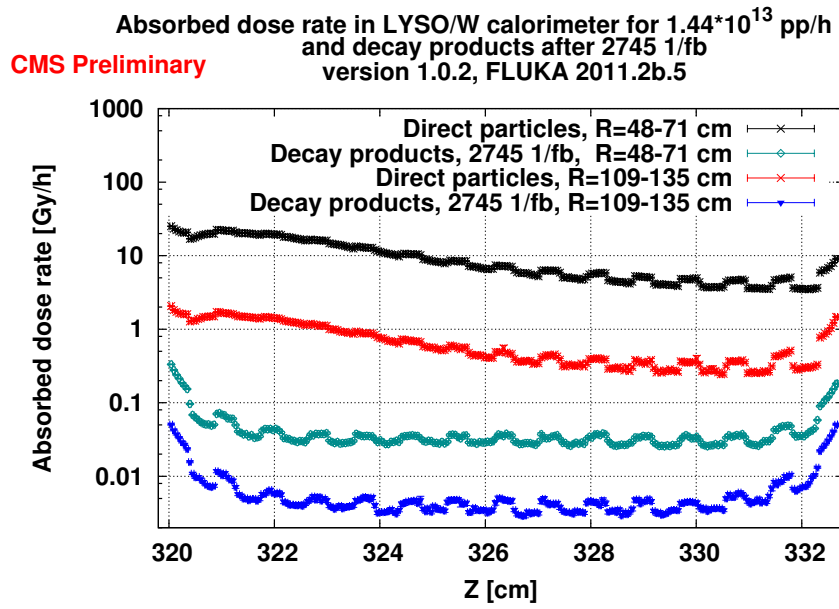
**Figure 20.13:** Monte Carlo estimation of the neutron fluence energy spectra for CMS in a CeF<sub>3</sub>, YSO and LYSO Shashlik calorimeter at the front boundary surface at  $2.2 < |\eta| < 2.6$  for 3000 fb<sup>-1</sup> (version 1.0.1-3).

For CeF<sub>3</sub>, the highest activity was observed for Fluoride isotopes, but all of these isotopes are short-lived with a half-life of smaller than a few hours and no built up of long-lived residual nuclei could be observed.

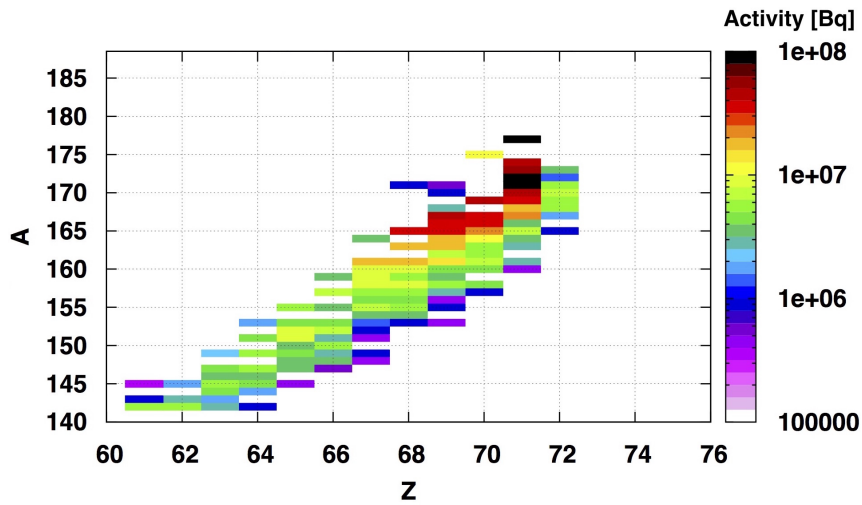
The residual activity of a single yttrium crystal is discussed in Section 19.2.4. The results obtained in the CMS environment are similar. Among the most radioactive isotopes is here also <sup>88</sup><sub>39</sub>Y with a half-life of 107 days. It contributes at a 1 % level to the overall activity among the decay products and is therefore not of particular importance.

The previous discussion about LYSO highlighted that lutetium shows the highest thermal neutron capture cross-section among all considered elements. The residual nuclei of a LYSO/W Shashlik calorimeter were therefore studied in more detail. Fig. 20.14 compares the absorbed dose rate during HL-LHC running ( $1.44 \times 10^{13}$  pp-int./h) with the absorbed dose rate of decaying particles after 2475 fb<sup>-1</sup>. The irradiation schedule and the FLUKA settings for activation studies are detailed in Chapter 17.2.2 and the parameters of the irradiation cycle are listed in Table B.2. The dose rate is visualized for two regions in R: 48 cm-71 cm and 109 cm-135 cm, corresponding to  $|\eta| = 1.6$ -1.8 and 2.2-2.6 at  $|Z| = 320$  cm. The dose rate in the higher  $|\eta|$ -region is on average one order of magnitude larger than for the lower  $|\eta|$ -region. Furthermore, the dose rate of the decay products is at a constant 1 % level of the prompt particles. This offset of deposited energy by decaying isotopes is at a manageable level for the HL-LHC running.

The overall activity of the created residual nuclei after 2475 fb<sup>-1</sup> in the first scintillator



**Figure 20.14:** Monte Carlo estimation of the absorbed dose rate due to the prompt electromagnetic shower and of the decay products for an LYSO/tungsten Shashlik calorimeter for the forward ECAL Shashlik calorimeter under HL-LHC conditions using FLUKA. The absorbed dose rate is projected to the calorimeter length in  $|Z|$ , from 320 cm-332.7 cm (version 1.0.2) [4].



**Figure 20.15:** Residual nuclei in the first scintillator layer at  $2.2 < |\eta| < 2.6$  of a LYSO/W Shashlik calorimeter at the irradiation stop after  $2475 \text{ fb}^{-1}$ . The residual nuclei with an atomic number above 60 and an activity above  $10^5 \text{ Bq}$  are shown (version 1.0.2).

**Table 20.10:** Long-lived lutetium isotopes with high activity. Possible decay channels are the  $\beta$  decay and the electron capture (EC).

| Isotope           | Decay channels       | Half life $\tau_{1/2}$ | Stable isotope    | Activity in layer (Bq)          |
|-------------------|----------------------|------------------------|-------------------|---------------------------------|
| $^{177}\text{Lu}$ | $\beta^-$            | 6.64 days              | $^{177}\text{Hf}$ | $1.9 \times 10^{10} \pm 1.4 \%$ |
| $^{174}\text{Lu}$ | $\beta^+, \text{EC}$ | 3.31 years             | $^{174}\text{Yb}$ | $3.7 \times 10^7 \pm 8.6 \%$    |
| $^{173}\text{Lu}$ | EC                   | 1.37 years             | $^{173}\text{Yb}$ | $1.5 \times 10^7 \pm 13.8 \%$   |

layer at  $2.2 < \eta < 2.6$  is  $A = 4.53 \cdot 10^{10} \pm 0.07 \text{ Bq}$ , the main drivers of this radioactivity are visualized in Figure 20.15. Nearly all of this radioactivity (96 %) is driven by residual nuclei created by low energy neutrons.

The dose rate of the decay products is dominated by short-lived radionuclides. The built up of deposited energy after the full run with  $2475 \text{ fb}^{-1}$  is a factor three higher than after a typical pp-run of 10 h. Responsible for this slight built-up is mainly the long-lived isotope  $^{177}\text{Lu}$  with an activity of  $A = 1.91 \pm 0.03 \times 10^{10} \text{ Bq}$  after  $2475 \text{ fb}^{-1}$  and with a half-life of  $\tau = 6.64 \text{ days}$ . The details of its decay are listed in Table 20.10 together with the other two most active lutetium isotopes.

## 21 | CHAPTER Summary and prospects

The high-luminosity upgrade of the LHC requires a new forward ECAL calorimeter and a complete redesign of the electronics for the ECAL barrel detector in CMS. The second part of this dissertation concentrated on Monte-Carlo studies, which were performed for this objective with the particle interaction and transport code FLUKA. The obtained results are shortly highlighted in this section.

The radiological studies for the upgrade of the electronic system in the ECAL barrel in Chapter 18 have been crucial for the planning of the LS3 and the preparation of the technical proposal for the phase-II upgrade [17]. In my role as the ECAL expert for FLUKA radiation simulations, I improved in collaboration with the BRIL project the ECAL description in FLUKA. My recommendations were and are being implemented in the different FLUKA versions and made for instance the tracking of a 'hot-spot' possible. Above all, these improvements will lead to a precise estimate of the radiological hazard and will likely reduce the expected residual dose.

A first conservative estimate of the ambient dose equivalent rate for human interventions on the supermodules in a low radiation environment classified this area most likely as a 'supervised radiation area'. Following the ALARA principles, personnel can be easily shielded from radioactive elements like the  $\text{PbWO}_4$  crystals and the backplate of the supermodules. This radiological study needs to be regularly updated, since the CMS description in FLUKA and the technical plans for the LS3 intervention are being constantly modified. Our radiological studies are the foundation for current and future radioactivity studies for the EB and will allow a precise estimate of the radiological quantities in this detector region.

The emphasis of this part of the dissertation lies on FLUKA studies for a Shashlik calorimeter, which was one option for a new forward ECAL in CMS at the HL-LHC. This Shashlik calorimeter consists of a heavy scintillator as its active medium and tungsten as its absorber. First, the suitability of LYSO, YSO and  $\text{CeF}_3$  crystals for such a Shashlik calorimeter was tested. These heavy scintillators were exposed to 24 GeV/c-proton fluences of up to  $5 \times 10^{14} \text{ cm}^{-2}$  to estimate their behavior in the radiation environment in

CMS at the HL-LHC. The radiological quantities of these scintillators were determined and compared to measurements. These simulations were used to benchmark the material description in FLUKA and were able to identify the main drivers of residual dose in the material. The simulated ambient dose equivalent rate for LYSO and  $\text{CeF}_3$  agreed with the measurement within their uncertainties, while a slight underprediction for YSO was observed. This might be explained by the simplified representation of the irradiation conditions in FLUKA. Overall, the comparison of the calculated and measured ambient dose equivalent rate indicated a reliable prediction of this quantity by FLUKA for the given setup. The  $\text{PbWO}_4$ ,  $\text{CeF}_3$  and LYSO crystals were enlarged to a length of  $26 X_0$  and their residual dose after a 24 GeV/c-proton irradiation were compared among each other. The residual radioactivity in LYSO agrees within uncertainties with the one in  $\text{PbWO}_4$ . For  $\text{CeF}_3$ , the residual dose is a factor two smaller, but leakage of the hadronic shower due to its smaller Molière radius has to be taken into account. Thus, the residual dose rates for LYSO and  $\text{CeF}_3$  are expected to be similar to the one of  $\text{PbWO}_4$  in a  $26 X_0$  deep and transversely extended calorimeter.

The envisaged Shashlik calorimeter was implemented in the FLUKA CMS description and its particle spectra and average particle fluences were calculated. The average particle fluence was found to be similar for all options. The charged hadron and neutron fluence induced by the 24 GeV/c protons in the single crystals irradiations were scaled to the corresponding expected fluences in a Shashlik calorimeter located in the CMS environment. These scale factors allow an extrapolation from the behavior of the crystals in proton-irradiations to the CMS radiation environment. They were of great interest towards the final decision of the future EE for CMS.

In a last step, I determined the absorbed dose and the main causes for radioactivity in the Shashlik calorimeter for each scintillator option. Even though the average absorbed dose is similar for all options, the high thermal neutron absorption cross-section of lutetium in LYSO leads to higher absorbed dose values for this option at the boundary surfaces of the sampling calorimeter.

It was determined that the background due to the activity of residual nuclei is at the percent level and as such at a manageable level for the signal readout of a Shashlik calorimeter. All three designs, using  $\text{CeF}_3$ , LYSO or YSO as the sensitive material and tungsten as the absorber material are suitable for a future Shashlik calorimeter.

Finally, a different design for the new forward electromagnetic calorimeter, the HGCAL, was preferred by the CMS collaboration [17]. The research program of the ETHZ group and collaborators for the Shashlik sampling calorimeter design is being completed at the moment. The usage of heavy inorganic scintillators for particle detection is however also commercialized in other fields of physics, for instance for nuclear and medical

physics applications. The results of the research and development of the Shashlik sampling calorimeter and my FLUKA radiation simulations in that context are therefore of great importance for future developments in these fields.





## APPENDIX

## Appendix of part I

## A.1 Uncertainties on photon selection efficiency

| Barrel               |            | Data      |          | MC         |
|----------------------|------------|-----------|----------|------------|
| p <sub>T</sub> [GeV] | Efficiency | Stat.Err. | Syst.Err | Efficiency |
| 20-30                | 0.7842     | 0.0011    | 0.0297   | 0.8331     |
| 30-40                | 0.8466     | 0.0004    | 0.0018   | 0.8820     |
| 40-50                | 0.8775     | 0.0002    | 0.0014   | 0.9092     |
| 50-60                | 0.8776     | 0.0005    | 0.0034   | 0.9115     |
| 60-80                | 0.8733     | 0.0012    | 0.0114   | 0.9109     |
| 80-110               | 0.8774     | 0.0024    | 0.0117   | 0.9107     |
| 110-150              | 0.8862     | 0.0037    | 0.0092   | 0.9158     |
| 150-200              | 0.8892     | 0.0059    | 0.0049   | 0.9160     |
| 200-270              | 0.8752     | 0.0090    | 0.07994  | 0.9256     |
| 270-350              | 0.8982     | 0.0150    | 0.0270   | 0.9238     |
| 350-500              | 0.8735     | 0.0260    | 0.0068   | 0.9255     |

| Endcap               |            | Data      |          | MC         |
|----------------------|------------|-----------|----------|------------|
| p <sub>T</sub> [GeV] | Efficiency | Stat.Err. | Syst.Err | Efficiency |
| 20-30                | 0.6202     | 0.0017    | 0.0175   | 0.6870     |
| 30-40                | 0.7059     | 0.0009    | 0.0017   | 0.7586     |
| 40-50                | 0.7547     | 0.0008    | 0.0032   | 0.8012     |
| 50-60                | 0.7702     | 0.0019    | 0.0016   | 0.8182     |
| 60-80                | 0.7816     | 0.0033    | 0.0093   | 0.8319     |
| 80-110               | 0.8042     | 0.0062    | 0.0063   | 0.8549     |
| 110-150              | 0.8131     | 0.0097    | 0.0115   | 0.8672     |
| 150-200              | 0.8189     | 0.0168    | 0.0159   | 0.8958     |
| 200-350              | 0.8961     | 0.0175    | 0.0162   | 0.9167     |

**Table A.1:** Photon selection efficiency measured in barrel and endcaps up to  $|\eta| < 2.1$  using the Tag and Probe method (all cuts except for electron rejection) [149].

| Barrel      |            | Data      |            | MC        |  |
|-------------|------------|-----------|------------|-----------|--|
| $p_T$ [GeV] | Efficiency | Stat.Err. | Efficiency | Stat.Err. |  |
| 20-30       | 0.738      | 0.008     | 0.7698     | 0.0009    |  |
| 30-40       | 0.809      | 0.003     | 0.8294     | 0.0003    |  |
| 40-50       | 0.864      | 0.002     | 0.8742     | 0.0003    |  |
| 50-60       | 0.863      | 0.004     | 0.8831     | 0.0006    |  |
| 60-80       | 0.881      | 0.008     | 0.8878     | 0.0009    |  |
| 80-110      | 0.89       | 0.02      | 0.896450   | 0.000007  |  |
| 110-150     | 0.90       | 0.02      | 0.8986     | 0.0002    |  |
| 150-200     | 0.91       | 0.03      | 0.8944     | 0.0006    |  |
| 200-270     | 0.88       | 0.07      | 0.913      | 0.007     |  |
| 270-500     | 0.9        | 0.1       | 0.90       | 0.01      |  |

| Endcap      |            | Data      |            | MC        |  |
|-------------|------------|-----------|------------|-----------|--|
| $p_T$ [GeV] | Efficiency | Stat.Err. | Efficiency | Stat.Err. |  |
| 20-30       | 0.73       | 0.01      | 0.758      | 0.001     |  |
| 30-40       | 0.799      | 0.004     | 0.8242     | 0.0005    |  |
| 40-50       | 0.849      | 0.003     | 0.8721     | 0.0004    |  |
| 50-60       | 0.844      | 0.008     | 0.8867     | 0.0008    |  |
| 60-80       | 0.83       | 0.02      | 0.897      | 0.001     |  |
| 80-120      | 0.904      | 0.009     | 0.902      | 0.003     |  |
| 120-500     | 0.89       | 0.04      | 0.918      | 0.003     |  |

**Table A.2:** Photon selection efficiency measured in barrel and endcaps using the Tag and Probe method (all cuts except for electron rejection) for 0 T [151].

## A.2 Additional list of test regions for the bias determination

| $m_{\gamma\gamma}$ min<br>(GeV) | $m_{\gamma\gamma}$ max<br>(GeV) | $m_{\gamma\gamma}$ min<br>(GeV) | $m_{\gamma\gamma}$ max<br>(GeV) | $m_{\gamma\gamma}$ min<br>(GeV) | $m_{\gamma\gamma}$ max<br>(GeV) |
|---------------------------------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|
| 500                             | 525                             | 1040                            | 1090                            | 2160                            | 2270                            |
| 525                             | 550                             | 1090                            | 1145                            | 2270                            | 2380                            |
| 550                             | 580                             | 1145                            | 1205                            | 2380                            | 2500                            |
| 640                             | 670                             | 1325                            | 1395                            | 2760                            | 2895                            |
| 670                             | 705                             | 1395                            | 1465                            | 2895                            | 3040                            |
| 705                             | 740                             | 1465                            | 1535                            | 3040                            | 3195                            |
| 740                             | 775                             | 1535                            | 1615                            | 3195                            | 3350                            |
| 775                             | 815                             | 1615                            | 1695                            | 3350                            | 3520                            |
| 815                             | 855                             | 1695                            | 1780                            | 3520                            | 3695                            |
| 855                             | 900                             | 1780                            | 1865                            | 3695                            | 3880                            |
| 900                             | 945                             | 1865                            | 1960                            | 3880                            | 4000                            |
| 945                             | 990                             | 1960                            | 2060                            |                                 |                                 |
| 990                             | 1040                            | 2060                            | 2160                            |                                 |                                 |

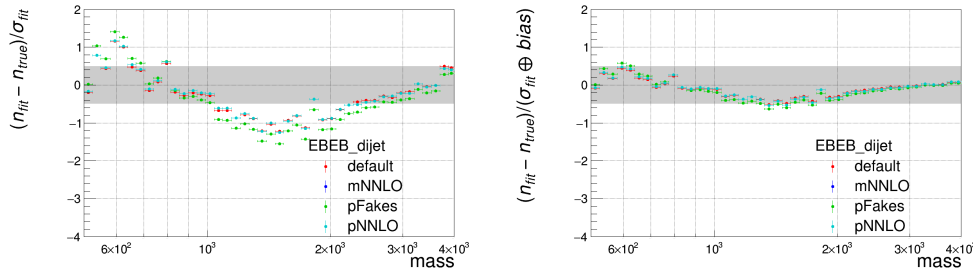
**Table A.3:** List of test regions considered for the bias determination with a bin width of 5 % [149].

| $m_{\gamma\gamma}$ min (GeV) | $m_{\gamma\gamma}$ max (GeV) | $m_{\gamma\gamma}$ min (GeV) | $m_{\gamma\gamma}$ max (GeV) |
|------------------------------|------------------------------|------------------------------|------------------------------|
| 500                          | 550                          | 1425                         | 1570                         |
| 550                          | 605                          | 1570                         | 1725                         |
| 605                          | 665                          | 1725                         | 1900                         |
| 665                          | 730                          | 1900                         | 2090                         |
| 730                          | 805                          | 2090                         | 2295                         |
| 805                          | 885                          | 2295                         | 2525                         |
| 885                          | 975                          | 2525                         | 2780                         |
| 975                          | 1070                         | 2780                         | 3060                         |
| 1070                         | 1180                         | 3060                         | 3365                         |
| 1180                         | 1295                         | 3365                         | 3700                         |
| 1295                         | 1425                         | 3700                         | 4000                         |

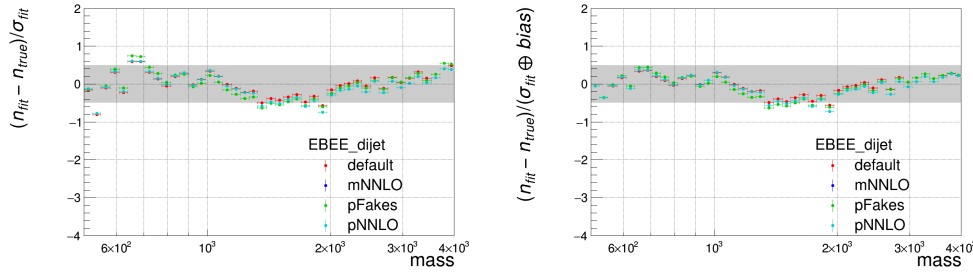
**Table A.4:** List of test regions considered for the bias determination with a bin width of 10 % [149].

| $m_{\gamma\gamma}$ min (GeV) | $m_{\gamma\gamma}$ max (GeV) | $m_{\gamma\gamma}$ min (GeV) | $m_{\gamma\gamma}$ max (GeV) |
|------------------------------|------------------------------|------------------------------|------------------------------|
| 500                          | 550                          | 900                          | 1000                         |
| 550                          | 600                          | 1000                         | 1200                         |
| 600                          | 650                          | 1200                         | 1800                         |
| 650                          | 700                          | 1800                         | 2500                         |
| 700                          | 750                          | 2500                         | 3500                         |
| 750                          | 800                          | 3500                         | 4500                         |
| 800                          | 900                          | 4500                         | 5500                         |

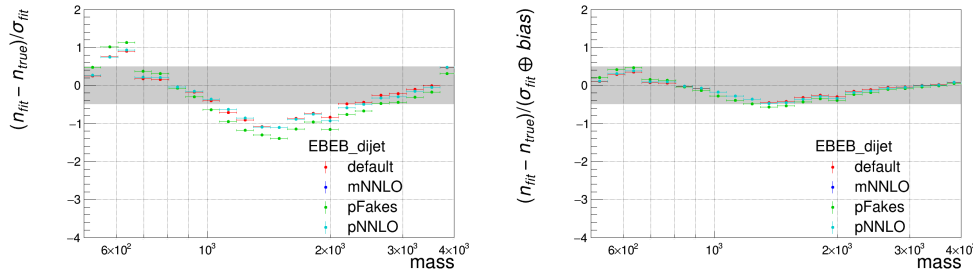
**Table A.5:** List of test regions considered for the bias determination used in Ref. [148] [149].



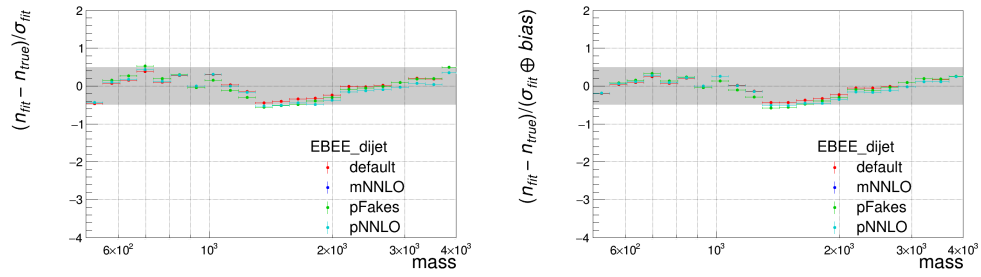
**Figure A.1:** Median of the pull  $p$  and modified pull  $\tilde{p}$  for all considered test regions according to Tab. A.3 for EBEB. Different datasets correspond to different MC shape variations as specified in the text [149].



**Figure A.2:** Median of the pull  $p$  and modified pull  $\tilde{p}$  for all considered test regions according to Tab. A.3 for EBEE. Different datasets correspond to different MC shape variations as specified in the text [149].

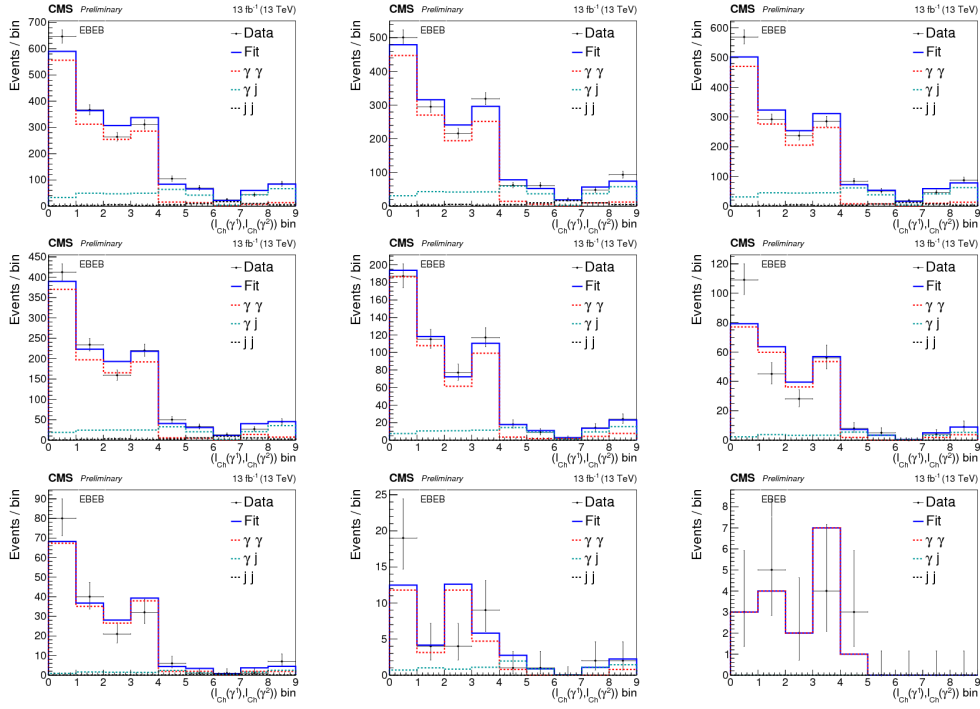


**Figure A.3:** Median of the pull  $p$  and modified pull  $\tilde{p}$  for all considered test regions according to Tab. A.4 for EBEB. Different datasets correspond to different MC shape variations as specified in the text [149].

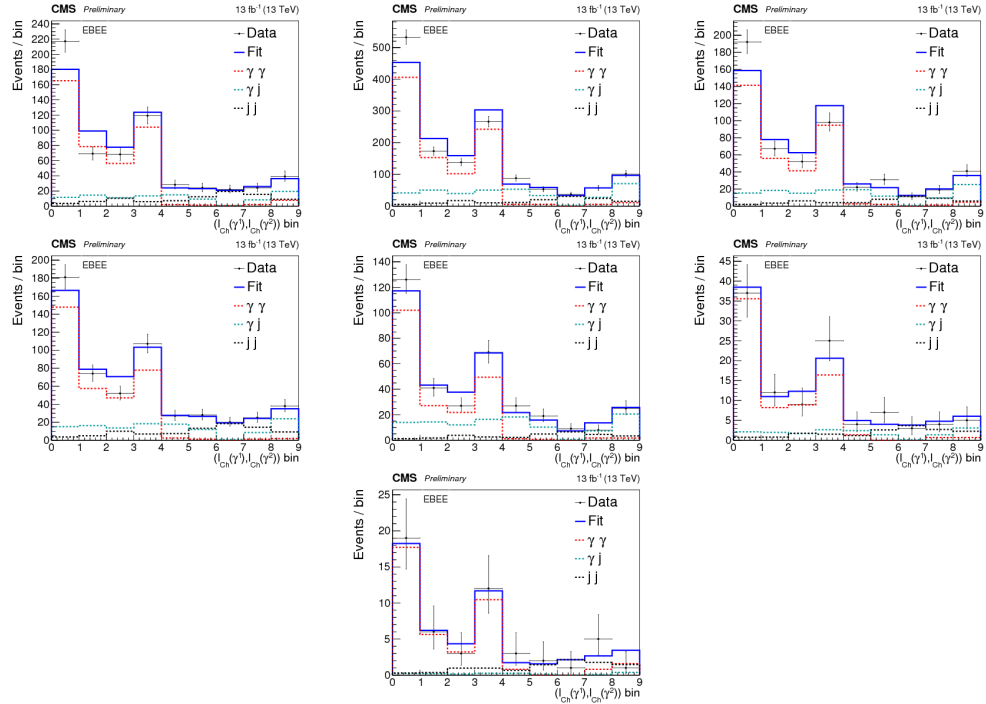


**Figure A.4:** Median of the pull  $p$  and modified pull  $\tilde{p}$  for all considered test regions according to Tab. A.4 for EBEE. Different datasets correspond to different MC shape variations as specified in the text [149].

### A.3 Additional fits of the background determination



**Figure A.5:** Fit of the  $\text{IsoCh}$ -distributions in data with the three components  $\gamma\gamma$ ,  $\gamma j$ ,  $j j$ -for all bins of the diphoton invariant mass spectrum in the EBEB category. The  $m_{\gamma\gamma}$  bin size is from left to right: 230 GeV, 253 GeV, 282 GeV, 332 GeV, 409 GeV, 500 GeV, 600 GeV, 800 GeV, 1 TeV, 1.6 TeV.



**Figure A.6:** Fit of the IsoCh-distributions in data with the three components  $\gamma\gamma$ ,  $\gamma j$ ,  $j j$ -for all bins of the diphoton invariant mass spectrum in the EBEB category. The  $m_{\gamma\gamma}$  bin size is from left to right: 320 GeV, 356 GeV, 444 GeV, 500 GeV, 600 GeV, 800 GeV, 1 TeV, 1.6 TeV.

**Table A.6:** Estimate of the  $\gamma\gamma$ -fraction ( $\bar{f}_{\gamma\gamma}$ ) to the overall background with statistical and absolute uncertainties.

| $\bar{f}_{\gamma\gamma}$ | $\sigma_{\text{stat}}$ | $\sigma_{\text{tot}}$ |
|--------------------------|------------------------|-----------------------|
| <b>EBEB</b>              |                        |                       |
| 0.88                     | 0.02<br>0.02           | 0.11<br>0.11          |
| 0.87                     | 0.02<br>0.02           | 0.11<br>0.11          |
| 0.88                     | 0.03<br>0.03           | 0.11<br>0.11          |
| 0.90                     | 0.03<br>0.03           | 0.11<br>0.11          |
| 0.92                     | 0.04<br>0.04           | 0.13<br>0.12          |
| 0.95                     | 0.07<br>0.07           | 0.14<br>0.13          |
| 0.97                     | 0.05<br>0.06           | 0.12<br>0.11          |
| 0.90                     | 0.10<br>0.12           | 0.16<br>0.17          |
| 1.00                     | 0.04<br>0.11           | 0.09<br>0.14          |
| <b>EBEE</b>              |                        |                       |
| 0.84                     | 0.05<br>0.05           | 0.16<br>0.16          |
| 0.80                     | 0.04<br>0.04           | 0.16<br>0.16          |
| 0.80                     | 0.08<br>0.09           | 0.17<br>0.17          |
| 0.79                     | 0.06<br>0.06           | 0.17<br>0.16          |
| 0.75                     | 0.07<br>0.07           | 0.17<br>0.17          |
| 0.84                     | 0.10<br>0.11           | 0.18<br>0.19          |
| 0.91                     | 0.10<br>0.11           | 0.22<br>0.20          |



## Appendix of part II

### B.1 Irradiation cycle for radioactivation studies with FLUKA

**Table B.1:** Irradiation cycle 'profile e' recommended by CMS BRIL FLUKA group. Based on the estimated luminosity per year.

| Year           | peak $\mathcal{L}$<br>$\text{cm}^{-2} \text{s}^{-1}$ | $\mathcal{L}$<br>$\text{fb}^{-1}$ | $\mathcal{L}$ per year<br>$\text{fb}^{-1}$ |
|----------------|------------------------------------------------------|-----------------------------------|--------------------------------------------|
| 2012           | $0.80 \times 10^{34}$                                | 30.0                              | 30.0                                       |
| LS1            |                                                      |                                   |                                            |
| 2015           | $0.5 \times 10^{34}$                                 | 50.0                              | 20.0                                       |
| 2016           | $1.50 \times 10^{34}$                                | 96.0                              | 46.0                                       |
| 2017           | $1.50 \times 10^{34}$                                | 132.0                             | 36.0                                       |
| 2018           | $1.50 \times 10^{34}$                                | 156.0                             | 24.0                                       |
| LS2            |                                                      |                                   |                                            |
| 2020 (Apr-May) | $1.50 \times 10^{34}$                                | 171.0                             | 15.0                                       |
| 2020 (Jun-Nov) | $2.00 \times 10^{34}$                                | 196.0                             | 25.0                                       |
| 2021           | $2.00 \times 10^{34}$                                | 251.0                             | 55.0                                       |
| 2022           | $2.00 \times 10^{34}$                                | 306.0                             | 55.0                                       |
| LS3            |                                                      |                                   |                                            |

**Table B.2:** Irradiation cycle 'profile d' recommended by CMS BRIL FLUKA group from LHC schedule beyond LS1 from 116th LHCC Meeting 4.12.13. Based on the estimated luminosity per year.

| Year | peak $\mathcal{L}$<br>$\text{cm}^{-2} \text{s}^{-1}$ | $\mathcal{L}$<br>$\text{fb}^{-1}$ | $\mathcal{L}$ per year<br>$\text{fb}^{-1}$ |
|------|------------------------------------------------------|-----------------------------------|--------------------------------------------|
| 2012 | $0.80 \times 10^{34}$                                | 30.0                              | 30                                         |
| LS1  |                                                      |                                   |                                            |
| 2015 | $1.45 \times 10^{34}$                                | 75.0                              | 45                                         |
| 2016 | $1.65 \times 10^{34}$                                | 120.0                             | 45                                         |
| 2017 | $1.75 \times 10^{34}$                                | 165.0                             | 45                                         |
| 2018 | $1.75 \times 10^{34}$                                | 187.5                             | 22.5                                       |
| LS2  |                                                      |                                   |                                            |
| 2020 | $2.00 \times 10^{34}$                                | 242.5                             | 55                                         |
| 2021 | $2.00 \times 10^{34}$                                | 297.5                             | 55                                         |
| 2022 | $2.00 \times 10^{34}$                                | 352.5                             | 55                                         |
| LS3  |                                                      |                                   |                                            |
| 2025 | $5.00 \times 10^{34}$                                | 427.5                             | 75                                         |
| 2026 | $5.00 \times 10^{34}$                                | 727.5                             | 300                                        |
| 2027 | $5.00 \times 10^{34}$                                | 1027.5                            | 300                                        |
| 2028 | $5.00 \times 10^{34}$                                | 1327.5                            | 300                                        |
| LS4  |                                                      |                                   |                                            |
| 2030 | $5.00 \times 10^{34}$                                | 1627.5                            | 300                                        |
| 2031 | $5.00 \times 10^{34}$                                | 1927.5                            | 300                                        |
| 2032 | $5.00 \times 10^{34}$                                | 2227.5                            | 300                                        |
| LS5  |                                                      |                                   |                                            |
| 2034 | $5.00 \times 10^{34}$                                | 2527.5                            | 300                                        |
| 2035 | $5.00 \times 10^{34}$                                | 2827.5                            | 300                                        |
| End  |                                                      |                                   |                                            |



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## Abbreviations

|              |                                                      |
|--------------|------------------------------------------------------|
| <b>ADD</b>   | Arkani-Hamed Dimopoulos Dvali extradimensional model |
| <b>ALICE</b> | A Large Ion Collider Experiment                      |
| <b>APD</b>   | Avalanche Photo Diodes                               |
| <b>ATLAS</b> | A large Toroidal LHC Apparatus                       |
| <b>BSM</b>   | Beyond Standard Model                                |
| <b>BDT</b>   | Boosted Decision Tree                                |
| <b>BTCP</b>  | Bogoroditsk Techno Chemical Plant                    |
| <b>BRIL</b>  | Beam conditions, Radiation and Luminosity Project    |
| <b>CERN</b>  | Conseil Européen pour la Recherche Nucleaire         |
| <b>CMS</b>   | Compact Muon Solenoid                                |
| <b>CMSSW</b> | CMS Software Framework                               |
| <b>CSC</b>   | Cathode Strip Chambers                               |
| <b>CSV</b>   | Combined Secondary Vertex                            |
| <b>C.L.</b>  | Confidence Level                                     |
| <b>DT</b>    | Drift Tubes                                          |
| <b>EB</b>    | Ecal Barrel                                          |
| <b>ECAL</b>  | Electromagnetic Calorimeter                          |
| <b>ED</b>    | Extra Dimension                                      |
| <b>EE</b>    | Ecal Endcap                                          |
| <b>EE</b>    | ElectroWeak Symmetry Breaking mechanism              |
| <b>ES</b>    | Ecal PreShower                                       |
| <b>eV</b>    | electron Volt                                        |
| <b>FLUKA</b> | FLUkturierende KAskade                               |

|               |                                                                                |
|---------------|--------------------------------------------------------------------------------|
| <b>FWHM</b>   | <b>F</b> ull <b>W</b> idth <b>H</b> alf <b>M</b> aximum                        |
| <b>GSF</b>    | <b>G</b> aussian <b>S</b> um <b>F</b> ilter                                    |
| <b>HL-LHC</b> | <b>H</b> igh- <b>L</b> uminosity <b>L</b> arge <b>H</b> adron <b>C</b> ollider |
| <b>HCAL</b>   | <b>H</b> adronic <b>C</b> alorimeter                                           |
| <b>HB</b>     | <b>H</b> cal <b>B</b> arrel                                                    |
| <b>HE</b>     | <b>H</b> cal <b>E</b> ndcap                                                    |
| <b>HF</b>     | <b>H</b> cal <b>F</b> orward                                                   |
| <b>HGCAL</b>  | <b>H</b> igh <b>G</b> ranularity <b>C</b> ALorimeter                           |
| <b>HLT</b>    | <b>H</b> igh <b>L</b> evel <b>T</b> rigger                                     |
| <b>HO</b>     | <b>H</b> cal <b>O</b> uter                                                     |
| <b>IP</b>     | <b>I</b> nteraction <b>P</b> oint                                              |
| <b>KK</b>     | <b>K</b> aluza- <b>K</b> lein                                                  |
| <b>LEP</b>    | <b>L</b> arge <b>E</b> lectron <b>P</b> ositron <b>C</b> olldier               |
| <b>LHC</b>    | <b>L</b> arge <b>H</b> adron <b>C</b> ollider                                  |
| <b>LHCb</b>   | <b>L</b> arge <b>H</b> adron <b>C</b> ollider <b>b</b> eauty                   |
| <b>LO</b>     | <b>L</b> eading- <b>O</b> rders                                                |
| <b>LS3</b>    | <b>L</b> ong <b>S</b> hutdown <b>3</b>                                         |
| <b>LT</b>     | optical <b>L</b> ongitudinal- <b>T</b> ransmission                             |
| <b>LY</b>     | <b>L</b> ight <b>Y</b> ield                                                    |
| <b>L1</b>     | <b>L</b> evel- <b>1</b> <b>T</b> rigger                                        |
| <b>MC</b>     | <b>M</b> onte- <b>C</b> arlo ( <b>S</b> imulation)                             |
| <b>ML</b>     | <b>M</b> aximum <b>L</b> ikelihood                                             |
| <b>MSSM</b>   | <b>M</b> inimally <b>S</b> upersymmetric <b>S</b> tandard <b>M</b> odel        |
| <b>NLO</b>    | <b>N</b> ext-to- <b>L</b> eading- <b>O</b> rders                               |
| <b>NNLO</b>   | <b>N</b> ext-to- <b>N</b> ext-to- <b>L</b> eading <b>O</b> rders               |
| <b>OOT</b>    | <b>O</b> ut <b>O</b> f <b>T</b> ime (pile-up)                                  |
| <b>PDF</b>    | <b>P</b> arton <b>D</b> ensity <b>F</b> unction                                |
| <b>PDF</b>    | <b>P</b> robability <b>D</b> ensity <b>F</b> unction                           |
| <b>PF</b>     | <b>P</b> article <b>F</b> low                                                  |
| <b>POG</b>    | <b>P</b> hysics <b>O</b> bject <b>G</b> roup                                   |
| <b>pp</b>     | <b>P</b> roton <b>P</b> roton                                                  |

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|             |                                                        |
|-------------|--------------------------------------------------------|
| <b>PS</b>   | <b>P</b> roton <b>S</b> ynchrotron                     |
| <b>PU</b>   | <b>P</b> ile <b>U</b> p                                |
| <b>QCD</b>  | <b>Q</b> uantum <b>C</b> hromo <b>D</b> ynamics        |
| <b>RF</b>   | <b>R</b> adio <b>F</b> requency                        |
| <b>RMS</b>  | <b>R</b> oot <b>M</b> ean <b>S</b> quare               |
| <b>RPC</b>  | <b>R</b> esistive <b>P</b> late <b>C</b> hambers       |
| <b>RS</b>   | <b>R</b> andall <b>S</b> undrum extradimensional model |
| <b>SC</b>   | <b>S</b> uper <b>C</b> luster                          |
| <b>SIC</b>  | <b>S</b> hanghai <b>I</b> nstitute of <b>C</b> eramics |
| <b>SM</b>   | <b>S</b> tandard <b>M</b> odel (of particle physics)   |
| <b>SM</b>   | <b>S</b> uper <b>M</b> odule                           |
| <b>SPS</b>  | <b>S</b> uper <b>P</b> roton <b>S</b> ynchrotron       |
| <b>SUSY</b> | <b>S</b> upersymmetry                                  |
| <b>VPT</b>  | <b>V</b> acuum <b>P</b> hoto <b>T</b> riode            |
| <b>WLS</b>  | <b>W</b> ave <b>L</b> ength <b>S</b> hifting (fiber)   |
| <b>2HDM</b> | <b>2-Higgs-Doublet-Model</b>                           |

